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MEMOIRS OF THE

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Scientific and
Industrial
Research



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Foreword

At the departure of the Network Collaboration Core for Materials & Devices Research Field”

Akihito Yamaguchi

Director, The Institute of Scientific and Industrial Research

At the 70th anniversary of The Institute of Scientific and Industrial Research (ISIR), ISIR has been reorganized on April 1st, 2009, to the institute composed of three major research divisions (information & quantum science, material & beam science, and biological & molecular science) and expanded & improved Nanotechnology Center, in order to contribute to the development of multidisciplinary science. In addition, Center for Research Education and Training, International Collaboration Center and Research Laboratory of Quantum Beam Science has been newly established and Materials Analysis Center has been reorganized to Comprehensive Analysis Center. These centers are expected to contribute graduate education of Osaka University and facilitate the domestic and international collaboration. This reorganization is the first big step toward the future of our institute.

ISIR was founded in 1939 on the basis of strong desire and the support of the business circles in KANSAI area. In order to perform our important mission, we started to construct the Nanotechnology Incubation Building in this April. It is a five-storied building having 5,000 m² floor space, which is composed of rental laboratories for business corporations and alliance laboratories for domestic and international collaboration. It is the first case of the on-campus Nanotechnology incubation facility in Japan.

In this June, our ISIR has been authorized as a headquarter of the new Network Collaboration Core for Material & Device Research Field composed of five national university institutes including IMRAM (Tagenken) in TOHOKU Univ., RIES (Denshiken) in HOKKAIDO Univ., and CRL (Shigenken) in Tokyo Institute of Technology, and IMCE (Sendouken) in Kyushu Univ. in addition to the four institutes described above. So, this year is a first step for a novel leading institute in Japan.

ISIR will continue to make contributions to the development of industry through basic science and technology and inspire the future.

Outline of ISIR

1. Research Activities

1) History and Organization

The Institute of Scientific and Industrial Research (ISIR) was founded in 1939 as a part of Osaka University, based on the strong desire of the business leaders of private enterprises in Osaka area. The purpose of the Institute is to study science necessary for industry and their applications. Since then, the institute had developed into one of the leading research organizations for science and engineering in Japan.

In 1939 ISIR had only 3 departments, however it had increased research areas and laboratories in the fields of electronic engineering, computer science, metallurgy and inorganic chemistry, organic chemistry, biochemistry, and beam science.

Modern industry in this country is, however, coming to a major turning point. There is a strong requirement to develop interdisciplinary sciences, or new fields which are away from conventional area in order to advance basic and applied sciences coping with social changes.

Since this Institute has researchers in a wide variety of fields and is suitable for making a new organization for interdisciplinary areas, it was restructured in 1995 to an Institute with 6 divisions with 24 departments for the purpose of promoting sciences on materials, information and biology. For solving problems related to energy, earth ecology, aging and advanced information technology, interdisciplinary and comprehensive studies have been conducted in the Institute. From 2002 through 2006, we have awarded as the best group in 21st Century COE program that is originally the top 20 group plan in Japan. This involves the positive exchange between different laboratories which yield results of the global level with respect to material, information and biotechnology.

In 2002, Nanoscience and Nanotechnology Center has started after restructuring Research Center for Intermaterials and Radiation Laboratory. The new Center focuses its research on nanomaterials and devices, beam science for nanotechnology and industrial nanotechnology. In 2003, the Center Building was constructed. In the new Center Building, there is a Nanotechnology Process Foundry for supporting the nationwide research in the nanotechnology field.

In 2006, Materials Science & Technology Research Center for Industrial Creation between ISIR and IMRAM (Tagenken) in Tohoku Univ. has started and then expanded to the Post-Silicon Materials and Devices Research Alliance including RIES

(Denshiken) in Hokkaido Univ. and CRL (Shigenken) in TIT next year. In 2006, Academia Industry Relation Office(AIR-Office) has been settled in order to strengthen cooperation between the institute and industries. In 2008, Division of special project has been founded for promotion of research by young faculties.

In 2009, we have made a great restructuring since 1995 in order to develop the novel interdisciplinary research fields and exercise leadership in nanotechnology research field into 3 great divisions (Division of Information and Quantum Sciences, Division of Material and Beam Sciences, and Division of Biological and Molecular Sciences) and expanded Nanoscience and Nanotechnology Center. We newly established the Center for Research Education and Training and the Center for International Collaboration. Former Materials Analysis Center was joined with Electron Microscope Laboratory and restricted into the Comprehensive Analysis Center. Research Laboratory for Quantum Beam Science was separated from Nanoscience and Nanotechnology Center for facilitating the collaboration in the beam science field.

In order to establish a core for academia-industry collaboration and open innovation, we started to construct the 5-story Nanotechnology Incubation Facility Building which will be completed in the next spring. ISIR Manufacturing Factory will be moved into the building. In addition, Nanoscience Techno-Core, Company Research Park and Osaka University Renovation Center will be settled in the building.

In 2009, the Network Joint Research Center for Materials and Devices including ISIR, IMRAM, RIES, CRL and IMCE (Sendoken) in Kyushu Univ. has been authorized by the Ministry of Education, Culture, Sports, Science and Technology. ISIR is a headquarter of this 5 institutes network. There is no precedent for such a great network of university institutes in Japan.

Divisions	Departments
Quantum Engineering	Quantum Molecular Devices Photonic and Electronic Materials Semiconductor Electronics Condensed Matter Physics
Advanced Materials Science & Technology	Structural Characterization and Design Metallic Materials Process Atomic Scale Science Functional Ceramic Materials Frontier Materials Creation Advanced-Energy Materials
Organic Molecular Science	Regulatory Bioorganic Chemistry Organic Fine Chemicals Organic Molecular Materials Molecular Excitation Chemistry Synthetic Organic Chemistry
Intelligent Systems Science	Knowledge Systems Intelligent Media Architecture for Intelligence Advanced Reasoning
Biological Science	Structural Molecular Biology Single Molecule Biophysics Cell Membrane Biology
Quantum Beam Science & Technology	Accelerator Science Beam Materials Science
Next Industry Generation	New Industrial Projection New Industry Generation Systems Intellectual Property Research
Division of Special Projects	Laboratories of First Project Laboratories of Second Project
Research Centers (Three Centers)	
Nanoscience and Nanotechnology Center	Nanomaterials and Nanodevices Artificial Nanomaterials for Bio-Information Systems Single-Molecular Integrated Devices Supramolecular Chemistry

Nanobiology
Nanosystem Design

Beam Science for Nanotechnology

Beam Science and Nanofabrication
Quantum Beams for Nanotechnology
Beam Processing for Nanotechnology
Ultrafast Spectroscopy of Nanostructures

Nanoscience and Nanotechnology for Industrial Applications

Nanomaterials and Environmentally Conscious Technology
Computational Nanomaterials Design
Nano-Bio-Intelligent Systems Science
Nanotechnology Transfer

Nanocharacterization

Advanced Nanostructural Characterization
Advanced Characterization for Nano-Processing
Quantum Materials and Devices Characterization

Open Laboratory

Radiation Laboratory

Electron Microscope Laboratory

Electronic Processing Laboratory

Nanofabrication Shop

Handai Multi-Functional Nanofoundry

Materials Analysis Center

Materials Science & Technology Materials Research Project

Research Center for Industrial Creation Hard Materials Research Group
Soft Materials Research Group

Human Interface Research for Safety and Security Project

Medical Sciences Research Group
Human Interface Research Group

**An alliance laboratory of
RIES, Hokkaido Univ.**

Quantum Information Optics

Service Facilities

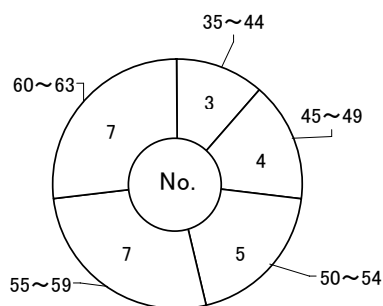
Workshop

**Laboratory for Radio-Isotope Experiments
Office of Information Network**

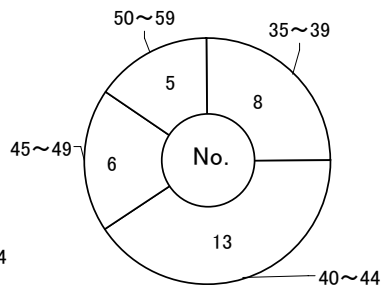
Academia Industry Relations Office
Public Relations Office
Library
Technical Division
Administrative Office

Staffs' Age (years old) –As of 3.31.2009

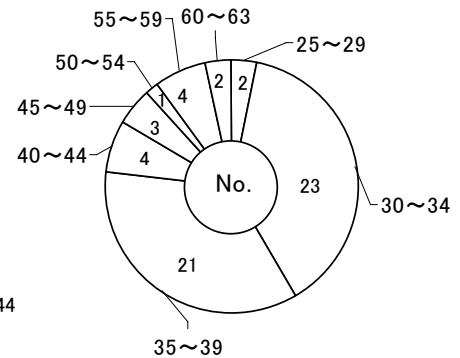
Professors



Associate Professors

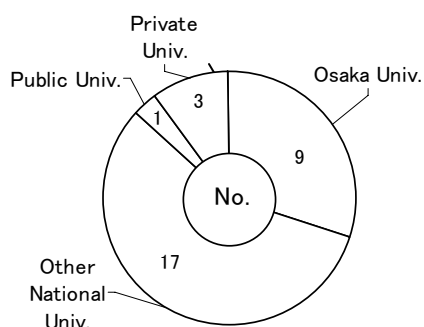


Assistant Professors

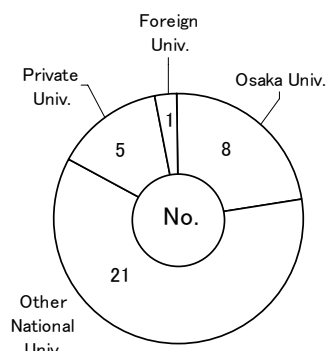


Staffs' Alma Mater –As of 3.30.2009

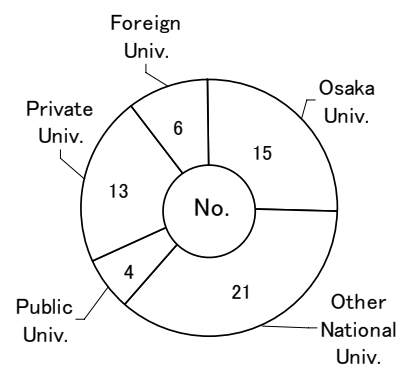
Professors



Associate Professors



Assistant Professors



2) Administration

Administration and management of ISIR are conducted by the Director elected from the full professors of ISIR. The term of the Director is two years. Reappointment is possible, but the Director can not be in the position for more than 4 years. Professor Akihito Yamaguchi has been a Director since April 1, 2008.

Important matters of ISIR are discussed and determined by the Faculty Council, which consists of the Director and all professors of ISIR. Various committees such as International Exchange, Self-Review, Circumstances and so on are working for each purpose.

Administration of the Institute-associated Centers is conducted by Director of each Center and its Executive Committee.

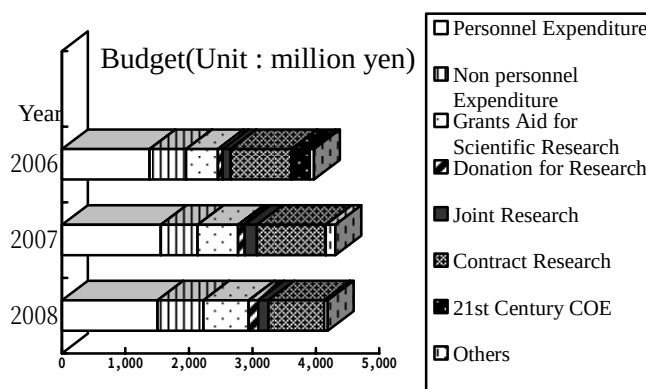
Evaluation Committee composed of outside experts in academic societies was established and the committee evaluated several items such as management, budget, facilities and research activities.

The new organization was highly evaluated, but with change of their structure to National University Agencies in April 2004, our management system needs reshaping. A Board of Directors under the Director has been formed, and Advisory Board has been set up to introduce opinions from outside into the Institute.

3) Research Budget

The budget of ISIR is mainly composed of Subsidy for operating expenses, Grants-in-Aid for Scientific Research of Ministry of Education, Sports, Culture, Science and Technology, Donations for Research, and Budget of Joint Research. The recent trend in the expenditure of ISIR is as follows.

Grants-in Aid for Scientific Research of Ministry of Education, Culture, Sports, Science and Technology are delivered to researchers and the total budget in 2008 is 716,327,000yen.



Donation for Research

Donation for Research is accepted after the Judgement of Committee and the amount in these three years are as follows. (Unit : kilo yen , () Number)

Division Year	Quantum Engineering	Advanced Materials Science and Technology	Organic Molecular Science	Intelligent Systems Science
2006	4,500 (3)	13,141 (17)	16,400 (13)	10,100 (8)
2007	500 (1)	22,600 (18)	34,999 (20)	19,614 (0)
2008	500 (1)	22,777 (19)	28,494 (22)	9,981 (11)

Division Year	Biological Science	Quantum Beam Science and Technology	Nanoscience and Nanotechnology center	Others	Total
2006	9,250 (7)	0 (0)	10,700 (9)	13,300 (5)	77,391 (62)
2007	11,350 (10)	1,600 (2)	17,570 (16)	300 (1)	108,533 (78)
2008	20,250 (9)	3,250 (4)	23,400 (16)	40,000 (1)	148,562 (83)

4) Cooperative Research

Cooperative Researches and Contract Researches in the fiscal year 2007-2008 are as follows: Cooperative Researches are carried out with 61 organizations. The budget for the fiscal year 2008-2009 is 188,574,000 yen. The number of Contract Researches are 43. The budget for the fiscal year 2008-2009 is 881,017,000 yen.

5) International Research

Structural Characterization and Design	Los Alamos National Laboratory	America	Materials Modification by Ion Beam Irradiation
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Structural Characterization and Design	Pacific Northwest National Laboratory	America	Ion-beam-induced structural changes in compound semiconductors studied by advanced electron microscopy
Knowledge System	University of Wales	England	Advanced Scientific Discovery Tools for Bioinformatics
Functional Ceramic Materials	Slovak Academy of Sciences	Slovakia	Defect Passivation Etchless (DPEL) and low temperature oxidation mechanism, and their application to solar cells.
Regulatory Bioorganic Chemistry	University of BERN	Switzerland	Studies on DNA switching devices
Molecular Excitation Chemistry	Korea University	Korea	The intramolecular charge transfer and the charge recombination between an electron donor and acceptor chromophores of dyad molecules were studied using femto second laser flash photolysis. The results were published in J. Phys. Chem. A 2008, 112(31), and 7208-7213, and Phys. Chem. Chem. Phys. 2008, 10(30), and 4393-4399.
Molecular Excitation Chemistry	Oregon State University	America	The emission from the charge recombination of the donor-acceptor type compound was studied by the pulse radiolysis in SANKEN. The results were published in J. Org. Chem. 2008, 73(9), 3551-3558.
Molecular Excitation Chemistry	Konkuk University	Korea	As the collaboration with Prof. Im Chan, emission properties of pi-conjugated polymers were studied, and the results were published in J. Photochem. Photobiol. A 2008, 200(2-3), 371-376.
Artificial Nanomaterials for Bio-Information Systems	Ewha Womans University	Korea	Fabrication of Nano-scale Oxide Heterostructures by Combination of Top-down and Bottom-up Nanotechnologies

Condensed Matter Physics	Research Center Jülich	Germany	JSPS POSTDOCTORAL FELLOWSHIP FOR NORTH AMERICAN AND EUROPEAN RESEARCHERS (Short-term) Theoretical study on electronic properties of magnetic molecules adsorbed on metal surfaces
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6) Symposia, Seminars, Workshops and Lectures

2008/4/17	Our Challenges in Local Image Feature Matching
2008/4/21	Design and Applications of General Imaging Systems
2008/5/20	Fabrication and properties of foamed magnesium alloys
2008/5/21	Theory on formation and growth of pores in lotus-type porous metals
2008/5/20-23	The Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD)
2008/6/17	Application of lead-free frits for display electrodes and solar cells
2008/7/1	Modified Nucleic acid systems for biomedical applications
2008/7/7	Magnetic properties of coupled and non-coupled Fe/Cr multilayers
2008/7/10	Toward New Sensors and Methodology in Computer Vision
2008/7/28	International Seminar on Data Mining
2008/8/1	1st regular meeting of the Workshop on new semiconductor chemical processes
2008/9/1	International Seminar on Data Mining
2008/9/24-27	2008 KOREA-JAPAN Symposium on Frontier Photoscience
2008/9/29-10/1	Nano-Advanced Materials and Devices -from Nano-fabrication to Nano-application -
2008/9/6-10	13th CMD Workshop
2008/9/9	Superconductivity of boron
2008/9/26	Study on high-strength porous TiAl-base intermetallic compounds
2008/10/9	Seminar on New Functional Nano-Electronics Research Group (G2) of Post-Silicon Materials and Devices Research Alliance
2008/10/17-18	Seminar on Molecular Nano-Mechanics & Bio-Mechanics Research Group (G3) of Post-Silicon Materials and Devices Research Alliance
2008/10/22	Workshop on porous materials 1
2008/10/23	1st Functional oxide electronics workshop
2008/10/24	Joint workshop between ISIR, Osaka University and Hiroshima Synchrotron Radiation Center, Hiroshima University
2008/10/27	Seminar on Molecular Nano-Electronics Research Group (G1) of Post-Silicon Materials and Devices Research Alliance

2008/10/30	Automating Biological Science
2008/11/7	Supramolecular Nano Structures Consisting of Organic π -Electron Systems
2008/11/21-22	37th Lectures on Thin Films and Surface Physics "Introduction to Computational Nanomaterials Design - Theoretical approach to give guidelines for synthesizing novel nano-structural materials and novel functional thin films
2008/12/1	64th Symposium on a special topic and a subsequent conference for presenting results of research activities made by the members of the Institute are held annually in November, they are open to the public.
2008/12/12	2nd regular meeting of the Workshop on new semiconductor chemical processes
2008/12/25-26	Symposium on 2008 Research Progress of Post-Silicon Materials and Devices Research Alliance
2009/1/22	12th SNKEN,7th Nanoscience and Nanotechnology Center,2nd MSTeC and 1st Post-silicon Materials and Devices Research Alliance International Symposium
2009/2/2-3	The 9th workshop on Radiation Laboratory
2009/2/3	Workshop on porous materials 2
2009/2/4	Joint Symposium between ISIR, Osaka University and Institute of Industrial Science, University of Tokyo
2009/2/20	Free volume in nanocrystalline bulk metals
2009/2/26	Joint Symposium between ISIR, Osaka University and Research Institute of Electronical Communication, Tohoku University
2009/3/2-6	14th CMD Workshop
2009/3/3-4	Special interest Group on Data Mining & Statistical Mathematics
2009/3/4	Symposium on Radiation Laboratory
2009/3/19	3rd regular meeting of the Workshop on new semiconductor chemical processes
2009/3/17	Workshop on porous materials 3

Other Lectures and Seminars

2008/4/24	Akira Hosomi	Laboratory of Selective Organic Syntheses and Natural Products, ENSCO, France	Assistant Professor	Advice for Creative Research
2008/4/25	Sylvain Jugé	Institute of Molecular Chemistry, University of Burgundy, France	Professor	P-Stereogenic Organophorus Compounds: From Chiral Ligands to Labelled Aminoacids

2008/5/14	Takahiro Harada	University of FUKUI, Department of Human and Artificial Intelligent Systems	Lecturer	
2008/5/15	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental of power devices
2008/6/19	Masakatsu Shibasaki	Graduate School of Pharmaceutical Sciences The University of Tokyo	Professor	Two-centered Asymmetric Catalysis: New Development and Pharmaceutical Synthesis
2008/6/24	Takeshi Arakawa	Center of Molecular Biosciences, University of the Ryukyus	Associate Professor	Seminar on the treatments for emerging viral diseases using bio-nanocapsules
2008/6/30	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental of TFT circuits and process
2008/7/10	Toru Nakayama	Laboratory of Applied Life Chemistry, Department of Biomolecular Engineering, Graduate School of Engineering, Tohoku University	Professor	Seminar on Biochemistry and Molecular Biology of Colour Development of Flowers
2008/7/29	Haruo Mizutani	Graduate school of Frontier Sciences, the university of Tokyo	Specially Appointed Assistant Professor	High-Resolution X-ray Microscopy for 3-Dimensional Reconstruction of Neural Network

2008/7/30	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	New system liquid crystal and process
2008/8/6	Nick Serpone	University of Pavia	Visiting Professor	Misoconceptions in TiO ₂ Photocatalysis(Addressing some outstanding issu)
2008/8/15	Kazuki Terauchi	Division of Biological Science, Graduate School of Science, Nagoya University	Lecturer	—
2008/8/21	Toshiaki Kaneko	Okayama university of science	Professor	Collective Energy Loss of Attosecond Electron Bunches
2008/8/27	Masaaki Wachi	University of Tokyo	Associate Professor	TolC-Dependent Exclusion of Porphyrins in Escherichia coli
2008/9/4	Stefan Matile	University of Geneva	Professor	Technical consulting for nucleic acids synthesis and application
2008/9/5	Jai Pal Mittal	University of Pune	Professor	Anti oxidants-Hype and Reality-Efforts to bioquantify with radiation chemistry ideas
2008/9/8	Tulsi Mukherjee	Bhabha atomic Research Centre	Professor	History and Perspective of Free Radical Research in BARC: Interface Among Chemistry, Biology and Medicine
2008/9/8	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental technology for system display
2008/9/8	Kenji Yoneda	Semiconductor Devices Development Center, Semiconductor Company, Matsushita Electric Industrial Co., Ltd.	Chief Engineer	New LSI process: high-k and low-k films

2008/9/9	Kenji Yoneda	Semiconductor Devices Development Center, Semiconductor Company, Matsushita Electric Industrial Co., Ltd.	Chief Engineer	New LSI process: cleaning method of semiconductor surfaces
2008/9/9	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental and new technology for system display
2008/9/10	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental of TFT circuit
2008/9/10	Kenji Yoneda	Semiconductor Devices Development Center, Semiconductor Company, Matsushita Electric Industrial Co., Ltd.	Chief Engineer	Fundamental of power devices
2008/9/18	Nathalie VAST	Commissariat à l'Energie Atomique, Direction des Sciences de la Matière	Senior researcher	Superconductivity from doping boron icosahedra
2009/10/14	Jan Dutkiewicz	The Institute of Metallurgy and Materials Science of the Polish Academy of science	Professor	Research on New Materials Produced by Mechanical Alloying and Hot Pressing and Tixocasting of Steel (in Frame of European Projects)
2008/11/6	Masahiko Iyoda	Graduate School of Science and Engineering, Tokyo Metropolitan University	Professor	Nanowire Formation of Stacked Organic Molecules

2008/11/7	Masahiko Iyoda	Graduate School of Science and Engineering, Tokyo Metropolitan University	Professor	Nanowire Formation of Stacked Organic Molecules
2008/11/12	John R. Miller	Brookhaven National Laboratory, U.S. Department of Energy	Senior Chemist	Charge Delocalization and Transport in Cojugated Molecules: "Molecular Wires" for Photovoltaics?
2008/11/13	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental of TFT process
2008/11/21	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Similarity and difference between TFT and LSI processes
2008/12/1	Akihisa Inoue	Tohoku University	president	Interesting research with potential of bulk metal glass at AIMR
2008/12/9	Joo-Hee Jung	Asian Medical Center, Seoul, Korea	Senior Researcher	Seminar on bio-nanocapsules conjugated with liposomes for in vivo pinpoint delivery of various materials
2009/1/31	Yoshio Furusho	Graduate School of Engineering, Nagoya University	Associate Professor	Synthesis and Application of Double Helical Molecules and Macromolecules Based on π -Conjugated Molecules
2009/2/4	André Charette	Department of Chemistry, Univ. de Montréal	Professor	New Methods for the Stereoselective Synthesis of Cyclopropane Derivatives Using Zinc-Based Reagents
2009/2/4	Ahmed A Busnaina	Northeastern University	Professor	Directed Assembly of Nanoelements for Devices and Sensors

2009/2/4	Park Jin-Goo	Hanyang University	Professor	Plastic, Glass and Metal Substrate Based (Bio-)MEMS Fabrication toward Commercialization
2009/2/5	Gu ManBok	Korea University	Professor	Aptamer Technorogies for Detection of Adipokines, Residual Pharmaceuticals,and EDCs
2009/2/6	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental of TFT circuit technology
2009/2/18	Toyoyuki Ose	Hokkaido University, Graduate school of life science	Specially Appointed Assistant Professor	Construction of Plasmid DNA Vectors for Protein Expression and Molecular Docking Simulation for Prediction of Protein-Ligand interaction
2009/2/20	Shigeki Imai	Systems Engineering Laboratories, Corporate Research and Development Group, Sharp Corporation	Director	Fundamental of TFT circuit technology
2009/3/7	Ken Tanaka	Department of Applied Chemistry, Graduate School of Engineering Tokyo University of Agriculture and Technology	Associate Professor	Organic Synthesis in Both Academia and Industry

7) Public Information Activity

Public information activity of ISIR in 2008 is as follows:

- Bulletin of ISIR (2008 (in both Japanese and English))
- Memoirs of the Institute of Scientific and Industrial Research, Osaka University (Vol.65 2008 (in English))
- Annual Report of ISIR (2008 (in Japanese))
- SANKEN News Letters, 34-36(in Japanese)

- Report on SANKEN TECHNO SALON (2008 (in Japanese))
- WWW home-page (<http://www.sanken.osaka-u.ac.jp/>)
(English version is available.)

8) Research Reports

The number of scientific and technological papers published in 2008 is 474.
The details are described in the part of activity of divisions and facilities.

9) Scientific Awards

K.NISHINO	Japanese Society of Chemotherapy Award	2008/1/8
T.MAJIMA T.TACHIKAWA	ISEPD2008 Poster Award	2008/1/8
R.IINO	Best presenter Award(The Institute of Electrical Engineers of Japan)	2008/3/1
ALONGHENG	The Research Incentive Award for Graduate Student of JSAE	2008/3/1
R.MIZOGUCHI Y.KITAMURA M.SASAJIMA	Best presentation award for freshmen of JSAI	2008/3/12
R.MIZOGUCHI Y.KITAMURA M.SASAJIMA	Best presentation award for freshmen of JSAI	2008/3/12
R.MIZOGUCHI K.KOZAIKI	Best presentation award for freshmen of JSAI	2008/3/12
A.YAMAGUCHI	Asakawa Award from Japanese Society for Bacteriology	2008/3/25
A.YAMAGUCHI	The Pharmaceutical Society of Japan Award	2008/3/25
H.NAKAJIMA	JIM Masumoto Hakaru Award	2008/3/26
M,ISHIMARU	JIM Meritorious Award	2008/3/26
K.NAKATANI	The Chemical Society of Japan Award for Creative Work for 2007	2008/3/27
H.ASAHI M.ISHIMARU	JJAP Editorial Contribution Award	2008/4/8
H.CHIBA	JSME Young Engineers Award	2008/4/8
M.TANIGUCHI	CSJ Presentation Award 2008	2008/4/10

K.KAIHATSU	Travel Grant Award(21st International Society for Antiviral Research (in Canada)	2008/4/14
K.NISHINO	The Young Scientists Prize by the Minister of Education, Culture, Sports and Technology, Japan	2008/4/15
K.NAKATANI	Ichimura Academic Award	2008/4/25
T.YANAGIDA	Young Best Presenter Award on 6th Society of NanoScience and Technology Symposium	2008/5/8
Y.YAGI R.SAGAWA	Finalist for Best vision Paper (2008 IEEE International Conference on Robotics and Automation)	2008/5/19
K.NISHINO	Ueda Memorial Award	2008/6/6
K.SUGANUMA M.INOUE	International Conference on Electronics Packaging 2007	2008/6/10
K.NISHINO	Japan Bifidus Foundation Award	2008/6/12
Y.YAGI Y.MUKAIGAWA	SSII07 Best Paper Award	2008/6/12
A.INOKUCHI	The JPA Lectureship Award	2008/6/12
ALONGHENG	2008 International Material Research Conference the Student Best Paper Award	2008/6/20
K.FUKUI	IEEE 8th International Conference on Computer and Information Technology, Best Paper Award	2008/7/9
H.NAKAJIMA	DSL2008 Award for Career Achievements	2008/7/10
T.KASUYA	The Highlights of Student Posters Session Best Poster Award	2008/7/13
K.SUGANUMA M.INOUE	ICEPT-HDP 2008 Best paper award	2008/7/29
Y.YAGI Y.MUKAIGAWA	MIRU2008 Best Paper Award	2008/7/30
H.SASAI S.TAKIZAWA	Tetrahedron: Asymmetry Most Cited Paper 2005 - 2008 Award	2008/8/18
M>NUMAO S.KURIHARA	DICOMO2008 Best Paper Award	2008/8/22
S.TAGAWA T.KOZAWA H.YAMAMOTO	APSRC-2008 Poster Award	2008/9/1
H.ASAHI T.KAWAI	JSAP Fellow	2008/9/2

K.MATSUMOTO		
T.MAJIMA	The Japanese photochemistry Associate Lectureship Award 2008	2008/9/12
K.KAWAI	The Japanese Photochemistry Association Prize for Young Scientist for 2008	2008/9/12
H.NAKAJIMA M.TANE	JIM Best Poster Award	2008/9/24
H.NAKAJIMA R.NAKAMURA	4th Handai Nanoscience and Nanotechnology International Symposium /Best Poster Award	2008/9/30
T.KOZAWA	Japanese Society of Radiation Chemistry, Science Award	2008/10/16
T.KAWAI	2008 Achievement Award	2008/10/21
S.TAGAWA T.KOZAWA	MNC Best Presenter Award	2008/10/28
K.NAKATANI	Osaka Science award	2008/10/29
H.NAKAJIMA R.NAKAMURA	DIMAT2008 /Best Poster Award	2008/10/31
S.KURIHARA etc.	DPS Workshop 2008 / Best Poster Award	2008/12/12
K.KAIHATSU	Jury's Special Award(Bio Business Competition of Japan)	2009/2/2
K.NAKATANI	Osaka University Award for Education and Research	2009/2/20
K.NISHINO	Osaka University Award for Education and Research	2009/2/20
H.NAKAJIMA M.TANE	Global COE program Paper Award	2009/3/18
S.TAKIZAWA	The PSJ Award for Young Scientists	2009/3/25
H.NAKAJIMA	JIM Distinguished Contribution Award	2009/3/28
Y.MORIKAWA etc.	14th JPS Award for Academic Papers on Physics	2009/3/29
H.NAKAJIMA R.NAKAMURA	JIM Best Poster Award	2009/3/29

2. Education

ISIR accepts graduate students (about 230) from the Graduate Schools of Science, Engineering, Engineering Science, Pharmaceutical Science, Information Science and Technology, and Frontier Biosciences, and also researchers for special training, including those from industry and from abroad.

Staff members also belong to various Faculties: Faculty of Science, Faculty of

Engineering, Faculty of Engineering Science, Faculty of Pharmaceutical Science, Faculty of Information Science and Technology, and Faculty of Frontier Biosciences. Some members belong to two Faculties. They give lectures for graduate and undergraduate students in each Faculty.

Number of graduate students as of March 31, 2009 is as follows.

G.S. Course	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Course	57	49	16	6	16	10	154
Doctor Course	17	33	7	4	7	4	72
Total	74	82	23	10	23	14	226

Number of students who had obtained Master's or Doctor's Degree in 2008 is as follows.

Field Degree	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Degree	23	19	6	2	9	8	67
Doctor Degree	1	6	0	2	4	1	14
Total	24	25	6	4	13	9	81

3. International Exchange

1) Exchange Agreement

Academic Exchange Agreements are now concluded with the following 17 organizations.

- Faculty of Natural Science, Otto-von-Gueriche University Magdeburg (Germany)
- College of natural Science, Chungnam National University (Korea)
- Forschungszentrum Jülich GmbH (Germany)
- University of Maryland at COLLEGE PARK (U.S.A.)
- University College London (U.K.)
- College of Natural Sciences, Pusan National University (Korea)
- Research Institute of Industrial Science, Hanyang University (Korea)
- College of Science, National Taiwan University (Taiwan)

- Pacific Northwest National Laboratory (U.S.A.)
- Centre National de la Recherche scientifique : CNRS (France)
- Rwth Aachen University (Germany)
- College of Engineering, Gyeongsang National University (Korea)
- College of Natural Science, Chungnam National University (Korea)
- Institute of Remote Sensing and Geographical Information System, Peking University (China)
- College of Science, National Taiwan Normal University (Taiwan)
- Faculty of Science, University of Geneva (Switzerland)
- Inner Mongolia Normal University (China)

2) Foreign Researchers and Students

Number of foreign researchers and students staying in ISIR as of March 31, 2009 is 64 in total. Details are, Research Associates (8), Visiting Researchers (9), Part-time Employee (14), Graduate Students (33: Doctor Course, 21, Master Course, 12). Their nationalities are: Korea (22), China (16), India (3), Viet Nam (3), U.K (1), Spain (1), Russia (1), U.S.A (1), Indonesia (1), Russia (1), Brazil (2), Bangladesh (3), Malaysia (1), Turkey (1), Venezuela (1), Egypt (1), Iran (1)

Foreign visitors in 2008 are as follows:

U.S.A. (5), Korea (54), U.K. (1), Germany (1), France (1), Italia (1), Russia (1), India (1), Slovak Republic (6), Thailand (3), Egypt (1), Bangladesh (2), China (2), Taiwan (1), Philippines (1) Total 85.

3) International Conferences and Symposiums

Number of presentations (plenary, invited, oral and poster in various international conferences and symposia) by staff of ISIR is 517 in total.

Number of ISIR staffs who have been working as committee members of International Conferences or Editorial Board of international academic journals are 184 in total. For more details, see the part of activity of divisions and facilities.

4. Concluding Remarks

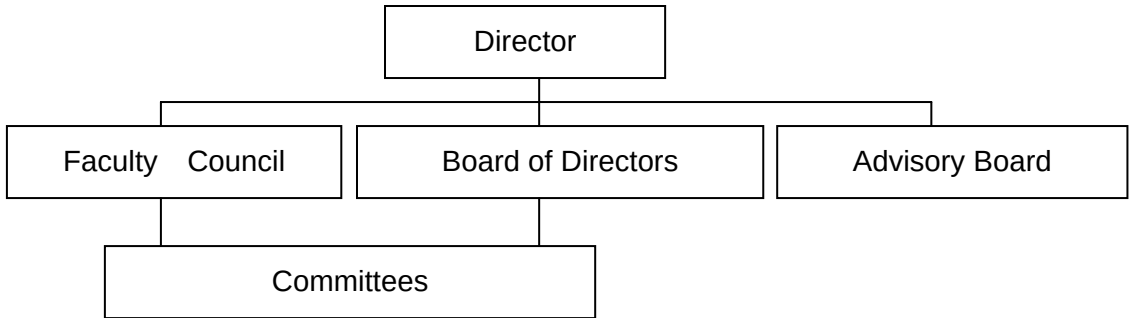
(1) Organization and Management System

After the reorganization in this spring (April 2009), ISIR has three major research divisions, Division of Information and Quantum Sciences, Division of Materials and Beam Sciences, and Division of Biological and Molecular Sciences, and one permanent

research center “Nanoscience and Nanotechnology Research Center”. In addition, ISIR contains two divisions for special purposes named “Division of Next Industry Creation” and “Division of Special Project Research”. The latter division contains independent laboratories supervised by associate professors with limited terms selected from young assistant professors of ISIR for promotion of young scientists. ISIR also has two research supporting centers, “Comprehensive Analysis Center” and “Research Laboratory for Quantum Beam Science”. Inter-institute project research, “Materials Science & Technology Research Center for Industrial Creation” and “Post-Silicon Materials and Devices Research Alliance” has reached the last year of its five year period. In the next year, the new inter-institute collaboration named “Network Collaboration Core for Materials & Devices Research Field” will be scheduled to start. In the ISIR, the following facilities are also installed; Workshop, Office of Information Network, Laboratory of Radio-isotope Experiments, Library, Academia-Industry Relation Office, Public Relations Office and Technical Division.

Management of ISIR is performed by the Director and the Board of Directors supervised by the Faculty Council composed of all ISIR professors. Advisory Board has been set up to introduce opinions from outside into the Institute. Advisory Board has been set up to introduce opinions from outside into the Institute.

【Organization of ISIR】



(2) Research Activities

In 1997, Harmonized Materials Research Group was designated as one of the Centers of Excellence (COE) of Ministry of Education, indicating the high research activity of the Institute.

From 2002 through 2006, we have awarded as the best group in 21 Century COE program that is originally the top 20 group plan in Japan. This involves the positive exchange between different laboratories which yield results of the global level with

respect to material, information and biotechnology.

In 2005, Materials Science & Technology Research Center for Industrial Creation has launched as a joint Center between ISIR and Institute of Multidisciplinary Research for Advanced Materials, Tohoku University. It was expanded to Post-Silicon Materials and Devices Research Alliance for collaboration with four university institutes in 2006.

In 2009, nationwide Network Joint Research Center for Materials and Devices including five university institutes has been authorized by Ministry of Education.

ISIR's research environment as facilities and equipments has been becoming better. A new building was constructed in 2001 and 2003 to the increased number of scientists and the development of Nanotechnology, respectively and Nanoscience and Nanotechnology Center started in April 2002. In addition, the old first research building will be reconstructed from autumn, 2007. In addition, a new building named "Nanotechnology Incubation Facility" has been under construction in 2009 for open innovation by academia-industry collaboration.

(3) Education

Considering objective of ISIR, supporting the graduate and undergraduate education is one of the important missions.

ISIR has over 200 graduate students coming from 6 different graduate schools and faculties such as Science, Engineering, Engineering Science, Pharmaceutical Science, Frontier Biosciences and Information Science and Technology.

In 2009, we have set up the Centre for Research Education and Training in order to promote the ISIR original education on research. We already have ISIR original lecture "Nano Engineering" in Graduate School of Engineering. We aim to expand the ISIR original lectures authorized by various graduate schools in Osaka University as a sub-program.

The Sanken Techno-Salon is one of forums to exchange information between our staff member and the people from industries specializing in electronics, organic chemicals, semiconductors, drugs, etc. We have also seminars for providing seeds of new technologies to the industrial communities. The Institute aim to grow researchers and students with the best humanity, capable of innovating their specific fields of research from basic point of view.

(4) Contribution to Societies

As the fast-paced advancement of science and technology and the rapid alteration of social and industrial structures, we must further recognize as the Institute open to

society and industry. We consistently strive to deepen our cooperation with society through positively opening of facilities, intellectual properties and achievements to meetings (ex. Sanken Techno Salon) and publications. Through them, we will be able to transfer our industrial seeds for new technology and exchange ideas for new materials. They have been highly evaluated that we have done joint researches with other university/industry.

In April 2005, AIR-office (Academia Industry Relations Office) has been settled in order to strengthen cooperation between the Institute and industries.

In 2008, Research Association of Industry and Science (RAIS), which is ISIR-supporting association having a history of 70 years, was reorganized, set up bureau office in ISIR and the bureau chief was adopted in order to promote and support the academia-industry cooperation.

(5) International Exchange

International Exchange is one of indispensable element for our Institute. We are trying to open the door widely to invite more researchers and students from other countries, and we have 3 kind of International exchange, Academic Exchange, Student Exchange and branches in France and USA. At present (March, 2008), 57 foreign researchers and students join in the Institute. International Conferences sponsored by our Institute have been held twice a year since 1998. It's so important to release our results towards all over the world and have a chance to exchange opinions with foreign scientists.

In 2009, Centre for International Collaboration was started for promoting the foreign exchange. Under the Centre, three collaborative laboratories between foreign universities has been set up or in preparation as follows: ICT Collaborative Laboratory between the School of Electronics Engineering and Computer Science, Peking Univ. And ISIR, Collaborative Laboratory between College of Science and Technology, Korea Univ. And ISIR, and Collaborative Laboratory between Faculty of Mathematical and Physical Sciences, Univ. College of London and ISIR in Areas Relating to Excited Surface Science.

(6) Future Plan and Prospect

At April in 2010, nationwide "Network Joint Research Center for Materials and Devices" will be started. It is a biggest collaboration network between university institutes in Japan. ISIR plays a leading role in the network as the headquarters. At the same time, our Nanotechnology Incubation Centre will open for the core of

academia-industry collaboration. So, we will advance to the next step of our ISIR in the next year.

In order to respond with flexibility to our quickly changing society, along with the rapid development of science and technology, we must understand our role of society and in order to stay effective and relevant Institute for industries, we must make independent researches and release widely our intellectual properties and achievement.

Keeping development of science and technology in Japan, we must cultivate researchers capable of producing academic and professional results that will benefit the people living on this planet. ISIR grow researchers and students who can active in the world.

You can see about ISIR on the following URL. (<http://www.sanken.osaka-u.ac.jp/>) The Institute of Scientific and Industrial Research keeps making efforts toward higher level contribution to science and industries, and keeps learning.

Activities of Divisions

Division of Quantum Engineering

Outline

New, advanced materials and fabrication techniques of nanostructures that allow the realization of the desired quantum effects of electrons, photons and spins are indispensable for the creation of novel electronic, photonic and spintronic devices. The Division of Quantum Engineering is engaged in experimental and theoretical research on these subjects aiming to establish the basis of future electronic/photonic/spintronic devices based on novel quantum effects. The Division of Quantum Engineering is composed of four departments: Quantum Molecular Devices, Photonic and Electronic Materials, Semiconductor Electronics and Condensed Matter Physics. Various approaches are being taken in the fields of electronic materials design and tailoring, surface physics, nanometer scale materials fabrication and characterization, semiconductor nanostructures for quantum devices, semiconductor-based new bio/chemical sensors and computational physics.

Research areas studied and techniques employed by the Division of Quantum Engineering include atomic and electronic structures of semiconductor surfaces and interfaces, nanofabrication processes using scanning probe microscopy, crystal growth of biomolecules, epitaxial growth of compound semiconductors by molecular beam epitaxy, characterization of structural, electric, optical and magnetic properties of semiconductor materials, formation and characterization of low-dimensional semiconductor quantum structures, fabrication of new semiconductor and quantum structure devices, control of the physical properties of carbon nanotubes and the fabrication of single electron transistor, and prediction of new functional materials and fabrication processes design using first principles and electronic structure calculations. Interdisciplinary researches in cooperation with other divisions are also pursued.

Achievements

- Understanding of the mechanisms of nanostructure relaxation, shape transformation of mesoscopic scale structures, and protein crystallization
- Crystal growth, characterization and device application of new semiconductors including III-nitride-based ferromagnetic semiconductors, Tl-III-V-N, III-nitride nanorod and quantum nanostructures
- Chirality & direction control of carbon nanotube growth
- Carbon nanotube quantum devices
- Integrated carbon nanotube biosensors
- Prediction of new functional materials, high efficient energy conversion materials and fabrication processes by first principles electronic structure calculations
- Materials and device design for semiconductor spintronics from the first principles
- Materials process design and quantum simulation by electronic excitations from the first principles
- Prediction of the electronic structure in organic-metal interfaces for organic-molecular electronics and materials design from the first principles

Department of Quantum Molecular Devices

Associate Professor: Koichi SUDOH
Graduate Student: Masakazu OKANO
Under Graduate Student: Kazuya MARUO
Supporting Staff: Kiyomi HIRASAWA

Outline

The Department of Quantum Molecular Devices is engaged in study of multi-scale surfaces/interfaces structures and nanoscale properties of materials for development of novel devices that integrate the quantum mechanical features of semiconductors and molecular functions of organic- and bio-molecules. In more concrete terms, we are studying dynamics of surface/interface structures under non-equilibrium conditions such as, relaxation, crystal growth, and interfacial reaction, using scanning probe microscopy.

Current Research Projects

Relaxation Dynamics of 2D Structures on Surfaces

Coarsening dynamics of two-dimensional (2D) morphologies on $\text{SrTiO}_3(001)$ surfaces have been studied using scanning tunneling microscopy. Forming submonolayer homoepitaxial films of various coverage by applying the STM nanofabrication technique, its relaxation process have been observed in real time by STM. The anomalous features of coarsening processes at coverages of around 0.5 have been revealed.

Shape Transformation of Silicon Micro-structures by Surface Diffusion

The mechanisms of shape transformation of silicon micro-structures by surface self-diffusion during hydrogen annealing have been studied. When high-aspect-ratio holes fabricated on $\text{Si}(001)$ surfaces are annealed at high temperatures, the hole inlets spontaneously close and voids are formed in the bulk Si. The mechanism of the void shape evolution during hydrogen annealing has been clarified. Different manners of shape transformation of 2D arrays of holes depending on the dimensions of the pattern have been shown, and the parameter window for formation of silicon-on-nothing (SON) structures have been obtained.

Interfacial Reaction during Annealing of Ultrathin SOI

Decomposition reaction during high temperature annealing of ultrathin silicon-on-insulator (SOI) substrates has been investigated. It has been found that, while continuous Si films are stable against the interfacial reaction, the interfacial reaction proceeds in dewetted regions where small Si islands scatter. Using TEM and AFM, the process of the reaction at Si island/ SiO_2 interfaces has been clarified.

Study on Growth Mechanism of Protein Crystals

Using sweet protein thaumatin as a model protein, the mechanism of protein crystal growth has been studied by in-situ atomic force microscopy (AFM) and Monte Carlo

(MC) simulation. It has been shown that our MC simulation can reproduce the AFM and optical microscope observations of growth of thaumatin tetragonal crystals. Through comparison between the experiments and the MC simulations, the fundamental information about the intermolecular interaction and the growth dynamics in thaumatin crystal growth has been obtained.

Publications

Original Papers

Smoothing of an atomically rough vicinal surface - STM observation and MC simulation, T. Irisawa, K. Matsumoto, K. Sudoh, H. Iwasaki, and M. Uwaha: Surf. Sci., 602 (2008) 2880-2885.

STM fluorescence of porphyrin enhanced by a strong plasmonic field and its nanoscale confinement in an STM cavity, H. W. Liu, R. Nishitani, T. Z. Han, Y. Ie, Y. Aso, and H. Iwasaki: Phys. Rev. B, 79 (2009) 125415-1-6.

International Conferences

Formation of Silicon on Nothing Structures by Hydrogen Annealing of the Hole Array on Si (100) (poster), R. Hiruta, H. Kuribayashi, R. Shimizu, K. Sudoh, and H. Iwasaki: 14th International Conference on Solid Films and Surfaces (2008 ICSFS), Dublin, Ireland, June 30- July 4, 2008.

Ostwald ripening of two-dimensional islands on SrTiO₃(001) (poster), M. Okano and K. Sudoh: International Symposium on Surface Science and Nanotechnology (ISSS-5), Tokyo, Japan, Nov. 9-13, 2008.

Structural relaxation of voids in Si substrates by high temperature hydrogen annealing (poster), R. Hiruta, H. Kuribayashi, R. Shimizu, K. Sudoh, and H. Iwasaki: 2008 MRS Fall Meeting, Boston, Massachusetts, USA, Dec. 1 – 5, 2008.

Publications in Domestic Meetings

The Physical Society of Japan	3 papers
The Japan Society of Applied Physics	2 papers
The Japanese Association for Crystal Growth Cooperation	1 paper

Sponsorships

Other Research Fund

K. Sudoh	Fuji Electric Device Technology Co., LTD	¥500,000
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Department of Photonic and Electronic Materials

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Assistant Professor: Shuichi EMURA
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Yusuke TANAKA, Katsuhiko TOKUDA, Yuya HONDA
Rina KAKIMI, Masane KIN, Yuji SAKAI, Motoki SOTANI
Hiroatsu TANI, Seiichi HAYASHI, Akio YAMANO
Jin-Qiang LIU
Undergraduate Student: Hiroya ICHIHARA
Research Student: Peng-Hang FAN
Support Staff: Akiko WATANABE

Outline

The department of Photonic and Electronic Materials makes research on materials, mainly semiconductors and related materials, and processing on them. Four steps are required in materials research, that is, materials design, materials synthesis (crystal growth) and processing, materials characterization, and device application. In materials design, study on finding required characteristics by changing the combination and ratio of atoms is conducted. In materials synthesis, study on molecular beam epitaxy growth is mainly carried out, in which the crystal growth is done by supplying molecules and atoms onto the substrate surface. In materials characterization, structure investigation by electron diffraction, X-ray diffraction, STM, EXAFS and Raman scattering, optical characterization by photoluminescence, optical absorption and so on, electrical characterization by Hall measurement, and magnetic characterization by SQUID are carried out. In device application, basic researches on photonic devices such as lasers, electronic devices such as field emission devices, and spintronic devices are conducted.

Current Research Projects

Crystal Growth and Properties of Diluted Magnetic Semiconductors

Diluted magnetic semiconductors are gathering great interest as a candidate for new functional materials. In 2001, we succeeded in the growth of GaCrN and observed the room temperature ferromagnetism as well as the PL emission. We also observed room temperature ferromagnetism and sharp PL emission for the rare-earth doped GaGdN. In 2005, tunnel magnetoresistance effect was observed at 77 K for the GaCrN/GaN/GaCrN tunnel diodes. Successful low temperature (300°C) growth of high Gd concentration (12%) GaGdN with improved ferromagnetism was also realized. Further increase of magnetization was obtained by Si co-doping. Together with the observation of enhanced magnetization in GaGdN/GaN superlattice structures these results were understood as carrier-induced ferromagnetism. In 2008, diameter-controlled growth of GaGdN nanorod was realized by changing the growth parameters to fabricate the nano-size spintronics devices. We have also observed the clear enhanced MCD signals and

hysteresis suggesting “real” ferromagnetic semiconductors.

Growth, Characterization and Device Application of Semiconductor-Semimetal Mixed Crystals; New Semiconductors Including Tl

In 1995, we proposed new semiconductors TlInGaAs in which the bandgap energy is independent of temperature. We have grown TlInGaAs by MBE and confirmed the small temperature variation of the bandgap energy and refractive index. In 2005, we obtained the small temperature variation of lasing peak wavelength as small as 0.06 nm/K for the TlInGaAs/TlInP/InP SCH LDs. We also proposed the TlInGaAsN/AlGaAs for both temperature-stable wavelength and threshold current LDs. In 2006, we found that the Tl incorporation is much improved by the use of Tl-contained cladding layers and barrier layers and by the co-doping of nitrogen (N) atoms. In 2008, by optimizing the layer structures of TlInGaAsN/GaAs/InGaP multi-quantum well (MQW) structures, relatively strong PL emission was obtained. We also obtained similar results for the TlInGaAsN/TlInP/InP MQW structures. These results show the possibility of fabrication of LEDs and LDs with these MQWs.

Growth of GaN Nano-Rods and Application to Field Emitter

III-V nitride semiconductors gather much interest from the viewpoint of application to light emitting devices as well as devices used in harsh environment. We have observed the strong PL emission from the grown polycrystalline GaN and proposed the wide variety of device applications. We also obtained the good electric field emission (FE) characteristics of electrons from GaN/metal samples, which is promising to fabricate the FE electron source devices. We also formed the GaN nano-rod structures on Si substrate and obtained the very small threshold voltage of 1.1 V/ μm for the FE. In 2008, based on the growth parameter dependence of GaN nano-rods, it was shown that their radii and spacing are controllable by varying the growth temperature. In addition, 2-dimensional (2D) field emitter arrays of nano-rods (10 μm spaced 10 μm square array and 1 μm spaced 1 μm square array) were fabricated on patterned SOI (Si/SiO₂/Si) substrates. It was found that the 1 μm spaced 1 μm square 2D-array of nanorods has better field emission characteristic than the 10 μm spaced 10 μm square 2D-array because of edge effect (enhancement of electric field at edges).

Growth of III-V Semiconductors on Sub-Micron Localized Areas of Si Surface

III-V semiconductors are attracting considerable attention as channel materials in the future advanced MISFETs with high performance (Beyond Si-CMOS), owing to their high electron mobility. To accomplish this, the formation of III-V-on-Insulator (III-V-O-I) on Si is mandatory. In 2008, the selective MBE growth of InP on sub-micron localized areas (800 nm and 400 nm in diameter) of Si substrate was successfully realized.

Spin Injection into Diluted Magnetic Semiconductors from Magnetic Metals and Their Nano-Magnetic Properties

Spin injection behavior from magnetic metals into diluted magnetic semiconductors (DMSs) is very important to realize semiconductor spintronics devices in addition to operate spin polarized scanning tunneling microscopy (SP-STM) to DMSs. So far, we have investigated crystal structures, growth mode, and magnetic properties of Fe

nanodots on GaN. In 2008, magnetic properties of Fe nanodots were studied using SP-STM. It was found that Fe nanodots with some ordered orientation show spin-dependent current-voltage characteristics.

XAFS Characterization of New Functional Materials

XAFS is a spectroscopy-based new characterization technique for analyzing atomic scale structures of materials and is only one technique directly analyzing the atomic arrangements/coordination for amorphous materials as well as very low density elements in materials. The atomic arrangements/coordination in the new functional materials, GaCrN and GaGdN, was characterized and it was showed that the Cr (Gd) atoms substitutionally occupy the group III sites. We also found the shift of the Cr atoms from the tetrahedron center in GaCrN, and the deformation ordering, which were considered to strongly affect the ferromagnetism of GaCrN. It was shown that the Cr atoms substitutionally occupy the group III sites in the GaCrN nano-rods grown at reduced temperatures.

Publications

Original Papers

Low temperature molecular-beam epitaxy growth of cubic GaCrN, S. Kimura, S. Emura, Y. Yamauchi, Y. K. Zhou, S. Hasegawa and H. Asahi: J. Cryst. Growth, 310 (2008) 40-46.

Large magnetization in high Gd concentration GaGdN and Si-doped GaGdN grown at low temperatures, Y.K. Zhou, S.W. Choi, S. Emura, S. Hasegawa and H. Asahi: Appl. Phys. Lett., 92(6) (2008) 6062505-1 - 6062505-3.

Growth and characterization of InCrN and (In,Ga,Cr)N, S. Kimura, S. Emura, K. Tokuda, Y. Hiromura, S. Hayakawa, Y.K. Zhou, S. Hasegawa and H. Asahi: Phys. Stat. Sol. (c), 5 (6) (2008) 1532-1535.

Molecular-beam epitaxy fabrication and analysis of GaN nanorods on patterned silicon-on-insulator substrate, J.U. Seo, S. Hasegawa, and H. Asahi: Phys. Stat. Sol. (c), 5(9) (2008) 3004-3007.

Selective growth of InP on localized areas of silicon (100) substrate by molecular beam epitaxy, K. Araki, S. Hasegawa and H. Asahi: Phys. Stat. Sol. (c), 5(9) (2008) 2766-2768.

Selective growth of InP on areas (1 μ m $\times$ 1 μ m) of silicon (100) substrate by molecular beam epitaxy, K. Araki, S. Hasegawa and H. Asahi: Proc. of the 20th Intern. Conf. on Indium Phosphide and Related Materials, (2008) WeP12-1 - WeP12-4.

Studies on TlInGaAsN Double Quantum Well Structures, D. Krishnamurthy, M. Ishimaru, M. Ozasa, Y. Tanaka, S. Hasegawa, Y. Hirotsu and H. Asahi: Proc. of the 20th Intern. Conf. on Indium Phosphide and Related Materials, (2008) WeP10-1 - WeP10-4.

Electronic structure of Ga_{1-x}Cr_xN and Si-doping effects studied by photoemission and X-ray absorption spectroscopy, G. S. Song, M. Kobayashi, J. I. Hwang, T. Kataoka, M. Takizawa, A. Fujimori, T. Ohkouchi, Y. Takeda, T. Okane, Y. Saitoh, H. Yamagami, F.-H. Chang, L. Lee, H.-J. Lin, D. J. Huang, C. T. Chen, S. Kimura, M. Funakoshi, S. Hasegawa, and H. Asahi:, (2008) 033304-1 – 033304-4.

Local Structural Change in paramagnetic and Charge-Ordered Phase of Sn_{0.2}Pr_{0.3}Sr_{0.5}MnO₃: an EXAFS Study, K.R. Priolkar, V. Kulkarni, P.R. Sarode, and S. Emura: J. Phys.: Condensed matter, 20 (2008) 335227 – 335231.

Review Papers

Advances and future prospects of semiconductor hetero-epitaxy, H. Asahi, Oyobutsuri, 77(5) (2008) 489-499 (in Japanese).

Books

Vacuum and Vacuum Evaporation, H. Asahi: in *Handbook of Thin Films* (Ohm-sha, 2008) 10-14 (in Japanese).

Patents

International Conferences

TlInGaAsN Novel Semiconductors and Temperature-Stable Lasing Wavelength Laser Diodes (invited), H. Asahi, S. Hasegawa, A. Fujiwara and D. Krishnamurthy: 2008 SPIE Photonics West Conference.

Selective growth of InP on areas (1 μ m $\times$ 1 μ m) of silicon (100) substrate by molecular beam epitaxy (poster), K. Araki, S. Hasegawa and H. Asahi: 20th International Conference on Indium Phosphide and Related Materials, Versailles, France,.

Studies on TlGaInNAs Double Quantum Well Structures (poster), D. Krishnamurthy, M. Ishimaru, M. Ozasa, Y. Tanaka, S. Hasegawa, Y. Hirotsu and H. Asahi,: 20th International Conference on Indium Phosphide and Related Materials, Versailles, France,.

Formation of aligned CrN nano-clusters in Cr-delta-doped GaN (poster), Y. K. Zhou, S. Kimura, S. Emura, S. Hasegawa and H. Asahi: International Conference on Quantum Simulators and Design 2008, Tokyo.

Crystal growth and characterization of GaCrN nanorods on Si substrate (poster), H. Tambo, S. Kimura, Y. Yamauchi, Y. Hiromura, S. Emura, S. Hasegawa and H. Asahi: The 2nd International Symposium on Growth of III-Nitrides, Izu, Japan.

Effects of morphologies on field emission characteristics of GaN nanorods grown on Si by MBE (poster), J. U. Seo, S. Hasegawa, and H. Asahi: The 2nd International Symposium on Growth of III-Nitrides, Izu, Japan.

Orbital ordering on dilute Cr³⁺ ions doped in GaN (poster), S. Emura, S. Kimura, K. Tokuda, Yi-Kai Zhou, S. Hasegawa and H. Asahi: 29th International Conference on Physics of Semiconductors, Brazil.

Third magnetic phase of GaGdN detected by SX-MCD (poster), M. Takahashi, Y. Hiromura, S. Emura, T. Nakamura Y.K. Zhou, S. Hasegawa and H. Asahi: 29th International Conference on Physics of Semiconductors, Brazil.

Structural properties of AlCrN, GaCrN and InCrN (poster), S. Kimura, K. Tokuda, Y. K. Zhou, S. Emura, S. Hasegawa and H. Asahi: 15th International Conference on Molecular Beam Epitaxy, Vancouver, Canada.

MBE growth and characterization of TlGaInNAs double quantum well structures (poster), D. Krishnamurthy, M. Ozasa, Y. Tanaka, S. Hasegawa and H. Asahi: 15th International Conference on Molecular Beam Epitaxy, Vancouver, Canada.

Annealing effect in GaDyN on optical and magnetic properties (poster), Y. K. Zhou, M. Takahashi, S. Emura, S. Hasegawa, H. Asahi: 5th International Conference on Physics and Applications of Spin-Related Phenomena in Semiconductors, Foz do Iguacu, PR, Brazil.

Magnetic properties of GaGdN studied by SQUID and SX-MCD (poster), M. Takahashi, Y.K. Zhou, S. Emura, T. Nakamura, S. Hasegawa, and H. Asahi: 5th International Conference on Physics and Applications of Spin-Related Phenomena in Semiconductors, Foz do Iguacu, PR, Brazil.

Structural properties of AlCrN, GaCrN and InCrN (poster), K. Tokuda, S. Kimura, Y. K. Zhou, S. Emura, S. Hasegawa and H. Asahi: XXI International Union of Crystallography, Osaka, Japan.

Crystal growth condition dependence of local structure around Gd in GaN nanorods (poster), S. Emura, H. Kameoka, H. Tambo, Y.K. Zhou, S. Hasegawa and H. Asahi: XXI International Union of Crystallography, Osaka, Japan.

Growth and characterization of GaN nanorods towards the application to field emitters (invited), S. Hasegawa, J.U. Seo and H. Asahi: 14th Seoul International Symposium on the Physics of Semiconductors and Applications, Jeju Island, Korea.

SX-MCD and XAFS Analysis on GaGdN (poster), M. Takahashi, Y. Hiromura, S. Emura, T. Nakamura, Y.K. Zhou, S. Hasegawa, and H. Asahi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Gd concentration dependence of local structures around Gd atoms in GaGdN nanorod (poster), H. Kameoka, S. Emura, H. Tambo, Y.K. Zhou, S. Hasegawa and H. Asahi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Growth and characterization of Fe nanostructures on GaN (poster), Y. Honda, M. Sotani, S. Hasegawa and H. Asahi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Growth and characterization of transition-metal and rare-earth doped III-nitride based

magnetic semiconductors for nano-spintronics (invited), H. Asahi, S. Hasegawa, S. Emura and Y.K. Zhou: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Influence of native silicon oxides on the growth of GaN nanorods on Si (001) (poster), S. Hasegawa, J. K. Seo, K. Uchida, H. Tambo, H. Kameoka, M. Ishimaru, and H. Asahi: International Workshop on Nitride Semiconductors (IWN-2008), Montreux, Switzerland.

Degradation mechanisms of GaAs PHEMTs under operation in high humidity conditions (poster), T. Hisaka, H. Sasaki, Y. Nogami, K. Hosogi, N. Yoshida, J.A. del Alamo, S. Hasegawa and H. Asahi: Reliability of Compound Semiconductors (ROCS) Workshop, Monterey, California, USA.

Growth and characterization of Fe nanostructures on GaN (poster), Y. Honda, S. Hayakawa, S. Hasegawa and H. Asahi: 4th Vacuum and Surface Sciences Conference of Asia and Australia, Matsue, Japan.

Ferromagnetism and Luminescence of Diluted Magnetic Semiconductors GaGdN and AlGdN (invited), S. Emura, M. Takahashi, H. Tambo, T. Nakamura, Y.K. Zhou, S. Hasegawa and H. Asahi: Materials Research Society Fall Meeting, Boston, MA, USA.

Field emission characteristics of GaN nanorods grown on Si by MBE (poster), S. Hasegawa, J. U. Seo and H. Asahi: International Symposium on Core University Program between Japan and Korea, Awaji, Hyogo, Japan.

Magnetic properties of GaCrN nanorods (poster), Y. K. Zhou, H. Tambo, S. Emura, S. Hasegawa and H. Asahi: International Symposium on Core University Program between Japan and Korea, Awaji, Hyogo, Japan.

Contributions to International Conferences and Journals

- | | |
|----------|---|
| H. Asahi | 2008 International Conference on Solid State Devices and Materials
(Program Committee member) |
| H. Asahi | 20th International Conference on Indium Phosphide and Related Materials
(International Steering Committee member) |
| H. Asahi | 15th International Conference on Molecular Beam Epitaxy
(International Advisory Committee member) |
| H. Asahi | Second International Symposium on Growth of III-Nitrides
(International Advisory Committee member) |
| H. Asahi | 4th Vacuum and Surface Science Conference of Asia and Australia
(Program Committee member) |
| H. Asahi | International Conference on Functional Materials for Advanced Technology
(International Organizing Committee member) |
| H. Asahi | 16th International Colloquium on Scanning Probe Microscopy
(Publication Committee member) |
| H. Asahi | 2009 International Conference on Solid State Devices and Materials
(Program Committee member) |
| H. Asahi | 21st International Conference on Indium Phosphide and Related Materials
(International Steering Committee member) |

H. Asahi	Journal of Crystal Growth (Editor)
H. Asahi	Current Applied Physics (Editorial Board member)
H. Asahi	J. Materials Science: Materials in Electronics (Editorial Board member)
H. Asahi	Journal of Ceramic Processing Research (Editor)
H. Asahi	Journal of Physics: Condensed Matter (Advisory Editorial Board member)
H. Asahi	e-Journal of Surface Science and Nanotechnology (Advisory Board member)
S. Hasegawa	Second International Symposium on Growth of III-Nitrides (Financial Committee member)
S. Hasegawa	22th International Conference on Indium Phosphide and Related Materials (Steering Committee member)
S. Hasegawa	14th International Conference on Modulated Semiconductor Structures (Local Arrangements Committee member)

Publications in Domestic Meetings

The Japan Society of Applied Physics	23 papers
PASPS Symposium	3 papers
Electronic Materials Symposium	2 papers
The Surface Science Society of Japan	1 paper
The Japan Institute of Metals	1 paper

Academic Degrees

Master Degree of Engineering

M. Takahashi	Study on formation and characterization of GaGdN/AlGaIn heteronanostructures
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Master Degree of Science

A. Kameoka	Fabrication and characterization of Gd-doped GaN nanorods
Y. Tanaka	Structural and optical characterization of TlInGaAsN on InP grown by molecular beam epitaxy
K. Tokuda	Crystal growth and their physical properties of Cr-doped III-nitride diluted magnetic semiconductors
Y. Honda	Formation of Fe dots on GaN and their I-V characteristics

Sponsorships

Grant-in-Aid for Scientific Research (B) (2)

H. Asahi	Study on Room Temperature Ferromagnetic Nitride Semiconductor Nanostructures and Application to Nanospintronics Devices	¥2,300,000
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Grant-in-Aid for Scientific Research on Priority Areas

H. Asahi	Study on Fabrication of InN-Based Long Wavelength Circular Polarized Semiconductor Lasers	¥3,900,000
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Grant-in-Aid for Creative Scientific Research

H. Asahi Development of properties and functionalities by precise ¥28,000,000
 control of rare-earth doping (Y. Fujiwara)

Department of Semiconductor Electronics

Professor:	Kazuhiko MATSUMOTO
Associate Professor:	Koichi INOUE, Kenzo MAEHASHI
Assistant Professor:	Yasuhide OHNO
Graduate Students:	Hideo NAGAHAMA, Yasuki YAMAMOTO, Shin IWASAKI, Yuichi TSUJITA, Satoshi NAGASO Tomoki TSUJI, Takaomi KISHIMOTO
Under Graduate Students:	Hideito ONODERA, Yusuke YAMASHIRO
Supporting Staff:	Misa KURIO

Outline

Semiconductors quantum structures, where electrons and photons play remarkable roles owing to quantum effects, are expected to show superior properties. We study the basic problems in the fabrication and the characterization of such quantum structures in the atomic scale. The research activities include applications to new devices based on the quantum effects with the coherent ballistic transport of carriers and electron-photon interactions.

Carbon nanotubes (CNTs), especially single-walled carbon nanotubes (SWNTs), are a promising material to realize quantum-effect devices because of their unique nano-structures. As a sensor of single charge or spin with the high sensitivity, the formation and characterization of field-effect transistors (FETs) and single electron devices using carbon nanotubes are studied using thermal chemical vapor deposition method, Raman scattering spectroscopy, scanning probe microscopy, and photoluminescence spectroscopy.

Current Research Programs

Resonant micro-Raman scattering study of SWNTs grown by the laser-irradiated chemical vapor deposition

In the laser-irradiated chemical vapor deposition process (LICVD), SWNTs are grown around a focus point of the laser light on substrate surfaces with Fe catalyst at an atmosphere of ethanol vapor. The local distribution of SWNTs was investigated by the resonant micro-Raman scattering measurement discriminating their chiralities. As the results, a doughnut-like pattern around the focus spot was obtained in the intensity distribution of radial breathing modes which were characteristic in SWNTs. Such patterns were different to a certain degree according to the Raman-excitation laser wavelength, which corresponded to the LICVD laser wavelength or not. By the consideration of the excitation power distribution, the result suggests that the growth of some SWNTs is resonantly promoted in a local area in the LICVD process.

Room-temperature-operating carbon nanotube single-hole transistors with significantly small gate and tunnel capacitances

Carbon nanotube single-hole transistors operating at room temperature were realized.

To obtain large charging energy, a 25-nm-long carbon nanotube channel was formed by shadow evaporation for small gate capacitance and an insulator was inserted between the channel and electrodes for small tunnel capacitances. A significantly small gate capacitance (0.06 aF) and small tunnel capacitance (0.3 aF) were obtained. The estimated charging energy of a carbon nanotube single-quantum dot was 108 meV. Drain current oscillation as a function of gate voltage was clearly observed while typical p-type field-effect transistor characteristics were obtained for the device without insulator. These results indicate that the small tunnel capacitance is necessary for the room-temperature-operating carbon nanotube single-charge transistors.

Horizontally-aligned SWNTs on patterned SiO₂/Si substrates

Horizontally-aligned SWNTs were fabricated on patterned SiO₂/Si substrates with groove-and-terrace or half-cylinder structures using electron-beam lithography and reactive ion etching. Scanning electron microscopy (SEM) observation revealed that the SWNTs were preferentially grown along the edges of terraces or along the sidewalls of the half cylinders. The results are consistent with calculations of the Casimir-Polder potential between the SWNTs and the patterned substrates. This method will be promising to control the directions of the SWNTs on SiO₂/Si substrates.

Microfluidic and label-free multi-immunosensors based on carbon nanotube microelectrodes

We fabricated microfluidic and label-free multi-immunosensors by the integration of CNT-arrayed electrodes and microchannels with pneumatic micropumps made of poly(dimethylsiloxane). In the microfluidic systems, four kinds of sample solutions were transported from each liquid inlet to microchannels using six pneumatic micropumps. As a result, two kinds of antibodies were immobilized onto different CNT electrodes using the microfluidic systems. Next, two kinds of cancer markers, prostate specific antigen and human chorionic gonadotropin in phosphate buffer solution, were simultaneously detected by differential pulse voltammetry. Therefore, microfluidic multi-immunosensors based on CNT electrodes and pneumatic micropumps are useful for the development of multiplex hand-held biosensors.

Publications

Original Papers

Electrical characterization of carbon nanotube field-effect transistors with SiN_x passivation films deposited by catalytic chemical vapor deposition, Kenzo Maehashi, Yasuhide Ohno, Koichi Inoue, Kazuhiko Matsumoto, Toshikazu Niki, and Hideki Matsumura: Appl. Phys. Lett., 92 (2008) 138111/1-3.

Carbon Nanotube Amperometric Chips with Pneumatic Micropumps, Yuichi Tsujita, Kenzo Maehashi, Kazuhiko Matsumoto, Miyuki Chikae, Soichiro Torai, Yuzuru Takamura, and Eiichi Tamiya: Jpn. J. Appl. Phys., 47 (4) (2008) 2064-2067.

High-Performance Carbon Nanotube Field-Effect Transistors with Local Electrolyte Gates., Taiji Katsura, Yasuki Yamamoto, Kenzo Maehashi, Yasuhide Ohno, and Kazuhiko Matsumoto: Jpn. J. Appl. Phys., 47 (4) (2008) 2060-2063.

Room-Temperature Coulomb Oscillations of Carbon Nanotube Field-Effect Transistors with Oxidized Insulators, Yasuhide Ohno, Yoshihiro Asai, Kenzo Maehashi, Koichi Inoue, and Kazuhiko Matsumoto: Jpn. J. Appl. Phys., 47 (4) (2008) 2056-2059.

Room-Temperature Carbon Nanotube Single-Electron Transistors Fabricated Using Defect-Induced Plasma Process, Shin Iwasaki, Masatoshi Maeda, Takafumi Kamimura, Kenzo Maehashi, Yasuhide Ohno, and Kazuhiko Matsumoto: Jpn. J. Appl. Phys., 47 (4) (2008) 2036-2039.

Suppression of current fluctuations in carbon nanotube field-effect transistors by applying alternating current, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, and Kazuhiko Matsumoto: Proc. of the 2008 International Conference on Nanoscience and Nanotechnology, (2008) 67-70.

Carbon nanotube field-effect transistor biosensors with high signal-to-noise ratio using alternating current measurement, Yasuki Yamamoto, Yasuhide Ohno, Kenzo Maehashi, and Kazuhiko Matsumoto: Proc. the IASTED International Conference on NANOTECHNOLOGY AND APPLICATIONS, 615-043 (2008) 21-26.

High-performance carbon nanotube field-effect transistors for high-sensitive bio sensors, Kenzo Maehashi, Kazuhiko Matsumoto: Proc. the IASTED International Conference on NANOTECHNOLOGY AND APPLICATIONS, 615-019 (2008) 1-5.

Controlling Direction of Growth of Carbon Nanotubes on Patterned SiO₂ Substrate, Takafumi Kamimura, Kazuhiko Matsumoto: Appl. Phys. Express, 2 (2009) 015005/1-3.

Transition between Particle Nature and Wave Nature in Single-Walled Carbon Nanotube Device, Takafumi Kamimura, Yasuhide Ohno, Kazuhiko Matsumoto: Jpn. J. Appl. Phys., 48 (2009) 015005/1-3.

Carbon Nanotube Fabry–Perot Device for Detection of Multiple Single Charge Transitions, Takafumi Kamimura, Yasuhide Ohno, Kazuhiko Matsumoto: Jpn. J. Appl. Phys., 48 (2009) 025001/1-4.

Room-temperature-operating carbon nanotube single-hole transistors with significantly small gate and tunnel capacitances, Yasuhide Ohno, Yoshihiro Asai, Kenzo Maehashi, Koichi Inoue, and Kazuhiko Matsumoto: Appl. Phys. Lett., 94 (2009) 053112/1-3.

International Conferences

High-Performance Carbon Nanotube Field-Effect Transistors Using Low-Energy Ion Implantation, *Kenzo Maehashi, Kohei Nishiguchi, Yasuhide Ohno, Koichi Inoue, Kazuhiko Yamamoto, and Kazuhiko Matsumoto: 66th Device Research Conference, Santa Barbara, USA, June, 23-25, 2008.

Convertible Transistor between Resonant Tunneling Transistor and Single Hole Transistor Using Single-Walled Carbon Nanotube., *Takafumi Kamimura, Yasuhide Ohno, and Kazuhiko Matsumoto: 66th Device Research Conference, Santa Barbara, USA, June, 23-25, 2008.

Transition from Carbon Nanotube Single-Hole Transistor Property to Resonant Tunneling Transistor Property by Controlling Thickness of Tunneling Barriers., *Takafumi Kamimura, Yasuhide Ohno, and Kazuhiko Matsumoto: TMS 50th Electronic Materials Conference, Santa Barbara, USA, June, 25-27, 2008.

High Sensitive Carbon Nanotube FET Biosensor with Micro Fluid System and AC Measurement System (poster), *Kazuhiko Matsumoto, Kenzo Maehashi, Yasuhide Ohno, and Yasuki Yamamoto: 9th International Conference on the Science and Application of Nanotubes, Montpellier, France, June 29 - July 4, 2008.

Low-Energy Oxygen Ion Irradiation Effects on Carbon Nanotube Field-Effect Transistors with Passivation Films., *S. Nagaso, Y. Ohno, K. Maehashi, K. Inoue, K. Yamamoto, and K. Matsumoto: 2008 International Conference on Solid State Device and Materials Tsukuba, Japan, September 23 - 26, 2008.

Conversion Between Particle Nature and Wave Nature of Hole in Single-walled Carbon Nanotube Transistor by Gate Voltage, *T. Kamimura, Y. Ohno, and K. Matsumoto: 2008 International Conference on Solid State Device and Materials Tsukuba, Japan, September 23 - 26, 2008.

Room Temperature Operation of Carbon Nanotube Single-Hole Transistors Fabricated by Shadow Evaporation Methods, *Y. Ohno, Y. Asai, K. Maehashi, K. Inoue, and K. Matsumoto: 2008 International Conference on Solid State Device and Materials Tsukuba, Japan, September 23 - 26, 2008.

Carbon Nanotube Field-Effect Transistor Biosensors with High Signal-to-Noise Ratio Using Alternating Current Measurement, *Y. Yamamoto, Y. Ohno, K. Maehashi, and K. Matsumoto: 2008 The IASTED International Conference on Nanotechnology and Applications, Crete, Greece, Sept. 29 - Oct. 1, 2008.

High-Performance Carbon Nanotube Field-Effect Transistors for High-Sensitive Biosensors, *K. Maehashi, and K. Matsumoto: 2008 The IASTED International Conference on Nanotechnology and Applications, Crete, Greece, Sept. 29 - Oct. 1, 2008.

Irradiation Effect of IR Laser on Carbon Nanotubes. (poster), *T. Tsuji, K. Inoue, Y. Ohno, K. Maehashi, and K. Matsumoto: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sept. 29 - Oct. 1, 2008.

Carbon Nanotube Amperometric Multi-Immunosensors with Pneumatic Micropumps (poster), *Y. Tsujita, K. Maehashi, K. Matsumoto, M. Chikae, Y. Takamura, and E. Tamiya: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sept. 29 - Oct. 1, 2008.

Evaluation of Ion Irradiation Effects on CNT-FETs with Passivation Films (poster), *S. Nagaso, Y. Ohno, K. Maehashi, K. Inoue, K. Yamamoto, and K. Matsumoto: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sept. 29 - Oct. 1, 2008.

Fabrication of CNT-FETs on Sapphire Substrate (poster), *T. Kishimoto, Y. Ohno, K. Maehashi, K. Inoue, and K. Matsumoto: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sept. 29 - Oct. 1, 2008.

Fabrication of the Catalyst Nanoparticle Arrays for Carbon Nanotube Growth (poster), *S. Iwasaki, Y. Ohno, K. Maehashi, and K. Matsumoto: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sept. 29 - Oct. 1, 2008.

Transition Between Particle Nature and Wave Nature of Hole in Single-Walled Carbon Nanotube Transistor by Gate Voltage, *Kazuhiko Matsumoto: AVS 55th International Symposium & Exhibition, Boston, USA, October 19 - 24, 2008.

Noise Reduction of Carbon Nanotube Field-effect Transistor Biosensors using Alternating Current Measurement, *Y. Yamamoto, Y. Ohno, K. Maehashi, and K. Matsumoto: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, October 27 - 30, 2008.

Microfluidic and Label-free Immunosensors based on Carbon Nanotube Microelectrodes, *Y. Tsujita, K. Maehashi, K. Matsumoto, M. Chikae, Y. Takamura, and E. Tamiya: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, October 27 - 30, 2008.

Carbon Nanotube Quantum Nanodevice., *K. Matsumoto, Y. Ohno and T. Kamimura: 13th Advanced Heterostructures and Nanostructures Workshop Hawaii, USA, December 7-12, 2008.

Carbon Nanotube Quantum Devices & Bio Sensor Application (invited), *K. Matsumoto: International Meeting on Frontiers of Physics 2009 Malaysia, January 12-16, 2009.

Carbon Nanotube Quantum Nanodevices & Bio Sensor Applications (plenary), *K. Matsumoto, T. Kamimura, K. Maehashi, and Y. Ohno: The 2nd International Symposium on Global COE Program of Center for Next-Generation Information Technology Based on Knowledge Discovery and Knowledge Federation, Hokkaido, Japan, January 20-21, 2009.

Aligned Single-Walled Carbon Nanotubes on Patterned SiO₂/Si Substrates (poster), *T. Kishimoto, S. Iwasaki, Y. Ohno, K. Maehashi, K. Inoue, and K. Matsumoto: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Vertically-Aligned Carbon Nanotube Arrayed Electrodes for Amperometric biosensors (poster), *H. Onodera, Y. Tsujita, K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Chirality Selection of Single-Walled Carbon Nanotubes by the irradiation of IR Laser (poster), *T. Tsuji, K. Inoue, Y. Ohno, K. Maehashi, and K. Matsumoto: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Multiplexed Immunosensors Based on Carbon Nanotube-Arrayed Microelectrodes and Pneumatic Micropumps (poster), *Y. Tsujita, K. Maehashi, and K. Matsumoto: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Detection of Negatively Charged Protein Using n-type Carbon Nanotube Field-Effect Transistors (poster), *Y. Yamamoto, K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Coulomb Oscillations in Graphene Quantum Dots (poster), *Y. Yamashiro, K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Total Integrated Immune Assay System Employing Simple and Accurate Check Valve-Pump Flow Control with Non-label High Sensitive Electrochemical Detection for Clinical Diagnosis (poster), *Yuzuru Takamura, Soichiro Torai, Miyuki Chikae, Yuichi Tsujita, Kenzo Maehashi, Kazuhiko Matsumoto and Eiichi Tamiya: the 12th Int. Conf. on Miniaturized Systems for Chemistry and Life Sciences (2008) Oct. 12 - 16, San Diego, USA.

Publications in Domestic Meetings

The Japan Society of Applied Physics

11 papers

Academic Degrees

Master Degree of Engineering

Shin IWASAKI	Aligned Growth of Carbon Nanotubes on the Patterned Surfaces of Silicon Substrates
Yuichi TSUJITA	Micro-Fluidic Multi-Biosensors based on Carbon Nanotube Micro-Electrodes
Satoshi NAGASO	Nano-Memory Devices with Carbon Nanotube Channels

Sponsorships

Grant-in-Aid for Scientific Research in Priority Areas

K. Matsumoto	Carbon Nanotube-Biosensor	¥33,800,000
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Grant-in -Aid for Basic Research (C)

K.Maehashi	Fabrication of High-Sensitive Multi-Biosensors based on Carbon Nanotube-Arrayed Microelectrodes	¥1,300,000
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Other Research Fund

K.Matsumoto	Japan Science and Technology Agency (CREST)	Quantum nano devices by controlling quantum nano interface	¥7,000,000
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Department of Condensed Matter Physics

Professor: Hiroshi KATAYAMA-YOSHIDA
Associate Professor: Yoshitada MORIKAWA
Research Technical Expert: Akira YANASE
Guest Professor: Mitsuhiro MOTOKAWA
Post Doctoral Fellows: Van An DINH, Ikutaro HAMADA, Susumu YANAGISAWA
Graduate Students: Hideki HAYASHIDA, Kenji TOYODA,
Haruhiko DEKURA, Kunihiko HARADA,
Jun ISHISADA, Akihumi UOZUMI,
Hideyuki JIPPOU, Hitoshi FUJII, Ryusuke TOMINAGA,
Shinya NAKAE, Hideyuki MORIMURA
Supporting Staff: Mika ASADA, Ryoko ITO

Outlines

The primary activities of this department are theoretical study of electronic properties of condensed matters, and materials design, which predicts novel materials possessing desired properties for applications. In addition to model analyses which extract the essence of materials properties, quantum simulations are used for the study, with the methods of computational physics reflecting a recent remarkable progress of computing ability. Theoretical approaches are tried to predict materials which meet requirements from application areas by first-principles calculations using atomic numbers only as parameters.

Current Research Project

Water/Metal Interfaces: Atomic Structures and Effect of Adsorbed Hydrogen

Understanding the interaction of water with metal surfaces is essential in corrosion, catalysis, and electrochemistry, as water plays important roles in chemistry at the water/metal interface. Ab initio electronic structure methods with the generalized gradient approximation (GGA) to density-functional theory (DFT) have been routinely used to study the water/metal interfaces. While DFT-GGA has been successfully applied to a variety of systems, there is a well known deficiency in describing the weak interaction, i.e., the van der Waals (vdW) forces. Though the vdW interaction is believed to be important in weakly interacting water/metal interfaces, there are no ab initio studies on this issue.

Herein we apply the van der Waals density functional (vdW-DF) to the H₂O bilayer on Rh(111) as an example of a water/metal interface, to study the influence of the vdW forces on the wetting H₂O layer on a metal surface. This interface can be considered to be an ideal interface to study the interaction of H₂O with the metal substrate, because of the close match between the lattice constants of Rh(111) and of ice Ih. The vdW-DF has been successfully applied to van der Waals complexes as well as the covalent solid and the adsorbed system, because the functional is seamless by construction, i.e., it can describe the nonlocal correlation at all length scale.

We also investigated the geometries, energetics, and electronic structures of the water

bilayer on Rh(111) and hydrogen preadsorbed Rh(111) [H/Rh(111)] surfaces investigated by DFT within a generalized gradient approximation (GGA), to clarify the interaction of water with adsorbed hydrogen (Hads) and the substrate.

Organic/Metal Interfaces

We have studied the interaction of benzene with Cu(111), Ag(111) and Au(111) surfaces using density functional theory (DFT) within a generalized gradient approximation (GGA) and the van der Waals density functional [vdW-DF, Dion *et al.*, Phys. Rev. Lett. 92 (2004) 246401]. The adsorption energies using vdW-DF are significantly more accurate than those using GGA, while the equilibrium adsorption distances between benzene and metal substrates (Z_C) calculated by both GGA and vdW-DF are almost identical. The work function changes induced by the adsorption of benzene are significantly underestimated compared with the experimental values, as a result of the overestimation of Z_C by both GGA and vdW-DF. Instead of determining the Z_C values from first-principles calculations, we deduced the most probable adsorption distances in such a way as to reproduce the experimentally-observed work function changes. The deduced Z_C (Z_C^{ded}) is shortest on Cu(111) while it is longest on Ag(111), reflecting the strength of the interactions between benzene and the metal surfaces. It turns out that the substrate dependence of the work function change is mainly ascribed to the difference in the metal-organic distance, Z_C . Charge transfers and work-function changes by the adsorption of benzene were analyzed by means of the induced density of interface states (IDIS) model [H. Vázquez *et al.*, Europhys. Lett. 65 (2004) 802], and compared with the self-consistent GGA calculations. The vacuum level shifts estimated by the IDIS model agree with the GGA results for $Z_C \geq 0.3$ nm. On the other hand, the discrepancy between the two methods becomes larger for $Z_C \leq 0.3$ nm, where the back donation from the metal substrates to the adsorbate becomes significant. We show that the IDIS model reasonably works well for benzene on Cu(111), Ag(111) and Au(111) surfaces because $Z_C^{\text{ded}} \approx 0.3$ nm on all surfaces. However, our analysis reveals that the actual charge density redistribution induced by the adsorption of benzene is more complicated than that assumed in the IDIS model.

Investigation of Switching Behavior of Molecules on Metal Electrodes for Molecular-scale Electronics

In this study, we studied the stable adsorption structure and the electronic structure of functionalized and nonfunctionalized OPE molecules on Au(111) by using a program package STATE (Simulation Tool for Atom TEchnology). Calculations are based on the density functional theory (DFT), within a generalized gradient approximation (GGA). Valence electrons are expanded in a plane wave basis set and Au(111) surface is represented by the repeated slab model. We also investigated the effect of electric field on the physical and electronic structure of OPE molecules of electric field by employing the Effective Screening Medium (ESM) method.

We found that the stable structure of OPE molecules switch from a bridge configuration to a fcc-hollow configuration under a strong electric field. The interaction between a static electronic field and a electronic dipole moment, and a dielectric polarization of OPE molecules play an important role in the conductance switching. We will also discuss the coverage dependence of OPE molecules for the switching behavior.

Elucidation of Mechanism of Intelligent Catalyst for Three-way Catalysts

The present study aims at clarifying the mechanism of the self-regenerative function by ab-initio thermodynamics calculations. The following figure shows the calculated relative grand potential of the reduced (segregated state of Pd) and the oxidized (solid solution) state as a function of the chemical potential of oxygen for Pd containing LaFeO₃ and CaTiO₃. As seen in the figure, the oxidized state is more stable than the reduced state above the critical O chemical potential (about 0.92 eV for LaFeO₃ and about -0.08eV for CaTiO₃) and the reduced state becomes more stable below the critical potential. The O chemical potential can be related to temperature and pressure of gas phase O. The critical O chemical potential for LaFeO₃ corresponds to 10⁻³ atom at 700K. On the other hand, Pd particles do not form solid solution with CaTiO₃ at realistic conditions. These results are in reasonable agreement with the experimental results.

Design of Co-doping Method in DMS

We have proposed co-doping method for increasing solubility of magnetic impurities in dilute magnetic semiconductors (DMS). The concentration dependences of the mixing energy of DMS, such as (Ga, Mn)N, (Ga, Cr)N, (Ga, Mn)As and (Zn, Cr)Te, show large convexity and these systems have a tendency toward spinodal decomposition. By introducing compensating impurities, e.g. O or Si, into these DMS, it is found that the mixing energy shows gradual transition from convex to concave concentration dependence resulting in negative mixing energy of magnetic impurities. This result suggests that the co-doping method dramatically increases the solubility of magnetic impurities in DMS, thus high concentration doping of magnetic impurities into DMS becomes possible.

However, the co-doped impurities kill the ferromagnetism of DMS. In order to remove the co-doped impurities after crystal growth, we propose interstitial impurities such as Li, Be, B, Na, Mg, K, Ca, Cu and Ag for co-dopants in (Ga, Mn)As. With these interstitials, the mixing energy of (Ga, Mn)As are strongly reduced and for low concentration of Mn it becomes negative. Next, to simulate low temperature annealing of Li-co-doped (Ga, Mn)As, we calculate binding energy between substitutional Mn and interstitial Li in GaAs by using STATE-SENRI package. The calculated binding energy is smaller than the binding energy between substitutional Mn and interstitial Mn. By performing kinetic Monte Carlo simulations with ab-initio binding energies, we have calculated effective diffusion constant of Li in (Ga, Mn)As. Due to the small binding energy, Li diffuse rather easily in (Ga, Mn)As and Li interstitials can be removed by the low temperature (lower than 580 degree C) annealing treatment. Thus, we have shown that by using the Li interstitials the solubility limit is enhanced and high concentration Mn doping becomes possible. Moreover, by low temperature annealing after the crystal growth Li can be diffuse out from the sample to recover the ferromagnetism.

Materials Design of Oxide Based Magnetic Materials for Spintronics

We have proposed a materials design of MgO based magnetic materials as a spin polarizer in semiconductor spintronics devices. By using the KKR-CPA method (MACHIKANNEYAMA2002 package) we calculate the electronic structure of Ni-, Co-doped MgO and N-doped MgO, CaO, SrO and BaO. By performing monte Carlo

simulations with ab-initio exchange interactions we estimate Curie temperature of these compounds. It is found that N-doped MgO, CaO, SrO and BaO are ferromagnetic inspite of the absence of magnetic impurities. In these compounds, N carries large part of the magnetization. Moreover, these compounds show half-metallic density of states, and this means that they are promising candidates for a spin polarizer. It is pointed out that to realize high-T_c the control of spinodal decomposition in these compounds is of significant importance.

Materials Design for Dilute Magnetic Semiconductors with IV-Group Elements

We have proposed a materials design of Si- and Ge-based dilute magnetic semiconductors. They are very much coherent with the present semiconductor electronics. In this sense, the fabrication of ferromagnetic DMS based on Si and Ge is very important. In order to design environmentally safe and cheap materials, we consider Fe and Mn as a magnetic impurity. By using the KKR-CPA method (MACHIKANNEYAMA 2002 package) we calculate the electronic structure of Mn- and Fe-doped Si and Ge. It is found that Mn atoms avoids nearest-neighbor configuration in Ge and in this configuration the Mn atoms couple ferromagnetically. Moreover calculated pair interactions between Mn are attractive and this result well explains the observed nano-column formation in Mn-doped Ge systems.

Publications

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Density functional theoretical study of hydrogen on Pt(111) in an electrochemical environment (poster), *I. Hamada, Y. Morikawa: The 1st International Conference of the Grand Challenge to Next-Generation Integrated Nanoscience June 3-7, 2008, Tokyo, Japan.

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Design of High Solubility of Magnetic Impurities for Semiconductor Spintronics by Codoping Method (poster), *T. Fukushima, K. Sato, and H.K.-Yoshida: Fifth International Conference on Physics and Applications of Spin-related Phenomena in Semiconductors, Aug 3-6, 2008, Bourbon Cataratas Resort & Convention Center, Brazil.

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Ab-initio Electronic Structure Calculations of $(\text{Ti,Co})\text{O}_2$ Within Self-interaction-corrected LDA (poster), *H. Kizaki, M. Toyoda, K. Sato, and H. Katayama-Yoshida: Fifth International Conference on Physics and Applications of Spin-related Phenomena in Semiconductors, Aug 3-6, 2008, Bourbon Cataratas Resort & Convention Center, Brazil.

First-principles molecular dynamics simulation of H adsorption at the water/Pt(111) interface (invited), *Y. Morikawa, I. Hamada, T. Ikeshoji, Y. Okamoto, M. Otani, and O. Sugino: 59th Annual Meeting of the International Society of Electrochemistry, Sep 7-12, 2008, School of Engineering, Spain.

Density-functional theoretical study of hydrogen on Pt(111) in an electrochemical environment (poster), *I. Hamada, Y. Morikawa: 59th Annual Meeting of the International Society of Electrochemistry, Sep 7-12, 2008, School of Engineering, Spain.

Computational Nano-materials Design for Semiconductor Nano-Spintronics (invited), *H.K.-Yoshida: Joint European Magnetic Symposia, Sep 14-19, 2008, Trinity College Dublin, Ireland.

An Investigation of Material Design for Gettering (poster), *K. Matsukawa, K. Shirai, H. Katayama-Yoshida: Pacific Rim Meeting 2008, Oct 12-17, 2008, Honolulu, Hawaii.

First-Principles Calculations of Electronic Structure on $(\text{Ti,Co})\text{O}_2$ within Self-Interaction-Corrected LDA, *H. Kizaki, M. Toyoda, K. Sato, H.

Katayama-Yoshida: 2nd International Symposium on Transparent Conductive Oxides, Oct22-25, 2008, Crete. Greece.

Density-functional theory study of hydrogen at the water/Pt(111) interface (poster), *I. Hamada, Y. Morikawa: The 12th SANKEN International Symposium, Jan. 22, 2009, Univ. Osaka, Japan.

Co-doing of interstitial impurities in dilute magnetic semiconductors (poster), *K. Sato, H. Fujii, H. Katayama-Yoshida: The 12th SANKEN International Symposium, Jan. 22, 2009, Univ. Osaka, Japan.

Theoretical investigation of the electronic structure of the Alq₃/metal interfaces (poster), *S. Yanagisawa, K. Lee, Y. Morikawa: The 12th SANKEN International Symposium, Jan. 22, 2009, Univ. Osaka, Japan.

First-principles molecular dynamics simulations of chemical reactions at electrode surfaces (invited), *Y. Morikawa: Supercomputing in Solid State Physics 2009, Feb. 16-19, 2009 ISSP Tokyo, Japan.

Theoretical investigation of the electronic structure of the Alq₃/metal interfaces (poster), *S. Yanagisawa, K. Lee, Y. Morikawa: The International Symposium "Simulations and Dynamics for Nanoscale and Biological Systems" March4-6, 2009 Univ. of Tokyo, Japan.

Contributions to International Conferences and Journals

- | | |
|-------------|--|
| Y. MORIKAWA | International Conference on Quantum Simulators and Design 2008(QSD2008), National Museum of Emerging Science and Innovation (Miraikan), (Tokyo), 31 May-3 Jun. 2008. (Organizing Committee) |
| Y. MORIKAWA | 4th Handai Nanoscience and Nanotechnology International Symposium: Nano-Advanced Materials and Devices, ~from Nano-fabrication to Nano-application~ Icho-Kaikan, Osaka University, Suita, (Osaka), 29 Sep.-1 Oct. 2008. (Organizing Committee) |

Publications in Domestic Meetings

The Physical Society of Japan	21 papers
The Japan Society of Applied Physics	4 papers
Publications in Domestic Meetings	10 papers

Academic Degrees

Master Degree for Engineering

- | | |
|-----------|---|
| A. Uozumi | Elucidation of self-regenerative function of intelligent catalyst by ab-initio thermodynamics calculation |
|-----------|---|

H. Jippou	First-principles electronic structure calculations of metal-organic interfaces
J.Ishisada	Effect of single lattice vacancy in Si on its elastic properties
K.Harada	Ab initio materials design for environmentally sustainable spintronics

Master Degree for Science

M.Fujii	Ab initio design of interstitial Li-co-doping method for high-Tc magnetic semiconductors Computational material design for high-Tc magnetic semiconductors by co-doping method
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Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

Y. Morikawa	Development and releasing of quantum simulator for submicron scale systems	¥2,300,000
Y. Morikawa	Development of efficient parallel quantum dynamics simulator	¥12,700,000
Y. Morikawa	Theory of nano-scale linked molecules	¥2,900,000
Y. Morikawa	Design of new multi-functional nanotube device	¥397,000

Entrusted Research

Y. Morikawa	Japan Science and Technology Corporation. Elements Science and Technology Project	Elucidation and design of self-organization for nano-scale catalysts from first-principles	¥8,104,235
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Other Research Fund

Y. Morikawa	Toyota Motors	Investigation of diffusion processes of Li ions by using high-quality electronic structure calculations.	¥5,000,000
Y. Morikawa	Matsushita Electric Industrial Co., Ltd.	First-principles investigation of metal/organic interfaces	¥1,540,000
Y. Morikawa	Kobe Steel Ltd.	First-principles investigation of atomic structures and electronic properties of interfaces.	¥1,045,000

Division of Advanced Materials Science and Technology

Outline

The Division of Advanced Materials Science and Technology is composed of six departments with research fields: Structural Characterization and Design, Metallic Materials Process, Atomic Scale Science, Functional Ceramic Materials, Frontier Materials Creation, and Advanced-Energy Materials. This division has a close relationship with Nanoscience and Nanotechnology Center of this Institute founded in 2002. The future highly functionalized materials can be obtained by hybridizing different kinds of materials which are well designed and controlled with respect to their structures, dimensions and physical and chemical properties. We are aiming at design, development and characterization of new functional or high strength and high performance materials by means of highly advanced processes with micro, nano and atomic scale controlled techniques we developed.

Achievements

- Local structural changes on annealing in Fe-based metallic glasses
- Thermally induced structural changes in radiation-induced amorphous phases
- Development of continuous casting technique for producing lotus-type porous carbon steel and aluminum alloys and application to functional materials
- Establishment of fabrication of lotus-type porous metals by thermal decomposition method
- Fabrication of nano-sized hollow sphere metals and nanotube by Kirkendall effect of atomic diffusion
- Construction of oxide nanowires and their application to ReRAM
- Nano-science by using of scanning probe microscopes towards high resolution imaging of a single molecule of DNA and a protein
- Development of bio-molecular device constructed from DNA.
- Development of low temperature fabrication method of SiO₂/Si structure by use of nitric acid oxidation and its application to TFT
- Development of defect passivation semiconductor cleaning method and improvement of device characteristics
- Development of low temperature oxidation method of SiC and improvement of characteristics of SiC-based MOS devices
- Crystal growth and characterization of novel ambipolar cuprates
- Crystal growth and carrier-density control of iron-pnictide high-temperature superconductors
- Transport and magnetic studies of spin Hall insulators
- Creation of novel sp³-bonded phases from graphite via fs-laser excitation
- Surface structural instability induced by hole injection from STP chips
- Ultra fast carrier dynamics on semiconductor surfaces
- Development of time-resolved ultrafast electron diffractometer

Department of Structural Characterization and Design

Associate Professor: Manabu ISHIMARU
Research Associate: Akihiko HIRATA
Graduate Students: Fumihiko NAKAMURA, Dai YAMAMOTO
Yuusaku NISHIYAMA
Supporting Staff: Shigeko TOMII

Outlines

In controlling structures of new functional materials, introduction of new local structure analysis techniques to the materials becomes necessary. Using high-resolution electron microscopy (HREM), electron diffraction and electron energy-loss spectroscopy, we are mainly analysing local atomic structures and electronic states of functional alloy nano-particles, amorphous alloys, ion-irradiated ceramics and multi-layered materials. We are also developing new local structure analysis techniques using nano-sized electron probe, energy-filter and imaging-plate. Molecular dynamics and Monte-Carlo calculations and electronic band structure calculations of new materials are carried out for predicting their structures and physical properties.

Current Research Project

Local structural changes on annealing in Fe-based metallic glasses

We have examined local structural changes on annealing including crystallization behavior especially in Fe-based metallic glasses by means of transmission electron microscopy. In an FeCrMoCBTm bulk metallic glass, well-defined diffraction peaks due to $M_{23}C_6$ were found in a X-ray diffraction profile after completing the crystallization. Before completing, however, we found various nanoscale intermediate states exhibiting pseudo-tenfold diffraction patterns by using a nanobeam electron diffraction method. Therefore the crystallization was found to proceed through a formation of such nanoscale intermediate states. In an FeCoSiNbB bulk metallic glass, moreover, we also found similar intermediate states exhibiting pseudo-tenfold diffraction patterns during the crystallization. These results imply that an appearance of the nanoscale intermediate states with pseudo-tenfold symmetries is one of the features for Fe-based bulk metallic glasses.

Thermally induced structural changes in radiation-induced amorphous phases

Thermally induced structural relaxation in amorphous silicon carbide (SiC) has been examined by means of *in situ* transmission electron microscopy (TEM). The amorphous SiC was prepared by high-energy ion-beam-irradiation into a single crystalline 4H-SiC substrate. Cross-sectional TEM observations and electron energy-loss spectroscopy measurements revealed that thermal annealing induces a remarkable volume reduction, so-called densification, of amorphous SiC. From radial distribution function analyses using electron diffraction, notable changes associated with structural relaxation were observed in chemical short-range order. It was confirmed that the structural changes observed by the *in situ* TEM study agree qualitatively with those of the bulk material.

On the basis of the alteration of chemical short-range order, we discussed the origin of thermally induced densification in amorphous SiC.

Publications

Original Papers

Ionization-induced effects in amorphous apatite at elevated temperatures, I.-T. Bae, Y. Zhang, W. J. Weber, M. Ishimaru, Y. Hirotsu, M. Higuchi: J. Mater. Res., 23 (2008) 962-967.

Low temperature thermal annealing-induced α -FeSi₂ derived phase in an amorphous Si matrix, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez, K. E. Sickafus: Appl. Phys. A, 91 (2008) 353-356.

Compositional analyses of ion-irradiation-induced phases in δ -Sc₄Zr₃O₁₂, K. E. Sickafus, M. Ishimaru, Y. Hirotsu, I. O. Usov, J. A. Valdez, P. Hosemann, A. L. Johnson, H. T. Thao: Nucl. Instrum. Meth. B, 266 (2008) 2892-2897.

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Unexpectedly low thermal conductivity in natural nanostructured bulk Ga₂Te₃, K. Kurosaki, H. Matsumoto, A. Charoenphakdee, S. Yamanaka, M. Ishimaru, and Y. Hirotsu: Appl. Phys. Lett., 93 (2008) 012101(1)-012101(3).

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Direct observations of thermally induced structural changes in amorphous silicon carbide, M. Ishimaru, A. Hirata, M. Naito, I.-T. Bae, Y. Zhang, W. J. Weber: J. Appl. Phys., 104 (2008) 033503(1)-033503(3).

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Review Papers

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International Conferences

Studies on TlGaInNAs double quantum well structures (poster), *D. Krishnamurthy, M. Ishimaru, M. Ozasa, Y. Tanaka, S. Hasegawa, Y. Hirotsu, H. Asahi: 20th Indium Phosphide and Related Materials Conference, Versailles, France (May 25-29, 2008).

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Local structure analysis of metastable iron silicides formed in the Fe ion implanted Si, *M. Naito, M. Ishimaru: 7th Polish-Japan Joint Seminar on Micro and Nano Analysis,

Warsaw, Poland (September 7-10, 2008).

Influence of native silicon oxides on the growth of GaN nanorods on Si(001) (poster), *S. Hasegawa, J.-U. Seo, K. Uchida, H. Tambo, H. Kameoka, M. Ishimaru, H. Asahi: International Workshop on Nitride Semiconductors, Montreux, Switzerland (October 6-10, 2008).

Structural relaxation in amorphous SiC studied by *in situ* transmission electron microscopy, *M. Ishimaru, A. Hirata, M. Naito, I.-T. Bae, Y. Zhang, W. J. Weber: 9th Asia-Pacific Microscopy Conference, Jeju, Korea (November 2-7, 2008).

Structural characterization of metastable iron silicides formed in the Fe ion implanted Si, *M. Naito, M. Ishimaru: 9th Asia-Pacific Microscopy Conference, Jeju, Korea (November 2-7, 2008).

Formation Process of χ -FeCrMo Structure in Fe-Cr-Mo-C-B-Tm Metallic Glass, *A. Hirata, Y. Hirotsu, K. Amiya, A. Inoue: 9th Asia-Pacific Microscopy Conference, Jeju, Korea (November 2-7, 2008).

Characterization of Natural Nanostructured Thermoelectric (Ga,In)₂Te₃ (poster), *K. Kurosaki, M. Ishimaru, A. Charoenphakdee, H. Matsumoto, H. Muta, S. Yamanaka: Materials Research Society 2008 Fall Meeting, Boston, USA (December 1-5, 2008).

Transmission electron microscopy study on electron beam irradiation induced phase transformation of niobium nitride (poster), *J. H. Won, J. A. Valdez, K. E. Sickafus, M. Ishimaru, M. Naito: Materials Research Society 2008 Fall Meeting, Boston, USA (December 1-5, 2008).

Natural nanostructured bulk Ga₂Te₃ as a new class of thermoelectric material (poster), *K. Kurosaki, M. Ishimaru, A. Charoenphakdee, H. Matsumoto, H. Muta, S. Yamanaka: The International Union Materials Research Society International Conference in Asia 2008, Nagoya (December 9-13, 2008).

Thermally induced structural changes of amorphous SiC, *M. Ishimaru: 16th International Conference on Microscopy of Semiconducting Materials, Oxford, UK (March 17-20, 2009).

Contributions to International Conferences and Journals

M. Ishimaru Japanese Journal of Applied Physics (Associate Editor)

Publications in Domestic Meetings

The Japan Institute of Metals	3 papers
The Japan Society of Applied Physics	2 papers
The Japanese Society of Microscopy	2 papers

Academic Degrees

Master Degree for Engineering

D. Yamamoto	Molecular Dynamics Study on Hetero-Epitaxial Growth of Si _{1-x} Ge _x Alloys
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Sponsorship

Grant-in-Aid for Scientific Research (C)

M. Ishimaru	Amorphization and chemical short-range order in SiC under radiation environments	¥1,500,000
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Grant-in-Aid for Encouragement of Young Scientists (B)

A. Hirata	Direct observation of nanoscale structure changes in Fe-based bulk metallic glasses	¥2,600,000
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Entrusted Research

M. Ishimaru	NEDO (Advanced Materials Technology Utilizing Glassy Metals for Commercial Uses)	Nano-structure Analysis for the Evaluation of Mechanical Properties in Glassy Metals	¥2,500,000
M. Ishimaru	Nissan Ltd.	Arc, Structural analysis of Li-ion battery	¥1,000,000
A. Hirata	Nissan Ltd.	Arc, Local structure analysis of amorphous states in Fe-based alloys	¥2,000,000

Department of Metallic Materials Process

Professor:	Hideo NAKAJIMA
Associate Professor:	Shinsuke SUZUKI
Assistant Professors:	Masakazu TANE, Ryusuke NAKAMURA
Designated Assistant Prof.:	Jae-Soung PARK (-2009.2), Takuya IDE
Post Doctoral Fellow:	Sang-Youl KIM (-2008.8)
Graduate Students:	Hiroshi CHIBA, Tae-Bum KIM, Yeong-Hwan SONG, Tae KAWASHIMA, Yuki KAWAMURA, Kohta TANIGUCHI, Rika OKAMOTO, Kohei SUGIHARA, Gen MATSUBAYASHI
Research Student:	Juan LOBOS
Supporting Staff:	Satoko MATSUMOTO

Outlines

Metals are fundamental materials indispensable to various structural and functional materials. The main purpose of this department is to investigate physics of metallic materials and develop novel processing of the metallic materials. The department has undertaken the following several topics of the metallic materials science and engineering.

Lotus-type porous metals (lotus metals) developed by this department are unique materials which exhibit extraordinary superior mechanical strength. The materials have been fabricated by unidirectional solidification of the melts under pressurized gases. Recently we developed a novel safe and low-cost method for fabricating lotus metals through thermal decomposition of gas compounds, which does not require pressurized gas. In this year, we investigated the fabrication of lotus copper, aluminum alloys and carbon steel using the thermal decomposition method and the continuous casting method. And the mechanical properties of lotus-type porous metals were investigated and a plastic deformation process for improvement of the mechanical properties was developed. Applications of lotus metals are investigated in the fields of machine parts, automobiles, electronics, leisure and medical engineering.

Furthermore, we are studying the formation mechanism on hollow nanoparticles and nanotubes to establish the principle for fabricating novel nanoporous materials. Our focus is on the use of generation and clustering of atomic vacancies, which are associated with diffusion phenomena, to introduce an interior nanopore into nanoparticles and nanowires. In this year, we showed that hollow nanoparticles were formed by annealing core/shell type nanoparticles composed of heterogeneous metals with large difference in diffusion coefficient and that oxide nanotubes were obtained via oxidation of metallic nanowires in air.

Current Research Project

Development of Thermal Decomposition Method to Fabricate Lotus-type Porous Metals

Lotus-type porous aluminum and its alloys with cylindrical pores were fabricated by

unidirectional solidification through thermal decomposition of $\text{Ca}(\text{OH})_2$, NaHCO_3 , or TiH_2 (gas compound). The elongated pores are evolved due to the solubility gap between liquid and solid when the melt dissolving hydrogen is solidified unidirectionally. The pore size decreases and the pore density increases with increasing amount of gas compound. The porosity and pore size decrease with increasing argon pressure, which is explained by Boyle's law. It is suggested that for this fabrication method, porosity and pore size can be widely controlled by kind and amount of gas compound and argon pressure.

Fabrication of Practical Lotus-type Porous Metals by Continuous Casting Technique

We fabricated lotus-type porous copper, aluminum alloys and carbon steel using the continuous casting technique through either the pressurized gas method or the thermal decomposition method. The porosity and the pore size in the lotus-type porous metals can be controlled by the temperature of the melt, atmosphere gas pressure, the solidification velocity and the amount of the gas compounds. This is a promising technique for low cost and mass-production for commercial application of the lotus metals and provides various products for applications.

High Strain Rate Compression Behavior of Lotus-type Porous Iron

High strain rate compression behaviors of lotus-type porous iron was investigated. In high strain rate compression along the orientation direction of pores, the stress-strain curve exhibit a unique plateau stress region where deformation proceeds with almost no stress increase. In high strain rate compression along the orientation direction of pores, lotus iron exhibits superior energy absorption characteristics due to the unique plateau stress region. The appearance of plateau stress region depends on the strain rate. In middle and low strain rates compression along the orientation direction of pores, the unique plateau stress region does not appear. The appearance of plateau stress region also depends on the compressive direction. In compression perpendicular to the orientation direction of pores, the unique plateau stress region does not appear even in the high strain rate compression.

Improvement of Mechanical Properties of Lotus-type Porous Copper

Surfaces of a plate sample of lotus-type porous copper were deformed plastically by a wire-cup brush rotating at a high speed. The processed surface had fine-grained crystals with a smaller grain size than 100nm and the ends of the pores were closed by a newly formed non-porous skin layer with fine-grained crystals. The ultimate tensile strength of the lotus-type porous copper sample was increased about 30% compared with the sample before processing.

Fabrication of Hollow Metallic Nanoparticles and Oxide Nanotubes Using the Kirkendall Effect

We studied the formation of hollow metallic nanoparticles through the Kirkendall effect, which is caused by the large difference in diffusion coefficient between two metals in interdiffusion. We found that hollow nanoparticles are formed by annealing Au nanoparticles with larger diffusion coefficients surrounded by Pd with smaller diffusion coefficients at 300~400°C. Our results show that hollow nanoparticles can be obtained

from core/shell nanoparticles composed by binary metals with large difference in diffusivity and solubility in a wide concentration range. Furthermore, we observed that Fe, Cu and Ni nanowires turned into oxide nanotubes via oxidation reactions.

Publications

Original Papers

Effects of Heating Rate, Holding Temperature and Holding Time on Porosity and Pore Morphology of Aluminum Foams by Powder Metallurgy Process, H. Seki, S. Sasaki, M. Otsuka, H. Nakajima: J. Jpn. Inst. Metals, 72 (4) (2008) 278-284.

Magnetization Process of Lotus-type Porous Metals, H. Onishi, S.K. Hyun, H. Nakajima, S. Mitani, K. Takanashi, K. Yakushiji: J. Appl. Phys., 103 (9) (2008) 93539.

Evaluation of physical Properties of Porous Metals with Unidirectional Pores, H. Nakajima, M. Tane, K. Nakata, S. Fujimoto, T. Ichitsubo, T. Tanaka, and Y. Yamada: Tetus to hagane, 13 (6) (2008) 368-374.

Peculiar elastic behavior of Ti-Nb-Ta-Zr single crystals, M. Tane, S. Akita, T. Nakano, K. Hagihara, Y. Umakoshi, M. Niinomi, and H. Nakajima: Acta Mater., 56 (12) (2008) 2856-2863.

Equal-channel Angular Extrusion Process of Lotus-type Porous Copper, S. Suzuki, H. Utshunomiya, H. Nakajima: Mater. Sci. Eng. A, 490 (1 - 2) (2008) 465-470.

Fabrication of Lotus-type Porous Metals through Hydride Decomposition, H. Nakajima: Adv. Eng. Mater., 10 (9) (2008) 816-819.

Shrinking of hollow Cu₂O and NiO nanoparticles at high temperatures, R. Nakamura, D. Tokozakura, J.-G. Lee, H. Mori and H. Nakajima: Acta Mater., 56 (18) (2008) 5276-5284.

In Vitro Corrosion Resistance of Lotus-type Porous Ni-free Stainless Steels, K. Alvarez, S.K. Hyun, S. Fujimoto, H. Nakajima: J. Mater. Sci.: Mater. Med., 19 (11) (2008) 3385-3397.

Fabrication of Lotus-Type Porous Al-Si Alloys Using the Continuous Casting Technique, J.S. Park, S.K. Hyun, S. Suzuki, H. Nakajima: Metal. Mater. Trans. A, 40 (2) (2009) 406-414.

New Fabrication Method for Lotus-Type Porous Metals and its Application, H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2007), (2008) 193-196.

Fabrication of Lotus-type Porous Carbon-steel by Continuous Casting Technique in Nitrogen Atmosphere, K. Kashiwara, S. Suzuki, S.K. Hyun, H. Yonetani, and H.

Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2008), (2008) 201-204.

Equal-channel Angular Extrusion of Lotus-type Porous Copper, S. Suzuki, H. Utsunomiya, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2009), (2008) 205-208.

Fabrication and Plastic Deformation Behavior of Lamellar Ti-Rich TiAl Crystals With Lotus-Type Aligned Pores, T. Nakano, S. Tachibana, K. Hagihara, Y. Umakoshi, T. Ide, M. Tane, H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2010), (2008) 213-216.

Fabrication of Lotus-type Porous Nickel with Atmospheric Pressure and Foaming Agents by Mold Casting Technique, S.Y. Kim, B.Y. Hur, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2011), (2008) 197-200.

Impact Properties of Lotus-type Porous Carbon Steel Measured by Instrumented Charpy Testing, T. Kujime, S. K. Hyun, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2012), (2008) 217-220.

Fabrication of Lotus-type Porous Al-Si by Continuous Casting Technique, J.S. Park, S.K. Hyun, S. Suzuki, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2013), (2008) 229-232.

Fabrication of Lotus-type Porous Magnesium by Continuous Casting Technique, S.K. Hyun, S. Suzuki, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2014), (2008) 233-236.

Effects of pore size distribution and loading direction on fatigue property of lotus-type porous copper with anisotropic pore structure, H. Seki, M. Tane, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2015), (2008) 237-240.

Fabrication of Lotus-type Porous Magnesium using Hydrogen Desorption from MgH_2 , M. Tane and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2016), (2008) 241-244.

Formation of a Nano-pore during Oxidation of Metal Nanoparticles, R. Nakamura, D. Tokozakura, J.-G. Lee, H. Mori, and H. Nakajima: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2017), (2008) 329-332.

Steady State Comparative-longitudinal Heat Flow (SCHF) Method Using Specimen of Different Thickness for Measuring Thermal Conductivity of Anisotropic and Thin Porous Metals, H. Chiba, T. Ogushi, H. Nakajima, K. Torii, T. Tomimura, F. Ono: Proceedings of 5th International Conference on Porous Metals and Metallic Foams (MetFoam2017), (2008) 521-524.

Plastic Deformation of Lotus-type Porous Copper through ECAE Process, S. Suzuki, H. Utunomiya, H. Nakajima: Journal of the JRI Cu, (47) (2008) 93-97.

Review Papers

Fabrication and Properties of Porous Metals with Directional Pores, H. Nakajima, M. Tane, S.K. Hyun, S. Suzuki: Materia, 47[4] (2008) 196-202.

Development of High-efficiency Water-cooled Type Heat Sink Using Lotus-type Porous Copper, H. Chiba, T. Ogushi, and H. Nakajima: Journal of the Heat Transfer Society of Japan, 47 (2008) 11-15.

Formation of Hollow Structures through Oxidation of Metallic Nanoparticles, R. Nakamura, D. Tokozakura, J.-G. Lee, H. Mori, H. Nakajima: Materia, 47[7] (2008) 368-374.

Diffusion Measurements in Liquid Metal, S.Suzuki: Materia, 47[6] (2008) 305-311.

Fabrication of Lotus-type Porous Ceramics by Unidirectional Solidification, S. Ueno, L.M. Lin, H. Nakajima: Materia, 47[8] (2008) 399-405.

Books

Method for Compression Test of Porous Metals (JIS H 7902), H. Nakajima: Japanese Industrial Standards Committee, (2008) 1-7.

Method for Thermal Conductivity Test of Porous Metals (JIS H 7903), H. Nakajima: Japanese Industrial Standards Committee, (2008) 1-16.

Glossary of Terms Used in Porous Metals (JIS H 7009), H. Nakajima: Japanese Industrial Standards Committee, (2008) 1-15.

Method for Measurement and Estimation of Thermal Conductivity and Thermal Diffusivity, H. Chiba, H. Nakajima: Science&Technology, (2009) 146-156.

High-temperature Measurements of Materials, (ed. by H. Fukuyama, Y. Waseda), S.Suzuki, Springer, (2009) 61-83.

Patents

Production Method for Porous Metal Body, H. Nakajima, JP4217865

Metal Porous Body Manufacturing Method, H. Nakajima, JP4235813

Metal Porous Body Manufacturing Method, H. Nakajima, Canada, No2473120

Sound Absorption Materials, H. Nakajima, Y. Okuda, Z.K. Xie and T. Ikeda, JP4196181

International Conferences

Hollow Oxide Formation via Oxidation of Metal Nanoparticles, R. Nakamura, H. Nakajima: The 3rd International Workshop on Nano and Amorphous Materials, Miyagi, Japan, August 7-8, 2008.

Formation of Hollow and Porous Oxides through Oxidation of Metallic Nanoparticles (poster), R. Nakamura, H. Nakajima: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sep. 29-Oct. 1, 2008.

Formation of Hollow Structure through Heat Treatment of Core-Shell Type Metal Nanoparticles (poster), K. Taniguchi, R. Nakamura, H. Nakajima: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sep. 29-Oct. 1, 2008.

Fabrication of Lotus-type Porous Carbon Steel by Continuous Casting Technique and Application to Machine Tools, M. Kashiara, H. Yonetani, S. Suzuki, S.Y. Kim, H. Nakajima: CELLMET2008, Cellular Metals for Structural and Functional Applications, 2nd International Symposium, Dresden, Germany, Oct. 8-10, 2008.

Lotus-type Porous Ni-free Stainless Steel Biomaterial Produced by Continuous Zone Melting Technique (poster), K. Alvarez, H. Nakajima: CELLMET2008, Cellular Metals for Structural and Functional Applications, 2nd International Symposium, Dresden, Germany, Oct. 8-10, 2008.

Formation of a Nano-hole via Oxidation of Metal Nanoparticles, R. Nakamura, H. Nakajima, H. Mori: 7th International Conference on Diffusion in Materials (DIMAT2008), Canary Islands, Spain, Oct. 28-31, 2008.

Shrinkage of Hollow Nanoparticles of Oxides of Cu and Ni at High Temperatures (poster), R. Nakamura, H. Nakajima, H. Mori: 7th International Conference on Diffusion in Materials (DIMAT2008), Canary Islands, Spain, Oct. 28-31, 2008.

Fabrication of Lotus-Type Porous Aluminum through Thermal Decomposition Method, H. Nakajima, S. Y. Kim, J. S. Park: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2008.

Structural Stability of Hollow Oxide Nanoparticles at High Temperatures (poster), R. Nakamura, H. Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2009.

Morphology Change of Core-Shell Type Metal Nanoparticles through Heat Treatment (poster), K. Taniguchi, R. Nakamura, H. Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2010.

Fabrication of Lotus-type Porous Magnesium through Thermal Decomposition Method (poster), M. Tane, H. Nakajima: International Conference on Advanced Structural and

Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2011.

Fabrication of Lotus-type Porous Copper by Thermal Decomposition Method using Titanium Hydride (poster), T.Ide, H. Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2012.

Fabrication of Lotus-type Porous Aluminum using Thermal Decomposition of Magnesium Hydroxide (poster), J.S. Park, H. Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2013.

Fabrication of lotus-type porous Al-Si alloy by continuous casting with using thermal decomposition method (poster), T.B. Kim, S.Suzuki, H.Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2014.

Mechanical property of lotus-type porous carbon steel fabricated by continuous casting method (poster), Y.Kawamura, S.Suzuki, S.Y.Kim, H.Nakajima, M.Kashihara, H.Yonetani: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2015.

Structure change and improvement of the mechanical properties of lotus-type porous copper by wire-brushing (poster), J. Lobos, S. Suzuki, H. Nakajima, Y. S. Ji, H. Fujii, D. Terada, N. Tsuji: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2016.

Fabrication of lotus-type porous Al-Cu alloys by continuous casting technique (poster), S.Suzuki, T.B.Kim, H.Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2016.

Fabrication of Porous Magnesium with Directional Pores through Thermal Decomposition of Magnesium Hydride (poster), M. Tane, H. Nakajima: International Conference on Advanced Structural and Functional Materials Design 2008, Osaka, Japan, Nov. 10-12, 2017.

Fabrication of Lotus-type Porous Aluminum through Thermal Decomposition Method (invited), H. Nakajima, T. Ide, S.Y. Kim: The 10th International Symposium on Eco-materials Processing and Design, Xi'an, China, Jan. 13-16, 2009.

Structure change and improvement of the mechanical properties of lotus-type porous copper by ECAE process, J. Lobos, S. Suzuki, H. Utunomiya, H. Nakajima: The 10th International Symposium on Eco-materials Processing and Design, Xi'an, China, Jan. 13-16, 2009.

Contributions to International Conferences and Journals

H. Nakajima Sixth International Conference on Porous Metals and Metal

	Foaming Technology (MetFoam2009) (International Advisory Board Member)
H. Nakajima	High Temperature Materials and Process (Editorial Board Member)
H. Nakajima	Diffusion and Defect Data (Editorial Board Member)
H. Nakajima	Materials Science Foundations (Editorial Board Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	5 th International Conference on Diffusion in Solids and Liquids (Organizing Committee Member)
H. Nakajima	International Conference on Eco-Materials Processing and Design 2010 (Organizing Committee Member)
H. Nakajima	3 rd International Symposium on Cellular Metals for Structural and Functional Applications (Program Committee)
H. Nakajima	International Conference on Advanced Structure and Functional Materials Design (Organizing Committee Member)
H. Nakajima	THERMEC 2009 International Conference on Advanced Materials (International Advisory Board Member)

Publications in Domestic Meetings

The Japan Institute of Metals	26 paper
Japan Heat Transfer Symposium	3 papers
The Japan Institute of Light Metals	2 papers
The Japan Copper and Copper Alloys Research Association	2 papers
The Iron and Steel Institute of Japan	1 paper
4 th Research Meeting on Physical Properties of Materials, Kansai Regional Office of The Iron and Steel Institute of Japan and The Japan Institute of Metals	1 paper
3 rd Research Meeting on Material Development, Kansai Regional Office of The Iron and Steel Institute of Japan and The Japan Institute of Metals	1 paper

Academic Degrees

Master Degree for Engineering

T. Kawashima	Fabrication of Lotus-type Porous Carbon Steel by Continuous Casting Technique and Its Mechanical Properties
Y. Kawamura	Strain-rate Dependence of Compressive Deformation Behavior and Energy Absorption Characteristics of Lotus-type Porous Iron
K. Taniguchi	Study on Formation of Hollow Nanoparticles through Interdiffusion of Core/Shell Type Metal Nanoparticles

Sponsorship

Grant-in-Aid for Scientific Research

H. Nakajima	Fabrication of Novel Nano-hollow Sphere Metals and Metallic Nano-tube and Elucidation of Physical Properties	¥11,050,000
S. Suzuki	Fabrication of Lotus Metals Consisting of Two Different Metals Using Continuous Casting Technique with Multiple Molds	¥1,300,000

Entrusted Research

H. Nakajima	Mori Seiki co.,Ltd.	Investigation for process of manufacture of lotus carbon steel (2008-2010)	Total ¥11,550,000
H. Nakajima	Japan Science and Technology Agency	Application for lightweight energy absorber of Lotus-type porous aluminum alloy fabricated by thermal decomposition method	¥2,000,000

Other Research Fund

H. Nakajima	The Japan Institute of Light Metals	Clarification of physical properties of lightweight metal	¥250,000
H. Nakajima	Nagaki Seiki Co., Ltd.		¥1,000,000
H. Nakajima	Lotus alloy Co.,LTD		¥27,000
H. Nakajima	Myoutoku LTD.		¥1,000,000
R. Nakamura	The Iron and Steel Institute of Japan	Formation Process of Hollow Oxides via Oxidation of Fe and Ni Nanoparticles	¥500,000
R. Nakamura	Foundation Advanced Technology Institute	Fabrication of Hollow Nanostructures Using Large Difference in Diffusivity between Heterogeneous Metals	¥1,200,000
R. Nakamura	Hosokawa Powder Technology Foundation	Fabrication and Control of Porous Nanostructures via Oxidation of Iron Nanoparticles	¥700,000
S. Suzuki	JFE 21st Century Foundation	Fabrication and Characteristics of Porous Carbon Steels with Controlled Micro and Macro Structures	¥2,000,000
H. Nakajima	College of Industrial		¥55,000

H. Nakajima	technology Toyota Motor Corporation (2008-2010)	Total ¥4,400,000
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Department of Atomic Scale Science

Professor:	Tomoji KAWAI
Associate Professor:	Masateru TANIGUCHI
Assistant Professor:	Hiroyuki TANAKA, Takeshi YANAGIDA
Visitor Professor:	Hea-Yeon LEE
Post Doctoral Fellows:	Masaki KANAI, Hitomi HOKONOHARA, Makusu TSUTSUI, Akihiko TAKAGI, Fumihiko YAMADA
Graduate Students:	Koji SUZUKI, Takumi KOBAYASHI, Kazumichi YOKOTA, Kazuki NAGASHIMA, Hideyuki KAWAGUCHI, Satoru YAMANAKA, Kouhei SHOJI, Kazuya GOTO, Keisuke OKA, Yuji SEGAWA, Masahito KAWANO, Kosuke MORIMOTO, Mitsunori KITTA
Under Graduate Students:	Yusuke IMAI
Supporting Staff:	Noriko FUJIBAYASHI

Outlines

This research group directs toward both nano-science and nanobio-technology in its activity. Main subjects are (1) Preparation of Function Harmonized Artificial Lattices, (2) Atomic Scale Surface Science, (3) Development of Bio-tip, and (4) Development of bio-molecular device constructed from DNA. By use of a laser molecular beam epitaxy technique under layer by layer growth conditions, we are challenging in development of highly sensitive IR –sensor by functional transition metal oxide nano-film. Observation and manipulation of a single atom or a molecule are undertaken on DNA molecules with Scanning Probe Microscopic (SPM) methods. And also we developed the ultrasensitive electrochemical gene sensing system by using nanowell array electrodes.

Current Research Project

Fabrication of Oxide Nanowires

We have succeeded in fabricating oxide heteronanowires by utilizing in-situ MBE method. The fabricated oxide heteronanowires showed the non-volatile memory switching effect within the confined nanoscale.

Identification of Single Molecules

We have succeeded in simultaneously identifying these characteristics of organic molecules within metal–molecule–metal junctions. Our strategy combines analyses of single molecule conductance and inelastic electron tunneling spectra exploiting the nanofabricated mechanically-controllable break junction (nano-MCBJ).

Electrical detection of individual DNA-sized particles in the microfluidics is accomplished by probing tunneling current across the nanogap electrodes whose gap size precisely controlled to the particle size at a sub-picometer resolution, using nano-MCBJ.

Nano-science and Nanotechnology by Using of Scanning Probe Microscopes

By using STM/STS measurements, a characteristic peak in dI/dV spectra of Guanine molecule has been detected.

By combination of extremely high resolution STM imaging with advanced STS at cryogenic temperatures that enables, for the first time, to distinguish single guanine bases from other bases in a long ssDNA strand and, by comparison to a known sequence, to identify the relevant part of the DNA sequence.

Self-Assembly Addressable Array of Single Molecular for Single Molecular Assay

These have been successfully demonstrated as highly sensitive and specific bimolecular assay devices using new electrochemical method. Also focused are on the development of biocompatible materials based nanopatterning, surface modification, self-assembly nanoarray, digital bionanochip device to address challenging problem in bio-nanoscience. These research works opened and accelerated the cutting-edge of new bio-nanoscience area.

Publications

Original Papers

Control of device characteristics of ambipolar organic field-effect transistors using the hydroxyl in organic insulator, H. Kawaguchi, M. Taniguchi, and T. Kawai: Synth. Met., 158 (2008) 355-358.

Thermodynamic stability of single molecule junctions, M. Tsutsui, K. Shoji, K. Morimoto, M. Taniguchi, and T. Kawai: Appl. Phys. Lett., 92 (2008) 223110-223112.

Metallic nature of metal-molecule interface formed by Au-Se bonds, K. Yokota, M. Taniguchi, H. Tanaka, and T. Kawai: Phys. Rev. B, 77 (2008) 165416-165420.

Hydration effects on the microwave dielectricity in dry poly(dA)-poly(dT) DNA, A. Hojo, H. Matsui, K. Iwamoto, T. Yanagimachi, H. Abdrurakhan, M. Taniguchi, T. Kawai, and N. Toyota: J. Phys. Spc. Jpn., 77 (2008) 04402-04408.

Local heating in metal-molecule-metal junctions, M. Tsutsui, M. Taniguchi, and T. Kawai: Nano Lett., 8 (2008) 3293-3297.

Measurement environment dependency of single molecule conductance, M. Taniguchi, K. Morimoto, M. Tsutsui, and T. Kawai: Chem. Lett., 37 (2008) 990-991.

Fabrication of 0.5 nm electrode gaps using self-breaking technique, M. Tsutsui, M. Taniguchi, and T. Kawai: Appl. Phys. Lett., 93 (2008) 163115-163117.

Control of threshold voltage and hysteresis in organic field-effect transistors, H. Kawaguchi, M. Taniguchi, and T. kawai: Appl. Phys. Lett., 94 (2009) 093305-093307.

Transverse field effects on DNA-sized particle dynamics, M. Tsutsui, M. Taniguchi, and T. Kawai: Nano Lett., 9 (2009) 1659-1662.

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International Conferences

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Metal-molecule interface for molecular electronics, *K. Yokota, M. Taniguchi, H. Tanaka, Tomoji Kawai: ACS National Meeting, Philadelphia.

Thermodynamic stability of atomic and molecular junctions, *M. Tsutsui, K. Shoji, M. Taniguchi, T. Kawai: ACS National Meeting, Philadelphia.

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High Resolution STM Imaging and Manipulation of Multi-decker Porphyrin, H. Tanaka, T. Ikeda, M. Takeuchi, S. Shinkai and T. Kawai: AVS 55th International Symposium & Exhibition, Boston, MA, USA, Oct.19-24, 2008.

Nanowire Morphology Control in Pulsed Laser Deposition (poster), Marcu, A., M.Goyat, T.Yanagida and T.Kawai,: 2nd INDLAS International Conference, Modern Laser Applications.

Nanochannels Fabrication Using Kirkendall Effect (poster), Marcu, A., T.Yanagida and T.Kawai: European Material Research Society, Fall Meeting,.

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Metal Oxide Nanowires: Synthesis, Nano-properties and Non-volatile Memory Applications (invited), Yanagida, T., K.Nagashima, K.Oka and T.Kawai,: Workshop on INL.

NanoWell based Electrochemical NanobioCHIP toward mult-Nanomedicine (invited), H.Y.Lee,T.Kawai: The 6th Japan-Korea Nanotech Industrialization Forum.

Integrated Biocompatible Nanobiochip (invited), H.Y.Lee: The 3rd CNU-SANKEN Joint Symposium on Advanced Materials Science.

Toward Digital NanoBioCHIP (invited), H.Y.Lee,T.Kawai: Invited Seminar, Department of veterinary and biomedical science, Penn State Neuroscience Institute, The Pennsylvania State University.

Well-Oriented NanoWell Array Metrics for Digital NanoBioChip (invited), H.Y.Lee,T.Kawai: Special invited seminar, Microbiochip Center, Hanyang University.

Well-Oriented NanoWell Array Metrics for Digital NanoBioChip (invited), H.Y.Lee,T.Kawai: Special invited seminar, Nanoscience and technology Institute, Seoul National University.

Well-Oriented NanoWell Array Metrics for Digital NanoBioChip (invited), H.Y.Lee,T.Kawai: Special invited seminar, Departemnt of bioengineering, Korea University.

Nano-Biochips Integrated through Soft lithography and Programmed Self-organization toward Single Molecular Analysis (plenary), H.Y.Lee,T.Kawai: The 2nd Thailand Nanotechnology Conference.

Advanced Bio-Devices Toward Single Molecular Assay (plenary), H.Y.Lee,T.Kawai: Biotronics2008.

Nanosocket Geometry based Digital BioChip-Devices (invited), H.Y.Lee: Special Invited Seminar, Department of Chemical Engineering Pohang University of Science and Technology (POSTECH).

Time-resolved Electrostatic Force Detection by Frequency Shift Mode (poster), T. Matsumoto, T. Kawai: 11th International Conference on Non-Contact Atomic Force Microscopy Madrid 2008,September 16-19, (2008), Madrid, Spain.

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Integrated NanoBiochip through Soft NanoLithography (invited), B.- K. Lee, H.- Y. Lee, T. Kawai: The 4th Handai Nanoscience and Nanotechnology International Symposium,September 29–October 1, (2008) , Osaka, Japan.

Time-resolved Electrostatic Force Detection by Frequency Shift Mode, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology,November 9-13, (2008), Tokyo, Japan.

Molecule Recognition Imaging by Frequency Shift Detection on Liquid (poster), T. Matsumoto, T. Kawahara, H. Hokonohara, M. Kawano, T. Kawai: International Symposium on Surface Science and Nanotechnology,November 9-13, (2008), Tokyo, Japan.

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Force Measurement between Protein, IL-6 and IL-6 Receptor, Immobilized at N-terminal (poster), H. Hokonohara, A. Takagi, T. Matsuura, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology,November 9-13, (2008), Tokyo, Japan.

Arrays Mn12 Complex with DNA Template, Y. Segawa, F. Yamada, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology,November 9-13, (2008), Tokyo, Japan.

Conduction through Biomolecular Arrays, T. Matsumoto, T. Kawai: 4th International Meeting on Molecular Electronics elecsmol'08, December 8-12, (2008) Grenoble, France.

Transverse Conduction DNA Probed by Simultaneous Measurements of STM and Non-contact AFM (poster), T. Matsumoto, Y. Maeda, T. Kawai: 4th International Meeting on Molecular Electronics elecsmol'08, December 8-12, (2008) Grenoble, France.

Metal Oxide Nano Physics (invited), T. Kawai: Department of Physics Bangladesh University of Engineering & Technology Seminar, Department of Physics Bangladesh University of Engineering & Technology, 2008.05.16.

Physical method for characterizing a single molecule, especially for DNA (invited), T. Kawai: Workshop in Bangkok, 2008.05.27.

NanoWell Array-based Digital BioChip Platform (invited), T. Kawai: 9th WSEAS Int. Conf. On MATHEMATICS AND COMPUTERS IN BIOLOGY AND CHEMISTRY(MCBC'08)ACADEMIA ROMANIA(Calea Victoriei 125, Sector 1, Bucharest, Romania)2008.06.24-26.

DNA Nanotechnology (invited), T. Kawai: Special Symposium on Emerging Science and Technology, Hanyang University, Seoul, Korea, 2008.06.30.

DNA Nanotechnology (invited), T. Kawai: Special Symposium on Emerging and Technology, Hanyang University, Korea, 2008.06.30.

Single-molecule sequencing of deoxyribonucleic acid using scanning tunneling microscopy, T. Kawai: Seeing at the Nanoscale VI, Maritim Proarte Hotel, Berlin, Germany, 2008.07.09-1.

Single-molecule sequencing of deoxyribonucleic acid using scanning tunneling microscopy, T. Kawai: 2008 International Conference on Nanoscience + Technology, Keystone Resort & Conference Center, Keystone, Colorado, USA, 2008.07.20-25.

Nano-Biochips Integrated through Soft Lithography and Programmed Self-organization toward Single Molecular Analysis (plenary), T. Kawai: The 2nd Thailand Nanotechnology Conference 2008 (Plenary Lecture), Phuket Graceland Resort and Spa Hotel, Phuket, Thailand, 2008.08.13-15.

Nano-fabrication and Nano-properties in Transition Metal Oxide Semiconductors (invited), T. Kawai: The 14th International Symposium on the Physics of Semiconductors and Applications, The Ramada Plaza Jeju hotel, 2008.08.26-29.

Heterostructured Nano-Oxides and Their Functionalities, T. Kawai: 15th International Workshop on Oxide Electronics, The Stanley Hotel(Estes Park, Colorado, USA), 2008.09.14-17.

Convergence of bio semiconductor technology (invited), T. Kawai: BIOTronics 2008 (International Conference on Biosensors, Biochips, and Bioelectronic Devices), Jeju, Korea, 2008.10.08.

Single Molecular Analysis of DNA and Protein (invited), T. Kawai: Special Invite Seminar, Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), 2008.09.29-10.01.

Biological processes on a membrane observed by atomic force microscopy, T. Kawai: AFM BioMed Conference, Hyatt Regency Monterey(Monterey, California, USA), 2008.10.15-18.

AFM Lithography for the Functional Metal Oxide Devices (plenary), T. Kawai: 2008 International Workshop on Tip-Based Nanofabrication (Plenary Lecture), Haward International House, Taipei, Taiwan, 2008.10.19-21.

Ferroelectric Control of Carrier Mediated Ferromagnetism in (Fe,Zn)3O4 with High Curie Temperature in Field Effect Transistor Structure, T. Kawai: MRS 2008 FALL MEETING, Hynes Convention Center and Sheraton Boston Hotel(Boston, Massachusetts, USA), 2008.12.01-05.

Minute Signaling Recognition for Smart Bio-Device Systems (invited), T. Kawai: BMMP-9, Npyori Conference Hall, Nagoya University, Nagoya, Japan, 2009.01.20-23.

DNA Nanotechnology toward Single Molecular Sequencing (invited), T. Kawai: INDO-JAPAN WORKSHOP ON "NANOBIOTECHNOLOGY & NANODEVICES", SASTRA University, Thanjavur, India, 2009.01.23-24.

Contributions to International Conferences and Journals

Tomoji Kawai Nanotech (Chairman)

Publications in Domestic Meetings

The Physical Society of Japan	5 papers
The Japan Society of Applied Physics	26papers
Japan Society for Molecular Science	5 papers
Japan Society of Chemical Engineering	4 papers
The Biophysical Society of Japan	4 papers
Society of Nano Science and Nanotechnology	1 paper

Academic Degrees

Master Degree for Science

K. Shoji Single-Molecule Identification Using Electrical Measurements

Master Degree for Engineering Science

K. Oka Fabrication of nanostructures of nickel oxides and their physical

S. Yamanaka	properties evaluations Magnetic Property of the highly integrated sipinel ferrite nano dot array and application of nano hetero spin device
K. Goto	The phase transition of magnetic nanowires fabricated by AFM lithography

Bachelor Degree for Engineering Science

Y. Imai	Fabrication and single molecule analysis of artificial cell
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Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

T. Kawai	Emergent Chemistry of Nano-scale Molecular System	¥ 9,880,000
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Grant-in-Aid for Scientific Research on Priority Areas

T. Kawai	Program Emergent Chemistry beyond Hierarchy in Transition Metal Oxide Nano Structure	¥19,890,000
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Grant-in-Aid for Scientific Research (A)

T. Kawai	Creation of DNA Nanostructure and the Study of Their Properties	¥10,140,000
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Grant-in-Aid for Scientific Research on Innovative Areas

M. Taniguchi	Development of DNA Sequencer Using Gating Solid-State Nanopore	¥11,830,000
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Grant-in-Aid for Young Scientists (B)

M. Taniguchi	Creation of Ballistic Conductance Organic Molecules	¥2,700,000
T. Yanagida	Fabrication of Oxide Nanowires	¥2,500,000

Entrusted Research

T. Kawai	MEXT	Handai Multi-Functional Nanofoundry	¥ 147,000,000
T. Kawai	NEDO	Development of the High Sensitivity Gene Polymorphism Detection Biochip system	¥ 6,600,000
T. Kawai	MEXT	Promotion of Novel Interdisciplinary Fields Based on Nanotechnology and Materials	¥6,470,000
T. Kawai	MEXT	Intelligent Artificial Agents	¥97,600,000

M. Taniguchi	Panasonic	and Information Systems Inspired by Biological Systems Dynamics Project Analysis and Evaluation of Rotaxane Molecular Devices	¥1,000,000
M. Taniguchi	Shin-Etsu Chemical Co., Ltd.	Development of Organic Polymer Devices	¥2,100,000
Other Research Fund			
M. Taniguchi	JST-PRESTO	Creation of Ultra-High Integrated Molecular devices Using Self-Organized Interconnect Method	¥27,300,000
H.Y. Lee	JST	Creation of Reliability and Bio-compatibility Nano Array Biochip for a Small Amount and Minute, Electric Signal Analysis	¥2,000,000
H.Y. Lee	Japan Securities Scholarship Foundation	Speed-up of Decomposition by Silicate/TiO ₂ /biodegrade Ability Lactic Acid Nanocomposite	¥1,300,000
H. Tanaka	JST-PRESTO	Nanopore-based Single-molecule DNA Sequencing	¥28,478,450
T. Yanagida	JST-PRESTO	Creation of Non-volatile Memory Using Oxide Heterostructured nanowires	¥1,000,000

Department of Functional Ceramic Materials

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Associate Professor:	Masao TAKAHASHI
Research Associates:	Kohji NOBUGAI, Taketoshi MATSUMOTO
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Undergraduates:	Yosuke FUKAYA
Support Staff:	Chika KUROSAKI, Reiko NOZAKURA

Outlines

The modern society is based on semiconductor technology. Our research is aiming to improve the characteristics of semiconductor devices and to develop semiconductor devices with new structures. For this purpose, we have developed new semiconductor chemical processes such as low temperature Si oxidation method by use of nitric acid and room temperature defect passivation method. Semiconductor devices studied in this department are: 1) Si solar cells, 2) Si or SiC-based metal-oxide-semiconductor (MOS) devices for LSI, 3) thin film transistors (TFT) for display devices.

Current Research Project

Low Temperature Fabrication of Thick SiO₂/Si and SiO₂/SiC Structures by Use of Chemical Method and its Application to Thin Film Transistors (TFT)

TFT is fabricated by the deposition of SiO₂ layers using a CVD method on polycrystalline Si thin films deposited on glass substrates. Due to the use of glass substrates, thermal oxidation which requires heat treatments at above 800 °C cannot be employed. SiO₂ layers formed by deposition methods possess poor characteristics, and moreover, it is impossible to form SiO₂ layers with uniform thickness on rough polycrystalline Si surfaces. Consequently, the formation of thick SiO₂ layers of ~50 nm thickness is required to achieve sufficiently low leakage current densities. Moreover, the interfacial characteristics of deposited SiO₂ layers are poor, resulting in a decrease in the mobility. Due to the large SiO₂ thickness, the electricity consumption for the TFT operation increases.

We have developed a low temperature formation method of thick SiO₂ layers by use of “two-step nitric acid oxidation method”. This method consists of the first immersion of Si in ~40% nitric acid solutions and the second immersion in 68% nitric acid (i.e., azeotropic mixture of nitric acid with water). Using this two-step nitric acid oxidation method, we have succeeded in the formation of SiO₂ layers with thickness more than 20 nm at ~120 °C. The SiO₂ layers formed by the first immersion possess

nano-size pores, and nitric acid is decomposed at the nano-size pores during the second immersion, leading to the generation of dissociated oxygen ions (O^-) with high oxidizing activity. The SiO_2/Si structure fabricated by use of the two-step nitric acid oxidation method possesses much superior electrical characteristics to those formed by CVD methods. SiO_2 layers formed by the two-step nitric acid oxidation method can be applied to gate oxide layers in TFT. Since the nitric acid oxidation is a direct oxidation method, SiO_2 layers with a uniform thickness can be formed even on rough surfaces, and moreover, excellent interfacial characteristics can be obtained, leading to lowering of electricity consumption for the TFT operation and improvement of TFT characteristics. Moreover, flexible TFT can be achieved by employing polymer substrates such as PET since SiO_2 layers can be formed at low temperature of $\sim 120^\circ C$ by use of the two-step nitric acid oxidation method.

We have improved an apparatus for nitric acid oxidation of poly-Si deposited on glass substrates with $30 \times 42 \text{ cm}^2$ in size for TFT. The surface concentration of metal contaminants was less than $3 \times 10^9 \text{ atoms/cm}^2$ (i.e., lower limitation of detection for total reflection X-ray fluorescence) which is sufficiently low for LSI (Large Scale Integration) fabrication. Using this apparatus, NAOS treatment for short time becomes possible because samples can be immersed in boiling HNO_3 .

We have developed a method of formation of atomically smooth Si/SiO_2 interfaces by oxidation of atomically flat $Si(111)$ surfaces by use of azeotropic nitric acid (HNO_3) aqueous solutions i.e., 68 wt % HNO_3 at $121^\circ C$. For the SiO_2 layer on the atomically smooth Si substrates, the concentration of suboxide species, Si^{2+} , is 50% of that on the rough Si substrates, and the valence band discontinuity is higher by 0.1 eV. In this case, the leakage current flowing through the 1.2 nm SiO_2 is low, and further decreased by postmetallization annealing at $250^\circ C$ in hydrogen e.g., 0.5 A/cm^2 at $V_G = 1 \text{ V}$.

A relatively thick (i.e., $\sim 9 \text{ nm}$) SiO_2 layer can be formed by oxidation of Si with nitric acid (HNO_3) vapor below $500^\circ C$. In spite of the low temperature formation, the leakage current density flowing through the SiO_2 layer is considerably low, and it follows the Fowler–Nordheim mechanism. From the Fowler–Nordheim plots, the conduction band offset energy at the SiO_2/Si interface is determined to be 2.57 and 2.21 eV for HNO_3 vapor oxidation at 500 and $350^\circ C$, respectively. From X-ray photoelectron spectroscopy measurements, the valence band offset energy is estimated to be 4.80 and 4.48 eV, respectively, for 500 and $350^\circ C$ oxidation. The band-gap energy of the SiO_2 layer formed at $500^\circ C$ (8.39 eV) is 0.68 eV larger than that formed at $350^\circ C$. The higher band-gap energy for $500^\circ C$ oxidation is mainly attributable to the higher atomic density of the SiO_2 layer of $2.46 \times 10^{22}/\text{cm}^3$. Another reason may be the absence of SiO_2 trap-states.

We have also characterized SiO_2 films on 3C-SiC surfaces formed by NAOS. SiC is known as compounds with wide band-gaps and good thermal conductivity suitable for power devices. SiC high-frequency devices are also expected because electron mobilities of SiC are much higher than that of Si. However, SiC MOS transistors with thermal oxide films show poor electrical characteristics due to accumulation of graphitic carbon at the SiC- SiO_2 interface. Two step NAOS can form a thick (e.g. 10 nm) and smooth SiO_2 layer on a 3C-SiC surface after heat treatment at $400^\circ C$ in pure hydrogen to flatten the SiC surface. The leakage current density was sufficiently low to use as insulating films for SiC MOS transistors.

Development of Semiconductor Defect Passivation Etch-Less Cleaning Method by Use of a New Chemical Reaction

We have developed the “semiconductor defect passivation etch-less cleaning method”. Metal contaminants on semiconductor surfaces are removed by the direct reaction of the developed semiconductor cleaning solution with metal contaminants to form stable complex ions. Consequently, re-adsorption of metal species in the cleaning solution does not occur, resulting in the complete removal of metal contaminants to the surface concentration below 10^9 atoms/cm² order. Due to the great cleaning ability of the solution, the semiconductor cleaning can be performed at room temperature (cf. conventional cleaning solutions: 50~80 °C), and moreover, the cleaning solutions even with concentration as low as 0.02 % possess sufficiently high cleaning ability. Furthermore, defect states such as Si dangling bonds are passivated by the cleaning solutions, leading to improvements of characteristics of semiconductor devices such as LSI, TFT, and solar cells.

Metal contaminants, such as Cu on SiC surfaces, cannot be completely removed by use of the conventional RCA cleaning method. After RCA cleaning, no chemical oxide is formed on the SiC surfaces, and this chemical stability is attributable to the incomplete removal of metal contaminants by the RCA method because it removes metal contaminants by oxidation and subsequent etching. Cleaning of metal-contaminated SiC with hydrogen cyanide (HCN) aqueous solutions followed by the RCA cleaning (or vice versa) can remove them completely. It is concluded that strongly adsorbed metals and metals in the bottom regions on the rough SiC surfaces cannot be removed by the RCA and HCN methods, respectively. The HCN method can remove strongly adsorbed metals because of the high reactivity of cyanide ions, while metals in the bottom regions cannot be removed because of the necessity of the formation of bulky metal-cyanide complex ions for the removal process.

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Contributions to International Conferences and Journals

H. Kobayashi Applied Surface Science (Editor)

H. Kobayashi 2008 SSSI International Conference (Chairman of Science

	Committee)
H. Kobayashi	International Symposium on Eco-materials and Design (Session Chairman)
H. Kobayashi	4 th Vacuum and Surface Science Conference of Asia and Australia (Publishing Committee)
M. Takahashi	Applied Surface Science (Guest Editor)

Publications in Domestic Meetings

The Chemical Society of Japan	1 paper
The Physical Society of Japan	2 papers
The Japan Society of Applied Physics	6 papers
Surface and Interface Spectroscopy	2 papers

Academic Degrees

Master Degree for Science

T. Iwata	Characterization of aluminum oxide thin films formed by nitric acid oxidation at low temperature
T. Yanase	Low temperature formation of SiO ₂ /Si structure with high quality by novel nitric acid oxidation

Sponsorship

Grand-in-Aid for Basic Scientific Research (A)

H. Kobayashi	Japan Science and Technology Organization	Low temperature formation of SiO ₂ /Si structure by nitric acid oxidation with using surface nano-pores	¥17,810,000
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Entrusted Research

H. Kobayashi	Japan Science and Technology Agency	Low temperature formation of TFT gate oxide layers and lower power consumption by the nitric acid oxidation method	¥62,400,000
H. Kobayashi	Japan Science and Technology Organization	Japan-Slovakia joint research project	¥2,500,000

Other Research Fund

T. Matsumoto	JGC-S Scholarship Foundation	High rate growth and nitric acid-reforming of gate insulating films on the substrates with low melting point	¥1,000,000
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T. Matsumoto	JFE Century Foundation	21st	Greening fabrication process	semiconductor	¥2,000,000
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Department of Frontier Materials Creation

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Outlines

The research of the Department of Frontier Materials Creation focuses on growths of high-quality single crystals and top-notch transport measurements of novel materials, such as high-temperature superconductors or spin Hall insulators. Our emphasis is on precise and systematic measurements of basic physical properties, which allows one to unveil the peculiar electronic states of novel materials. This is achieved by combining the expertise in solid-state physics and applied chemistry. Our goal is two-fold: Creating innovative materials for solving urgent issues of the human society, while exploring fundamental new physics in condensed matter.

Current Research Project

Basic Research of High-T_c Superconductors

The mechanism of the high-T_c superconductivity remains one of the most challenging problems in modern condensed-matter physics. This project focuses on the physics of the high-T_c cuprate materials to understand why superconductivity occurs in these materials at notably high temperatures, the answer to which might help us find a blueprint for “room-temperature” superconductors. To elucidate the mechanism of the high-T_c superconductivity, it is important to understand the normal state from which the superconductivity emerges, because it has turned out that the “normal” state of the cuprate materials is actually quite anomalous, while the superconducting state appears to be rather ordinary except for the d-wave nature of the gap. Since the peculiarity of the normal state is strongly manifested in the transport properties, we conduct high-accuracy measurements of the anisotropic resistivity, magnetoresistance, Hall coefficient, thermal conductivity, and thermopower. Furthermore, to corroborate those transport measurements, we also measure the magnetic susceptibility and specific heat, covering most of the basic material properties. Besides, we devote a lot of effort to growing high-quality single crystals of various cuprate materials. The crystals are used for our own transport measurements as well as for various other measurements through world-wide collaborations. The in-house crystal growths are very important for our own transport properties research, because systematic controls of various parameters (such as

carrier concentration, impurity concentration, and chemical pressure) are indispensable for deducing useful information from the transport data. In addition, with the discovery of new iron-based high-T_c superconductors in 2008, we have started new efforts to grow single crystals of iron-pnictide superconductors and to precisely control their carrier concentrations.

Basic Research of Spin-Hall Insulators

This project explores new avenues of the spintronics to utilize the intrinsic and dissipationless spin current that is expected to flow in spin Hall insulators. This is quite a different approach from the mainstream spintronics research to utilize magnetic materials or conventional semiconductors, where energy dissipation is inevitable. The idea of the spin Hall insulator was theoretically proposed a few years ago but is yet to be experimentally explored, so the primary objective of this project is to detect the intrinsic spin currents in candidate insulators. In addition, we investigate the fundamental nature of quantum spin Hall insulators (also called “Topological insulators”), which is expected to be a new state of matter with helical surface states, while exploring ways to utilize intrinsic spin currents for spintronics applications. To take advantage of our expertise, this project focuses on clean bulk samples, which makes it distinguished from many other projects that are based on thin films.

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One-Step Synthesis of the Core-Shell Structure Titania/Polyaniline Hybrid Materials: The Effect of the SDS Surfactant (poster), *Y.-G. Han, T. Kusunose, T. Sekino: The 1st International Symposium on Hybrid Materials and Processing (HyMaP 2008), Korea, Busan, Oct. 2008.

Synthesis, Nanostructures and Physico-Chemical Properties of Ce-Modified TiO_2

Nanotubes (poster), *D.-J. Park, T. Sekino, T. Kusunose, S.-I. Tanaka: The 1st International Symposium on Hybrid Materials and Processing (HyMaP 2008), Korea, Busan, Oct. 2008.

Synthesis and Phase Transfer of Organic Bilayer-Protected Gold Nanocrystals in Different Media (poster), *S.-Y. Moon, T. Sekino, T. Kusunose, S.-I. Tanaka: 1st Workshop Tohoku University – EMAC – INSA, France, Albi, Dec. 1-2, 2008.

Direct Synthesis and Biocompatibility of Titania Nanotube Layers on Metal Substrates for Implant Biomaterial (poster), *T. Miwa, H. Nishida, H. Egusa, D.-J. Park, T. Sekino, S.-I. Tanaka: International Symposium on Core University Program between Japan and Korea, - New Processing and Nanostructure/Property Relationship for Multi Functional Materials - (The 21st JSPS-KOSEF Core University Program (CUP) Seminar between Japan and Korea), Awaji, Japan, Dec. 14-16, 2008.

Thermoelectric Properties of Rare Earth Cobalt Oxide Solid Solutions $R_{1-x}R_2CoO_3$ (poster), *H. Hashimoto, T. Kusunose, S. Tsukuda, T. Sekino, S.-I. Tanaka: International Symposium on Core University Program between Japan and Korea, - New Processing and Nanostructure/Property Relationship for Multi Functional Materials - (The 21st JSPS-KOSEF Core University Program (CUP) Seminar between Japan and Korea), Awaji, Japan, Dec. 14-16, 2008.

Effects of Substituting A-Site Ions on Thermoelectric Properties of Perovskite-Type Rare Earth Cobalt Oxides $R_{1-x}R_2CoO_3$, *H. Hashimoto, T. Kusunose, T. Sekino: Eco-Materials Processing and Design (ISEPD 2009), Grand New World Hotel, Xian, China, Jan. 13-16, 2009.

Synthesis, Functionalization, Processing and Assembly of Nanostructures (poster), *S.-Y. Moon, T. Sekino, S.-I. Tanaka: 33rd International Conference and Exposition on Advanced Ceramics and Composites, Hilton Daytona Beach Resort & Ocean Center, Daytona Beach, Florida, USA, Jan. 18-23, 2009.

Visual Observation of Solid Helium Samples Grown at Constant Volume, *S. Sasaki, F. Caupin, S. Balibar: International Conference of Low Temperature Physics 25th.

Optical Observations of Defects in Solid ^4He ~What is Supersolidity?~ (poster), *S. Sasaki, F. Caupin, S. Balibar: The 12th Sanken International Symposium, Osaka, Japan, January 22, 2009.

Contributions to International Conferences and Journals

Y. Ando	9th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors (Japan Committee)
Y. Ando	12th Sanken International Symposium (Conference Chair)

Publications in Domestic Meetings

Physical Society of Japan
Ceramic Society of Japan

9 papers
4 papers

Academic Degrees

Doctor Degree for Engineering

Y.-G. Han Design and Development of Polymer-based Nanohybrids with Advanced Electrical Functions

Master Degree for Engineering

D.-J. Park Development and Multi-Functions of Rare Earth Modified TiO₂ Nanotubes by Soft Chemical Method
T. Miwa Direct Synthesis and Biocompatibility of Titania Nanotube Layers on Metal Surface

Bachelor Degree for Engineering

D. Hama Crystal Growth of Na_xWO₃ by Chemical Vapor Transport and Its Characterizations
T. Minami Synthesis of Polycrystalline Iron-Pnictide High-Tc Superconductors and Efforts towards Their Crystal Growth

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

Y. Ando Search for Quantum Oscillations in a La-based Cuprate ¥2,100,000

Grant-in-Aid for Young Scientists (S)

Y. Ando Mott Insulator and Spin Hall Insulator: Elucidating the Physics of Nontrivial Insulators ¥31,980,000

Grant-in-Aid for Young Scientists (B)

K. Segawa Creation and Physical Properties of PIN Junction in Parent Compound of High-Temperature Superconductors ¥2,340,000

Grant-in-Aid for Scientific Research (B)

T. Kusunose Multiple Structuralization and Functionalization of Oxide Nanotubes Aiming for Environmental and Energy Application ¥520,000

Entrusted Research

Contribution to Research

T. Kusunose	Sumikin Ceramics & Quartz Co., Ltd.	¥1,000,000
T. Kusunose	Nippon Tungsten Co., Ltd.	¥500,000
T. Kusunose	Denki Kagaku Kogyo Co., Ltd.	¥950,000

Cooperative Research

Y. Ando	Central Research Institute of Electric Power Industry	Development of new materials by physically understanding transition metal oxides	¥1,000,000
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Other Research Fund

Y. Ando	US AFRL Asian Office of Aerospace Research and Development, Special Grant	Exploration of New Principles in Spintronics Based on Spin Hall Insulators	¥5,350,000
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Department of Advanced-Energy Material

Professor:	Katsumi TANIMURA
Associate Professor:	Shin'ichiro TANAKA
Research Assoc.	Ei'ichi INAMI,
Research Assoc.	Nobuyasu NARUSE
Graduate Students:	Taku Ichibayashi
Support Staff:	Masanobu NUNOGAKI
	Sachiyo NOZAWA,

Outline

For fabricating highly functional nano-structured devices in future technology, it is essential to establish the ways to control structures and compositions of materials at the atomic level. In this department, we aim to establish the fundamentals for controlling the modes of *atomic binding in solids* via excitation-induced atomic reactions. For this purpose, we have carried out extensive experimental studies in the following three categories:

- 1) the primary processes of the structural changes induced by photoexcitation of solids,
- 2) ultrafast carrier dynamics on semiconductor surfaces,
- 3) excitation-induced structural changes of semiconductor surfaces,

In our studies, the main emphasis is placed on *direct experimental determination of photoinduced changes of electronic and lattice systems at ultrafast temporal domains and at the atomic levels*. As topics in the first category, we have studied the primary processes of the dynamics of the photoinduced phase transition in low dimensional crystals, like quasi one-dimensional organic solids and two-dimensional solids like graphite. As topics of the second categories, we have studied carrier dynamics on Si surfaces by means of femtosecond two-photon photoemission spectroscopy. And as the third topic, we have studied laser- or low-energy electron induced structural changes of clean surfaces of Si and InP by means of not only the direct imaging of the surface atomic structure and its changes by STM, but also highly sensitive detection of Si atoms emitted from surfaces in the time scale of femtosecond. Also, in order to achieve direct determination of crystalline structural changes in femtosecond temporal domains, we have developed a ultrafast high-energy electron diffractometer with 100-fs temporal resolution.

Current Research Projects

Excitation-Induced Instability on Semiconductor Surfaces

Based on our systematic studies on laser-induced and tunneling-current-induced electronic processes of structural changes on semiconductor surfaces, detected by using STM for revealing the changes on surfaces from atomic level, we have established a unified theoretical mechanism of the instability that can describe quantitatively the efficiency of surface bond breaking successfully. The mechanism is based on the two-hole localization of valence holes at intrinsic surface sites.

As extensions of the series of studies to establish the new fabrication methods, we have studied further the following two topics in this year:

- (1) Stochastic resonance effects of photoinduced surface bond rupture on Si(111)-(7x7),

- (2) Mechanism of surface bond rupture on Si(111)-(7x7) induced by low-energy electron beam excitation.

In the first topic, we have studied the temperature dependent effects on the fs-laser induced bond rupture rate to reveal synergistic effects of thermal fluctuation of the lattice system and dynamical relaxation process of two-hole localization. We have found an exponential type enhancement of the bond rupture rate on temperature, which proves a type of stochastic resonance of the dynamical process with the thermal fluctuation effects. In the second topic, we have found that surface plasmons excited by low-energy electrons induce surface bond rupture effectively. Based on the similarities of the structural changes induced, we have proposed the two-hole localization mechanism which underlies in the plasmon-induced effects.

Ultra-fast surface carrier dynamics on semiconductor surfaces studied by femtosecond two-photon photoemission spectroscopy

The excitation induced structural instabilities are triggered by several modes of ultrafast relaxation of electronic excited states, like carriers, excitons, and electron-hole plasma. In order to elucidate the dynamics of photogenerated surface carriers, which play crucial roles in several photoinduced reactions in solids and on solid surfaces, it is essential to study the ultrafast carrier dynamics with resolving their evolutions in momentum and energy spaces. Use of femtosecond laser for pump and probe pulses has a strong advantage for resolving the carrier dynamics directly. In particular, the new system based on a tunable OPA laser for pump pulses of 100-fs temporal width has opened a new breakthrough for studying the dynamics extensively.

By probing electrons populated near the conduction band minimum of Si directly, we have elucidated directly the ultrafast processes of intravalley relaxation and energy relaxation of hot electrons and L-to-X intervalley scattering of highly excited hot electrons. Also, by probing both the electrons in the bulk conduction band and those in surface-specific states of the Si(001)-(2x1) and Si(111)-(7x7) surfaces, we have found for the first time an ultrafast electron-hole recombination via surface localized states with 1 ps of excitation. Also, the lifetime of the surface D_{down} state is 15 ps, and has an effective surface electron-hole recombination, thus leading to strong density-dependent kinetics of carrier dynamics on this surface. At longer time delays, the transition from bulk-to-surface states is rate-determining of the surface-state population. Consequently, apparent decay of electrons at the surface D_{down} state shows a strong excitation-wavelength dependent feature.

Furthermore, by using 6-eV probe photons, we can study the dynamics of photogenerated holes in surface occupied states and in bulk valence band, which can be probed as a small depression of occupied-state photoemission intensities. Holes generated in surface states S2 and S3 on Si(111)-(7x7) decays via two modes; one is the dynamical recombination with 1 ps after excitation, and the other is the transfer-limited process of electron-hole recombination. Extensions to other surface states are now underway.

Photoinduced structural phase transformation of graphite: discovery of a novel sp^3 -bonded phase of carbons, *Diaphite*

By combining fs-laser excitation and STM probing at the atomic levels, we have found the formation of a novel phase of sp^3 -bonded carbons by fs-laser excitation of graphite. The structure is unique; it is just an intermediate between graphite and diamond,

diaphite. The novel phase is formed as nano-scale clusters with a typical dimension of 5 nm, only under a specific excitation conditions that laser light has to be fs-temporal duration, p-polarized and a high energy intensity more than 60 mJ/cm². Theoretical study of total energy calculations with LDA method have confirmed the diaphite phase as a metastable phase of graphite, separated by a barrier of 0.5 eV, which is sufficient to stabilize the phase once formed at room temperature, and predicted the atomic structures just determined by STM-image analysis. The new phase is formed under the inter-layer compression and shear displacement, both of which can be inherently excited under intense fs-laser excitation.

Highly functional Surface-layer formation by Means of Charged-particle Injection under Plasma Processing

We have developed a multiplex surface processing for creating “a new type metal ceramics” which have the properties of high thermal loading and extreme high hardness. The multiplex processing is the sequential process of the reactive modification of metal surfaces by irradiation with charged particle beams, followed by plasma processing for carburization, nitridation or oxidation. For establishing the method of this unique processing, we have constructed moving electrodes, which make it possible of ion-beam irradiation and plasma processing for the same samples without breaking high vacuum condition. The electrodes have shown a reasonable performance in intensity and in stability. A very stable firing of plasma is now possible, giving a strong possibility for real use of this method for creating new type metal ceramics.

Publications

Original Papers

- 1) Excitation-induced atomic desorption and structural instability of III-V compound semiconductor surfaces, K. Tanimura and J. Kanasaki, Surf. Sci. **602**, 3162–317 (2008).
- 2) Electronic properties and electron dynamics on the Si(001)-(2x1) surface with C-defects, S. Tanaka and K. Tanimura, Phys. Rev. B **77**, 195323-1-8 (2008).
- 3) Local bond rupture of Si atoms on Si(111)-(2x1) induced by the surface π - π^* excitation, E. Inami and K. Tanimura, Surf. Sci. **603**, L63-L65 (2009).
- 4) Formation of sp³-bonded carbon nanostructures by femtosecond laser excitation of graphite. J. Kanasaki, E. Inami, K. Tanimura, H. Ohnishi, and K. Nasu, Phys. Rev. Lett., **102**, 087402-1-4 (2009).
- 5) Ultrafast carrier relaxation in Si studied by time-resolved two-photon photoemission spectroscopy: Intravalley scattering and energy relaxation of hot electrons, T. Ichibayashi and K. Tanimura, Phys. Rev. Lett., **102**, 087403-1-4 (2009).
- 6) Dynamics of bulk-to-surface electron transitions on Si(001)-(2x1) studied by time-resolved two-photon photoemission spectroscopy, S. Tanaka, T. Ichibayashi, and K. Tanimura, Phys. Rev. B **79**, 155313-1-8 (2009).
- 7) Ultrafast carrier dynamics in Si and Si surfaces studied by femtosecond time-resolved two-photon photoemission spectroscopy, K. Tanimura and T. Ichibayashi, Proc. of SPIE, **7214**, 72141M-1-13 (2009).
- 8) 100-femtosecond MeV electron source for ultrafast electron diffraction, J. Yang, K. Kan, N. Naruse, Y. Yoshida, K. Tanimura, Radiat. Phys. Chem. in press.

International Conferences

Ultrafast carrier dynamics in Si and on Si surfaces studied by time-resolved twophoton photoemission spectroscopy (invited), K. Tanimura, 6th International Conference on Ultrafast Surface Dynamics, Kloster Banz, Germany, July 20-25, 2008

Ultrafast carrier dynamics on Si surfaces studied by time-resolved two-photon photoemission spectroscopy (invited), K.Tanimura, Ultrafast Phenomina in Semiconductors and Nanostructure Materials XIII, San Jose, USA, January25-28, 2009

Local bond rupture on Si surfaces induced by low-energy electron-beam excitation, J. Kanasaki and K. Tanimura, International workshop on “Low-Energy Electron Molecule Interaction:LEEMI-EIPAM'08, Roscoff, France, May7-11, 2008.

Interlayer bond formation of graphite crystals induced by femtosecond laser excitation, Kanasaki, E. Inami, K. Tanimura, and K. Nasu, 25th European Conference on Surface Science, Liverpool, UK, July 27-Aug.1, 2008.

Surface-carrier dynamics on Si(001)-(2x1): roles of electron transfer from bulk- to surface-electronic states, S. Tanaka and K. Tanimura, 25th European Conference on Surface Science, Liverpool, UK, July 27-Aug.1, 2008.

Quantum-confinement effect in individual GeSn nanodots observed by Fourier-transform photoabsorption spectroscopy combined with scanning tunneling microscopy, N. Naruse, Y. Mera, Y. Nakamura, M. Ichikawa, and K. Maeda
25th European Conference on Surface Science, Liverpool, UK, July 27-Aug.1, 2008.

Hot-hole and hot-electron dynamics at Si surfaces studied by time-resolved twophoton photoemission spectroscopy, T. Ichibayashi and K. Tanimura, 6th International Coonference on Ultrafast Surface Dynamics, Kroster Banz, Germany, July 20-25, 2008.

Image-potential induced surface-resonance states at Si(100)-(2x1), T. Ichibayashi and K.Tanimura, 25th European Conference of Surface Science, Liverpool, UK, July 27-Aug.1, 2008..

Taku ICHIBAYASHI and Katsumi TANIMURA

Ultrafast carrier dynamics in Si studied by time-resolved two-photon photoemission spectroscopy, T. Ichibayashi and K. Tanimura, 3rd International Conference on Photo-Induced PhaseTransitions and Cooperative Phenomena,Osaka, Japan, Nov. 11-13, 2008.

Ultrafast Electron NanoCrystallography, Y. Murooka, R.K. Raman, R.A. Murdick, and C.-Y. Ruan,

IUCR2008 Satellite Meeting at Nagoya University (IUCR=XXI Congress and General Assembly of the International Union of Crystallography), Nagoya, Japan, September 1-2, 2008

Publications in Domestic Meetings

The Physical Society of Japan

12
papers

Academic Degrees**Doctor Degree for Science**

T. Ichihashi Ultrafast carrier dynamics on Si surfaces studied by femtosecond
time-resolved two-photon photoelectron spectroscopy

Sponsorships**Grant-in-Aid for Specially Promoted Research**

K. Tanimura	Dynamical studies of photoinduced structural phase transitions	¥175,760,000
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Division of Organic Molecular Science

Outline

Division of Organic Molecular Science has five departments: Dep. of Regulatory Bioorganic Chemistry, Dep. of Organic Fine Chemicals, Dep. of Organic Molecular Materials, Dep. of Molecular Excitation Chemistry, Dep. of Synthetic Organic Chemistry, and Dep. of Analytical Molecular Chemistry (started from April 2004). The research field in the division covers organic chemistry, bioorganic chemistry, organometallic chemistry, physical organic chemistry, material chemistry, physical chemistry, analytic chemistry, photochemistry, and reaction kinetics. In each department research on own original subject is going on and in some cases joint projects between several departments are carried out.

Achievement

- Development of photoswitchable molecular glue for DNA
- Synthesis of DNA bearing transition metal chain
- Development of Technology for Single Nucleotide Polymorphisms
- Molecular Design of Ligand Selectively Binding to the Human Telomeric Repeat Sequence
- Design and functional evaluation of dual inhibitors for prenyltransferases
- Inhibition of influenza virus infection by novel tea catechin derivatives
- Development of new synthetic procedure of 4-carbamoylimidazolium 5-olate
- Development of p-type and n-type semiconductors for organic electronics
- Construction of molecular wires with switching and insulation-covering functions
- Beam-controlled DNA chemistry
- Multi-laser photochemistry
- Photocatalytic reactions of TiO_2
- Chemistry of metal clusters and nanoparticles
- Development of novel enantioselective reaction via Pd(II/IV) catalysis
- Design and synthesis of novel spiro chiral ligands
- Highly efficient chiral dinuclear vanadium(V) catalysts for oxidative coupling of 2-naphthols
- Catalytic enantioselective synthesis of spiro compounds

Department of Regulatory Bioorganic Chemistry

Professor:	Kazuhiko NAKATANI
Assistant Professors:	Da-Yang ZHOU, Masaki HAGIHARA, Chikara DOHNO, Fumie TAKEI
Post Doctoral Fellows:	Hanping HE, Kensuke MAEKAWA, Yoshimi OKA
Graduate Students:	Gosuke HAYASHI, Shin-nosuke UNO, Shiori UMEMOTO, Tomohiro DOURA, Changfeng HONG, Tsuyoshi YAMAMOTO, Masami IMAMURA, Masatsugu OKAZAKI, Shun SAKAI, Tomonori SHIBATA
Under Graduate Students:	Keisuke YONEDA
Research Assistance:	Akiko SEO, Risa YAMAUCHI
Supporting Staff:	Yuriko YAGUCHI

Outlines

We have studied on “Chemical Biology” and “Nano-Technology” based on synthetic organic chemistry. For chemical biology, we focused our attention on 1) molecular design of mismatch binding ligands, and 2) in vitro selection of RNA aptamer binding specific nucleic acid structure. Because DNA is not only a genetic materials but also an important organic materials consisting of C, H, O, N, and P atoms with ability of spontaneously forming a double helix. To use DNA as precision organic materials in nano-technology, we have studied on the chemical properties of DNA and on the synthesis of chemically modified DNA.

Current Research Project

Development of Technology for Single Nucleotide Polymorphisms

The technique for promptly detecting the genetic mutation is expected as a basis technology that supports the personalized medicine. In this laboratory, we have proposed the technology for genetic mutation detection that uses a small molecule binding to the mismatch and the bulge structure in the duplex DNA. The practical technology must be handy, accurate, and cheap in cost. To meet this demand, we did not study the chemical modification of DNA, but used the molecule selectively binding to the cytosine bulge. Upon binding to cytosine bulge, the fluorescence wavelength shifted the long wavelength by 30 nm. By using this characteristic fluorescence, we have succeeded to develop the method detecting single nucleotide polymorphisms. A primer having a cytosine bulge site in a hairpin structure and SNP recognition site at the end of 3' was prepared for PCR. Using this primer and fluorescent molecules, allele specific PCR was monitored in order to do SNP typing.

Molecular Design of Ligand Selectively Binding to the Human Telomeric Repeat Sequence

The telomeric sequence d(TTAGGG)_n located at the 3' end of human genomic DNA

plays important roles in protecting chromosomal ends from fusion, rearrangement, and translocation. In cancer cells the enzyme telomerase is activated maintains the length of the telomere for achieving the immortality. Therefore, the ligands that bind to telomere and inhibit its elongation are expected to be potential anti-cancer drugs. The single-stranded region of the d(TTAGGG)_n repeat is known to form G-quadruplex structures *in vitro*. We synthesized a novel ligand naphthyridine tetramer (**NT**) and evaluated its specific binding to the human telomeric repeat sequences. The results from enzymatic analyses together with spectroscopic measurements clearly showed that **NT** did not inhibit telomerase but interfere the telomere elongation by a formation of unique hairpin structure on the template. The novel mode of **NT** binding to the human telomere sequence would be useful for the design of molecules in a next generation.

Development of photoswitchable molecular glue for DNA

DNA molecular glue is a small synthetic ligand that can adhere two single-stranded DNAs that do not spontaneously hybridize with each other. For reversible control of DNA hybridization by an external light stimulus, we have developed a photoswitchable molecular glue for DNA. The photoswitchable molecular glue, **NCDA**, consists of two guanine-recognizing naphthyridine moieties connected with a photochromic azobenzene unit. Azobenzene undergoes a reversible cis/trans isomerization by photoirradiation, which changes the relative orientations and positions of the naphthyridine moieties, resulting into photoswitching of **NCDA** binding to the DNA containing GG-mismatch. **NCDA** in the cis configuration binds to a GG-mismatch sequence, and induces the formation of the DNA duplex. Using the photoswitchable binding property of **NCDA**, the hybridization event of two natural unmodified DNAs can be reversibly controlled by an external light stimulus.

Synthesis of DNA bearing transition metal chain

Synthesis of DNA containing metal molecular chain is important in terms of production of novel materials. We have studied to synthesize a DNA which include a transition metal molecular chain.

Publications

Original Papers

Genotyping by allele-specific L-DNA-tagged PCR, Gosuke Hayashi, Masaki Hagihara, Kazuhiko Nakatani: J. Biotechnol., 135 (2008) 157-160.

Synthesis of Dimeric 2-Amino-1,8-naphthyridine and Related DNA-Binding Molecules, Kazuhiko Nakatani, Hanping He, Shin-nosuke Uno, Tsuyoshi Yamamoto, Chikara Dohno: Current Protocols in Nucleic Acid Chemistry, 2 (2008) 1-21.

DNA Labeling by Ligand Inducible Secondary Structure, Tao Peng, Hanping He, Masaki Hagihara, Kazuhiko Nakatani: ChemBioChem, 9 (2008) 1893-1897.

Ligand Binding to Tandem G-quadruplex from Human Telomeric DNA, Li-Ping Bai, Masaki Hagihara, Zhi-Hong Jiang, Kazuhiko Nakatani: ChemBioChem, 9 (2008) 2583-2587.

Site-specific binding of chelerythrine and sanguinarine to single pyrimidine bulges in hairpin DNA, Li-Ping Bai, Zongwei Cai, Zhong-Zhen Zhao, Kazuhiko Nakatani, Zhi-Hong Jiang: *Anal. Bioanal. Chem.*, 392 (2008) 709-716.

Dimer of 2,7-diamino-1,8-naphthyridine for the detection of mismatches formed by pyrimidine nucleotide bases, Akio Kobori, Kazuhiko Nakatani: *Bioorg. Med. Chem.*, 16 (2008) 10338-10344.

RNA Aptamers That Reversibly Bind Photoresponsive Azobenzene-Containing Peptides, Gosuke Hayashi, Masaki Hagihara, Kazuhiko Nakatani: *Chem. Eur. J.*, 15 (2009) 424-432.

The effect of linker length on binding affinity of a photoswitchable molecular glue for DNA, Chikara Dohno, Shin-nosuke Uno, Shun Sakai, Mika Oku, Kazuhiko Nakatani: *Bioorg. Med. Chem.*, 17 (2009) 2536-2543.

Synthesis and Reaction of DNA Oligomers Containing Modified Cytosines Related to Bisulfite Sequencing, Yoshimi Oka, Tao Peng, Fumie Takei, Kazuhiko Nakatani: *Org. Lett.*, 11 (2009) 1377-1379.

International Conferences

Synthesis and evaluation of photoresponsive molecular Glue for DNA (poster), *Shin-nosuke Uno, Chikara Dohno, Mika Oku, Shun Sakai, Kazuhiko Nakatani: IUPAC ICOS-17, 17th International Conference on Organic Synthesis.

Small molecule affecting the synthesis of trinucleotide Repeat (GAA)_n, *Hanping He, Masaki Hagihara, Kazuhiko Nakatani: 26th Chinese Chemical Society (CCS) Congress.

Preparation and evaluation of small molecule binding to trinucleotide repeat d(GAA)_n (poster), *Hanping He, Masaki Hagihara, Kazuhiko Nakatani: Ninth Tetrahedron Symposium.

THE FLUORESCENT DETECTION OF SINGLE NUCLEOTIDE DIFFERENCE USING CYTOSINE BULGE HAIRPIN PRIMERS (poster), *Fumie Takei, Masaki Hagihara, Yoshimi Oka, Kazuhiko Nakatani: XXII IUPAC SYMPOSIUM ON PHOTOCHEMISTRY 2008.

Switching DNA hybridization by a molecular glue for DNA (poster), *Chikara Dohno, Uno Shin-nosuke, Kazuhiko Nakatani: XXII IUPAC SYMPOSIUM ON PHOTOCHEMISTRY 2008.

Fluorescent Ligand as a molecular probe for the RNA structure (poster), *Shiori Umemoto, Jinhua Zhang, Chikara Dohno, Kazuhiko Nakatani: Joint Symposium of 18th International Roundtable on Nucleosides, Nucleotides and Nucleic Acids (IRTXVIII) and 35th International Symposium on Nucleic Acids Chemistry.

The reaction of cytosine with bisulfite by base flipping from the duplex (poster), *Yoshimi Oka, Tao Peng, Fumie Takei, Kazuhiko Nakatani: Joint Symposium of 18th International Roundtable on Nucleosides, Nucleotides and Nucleic Acids (IRTXVIII) and 35th International Symposium on Nucleic Acids Chemistry.

RNA aptamers that reversibly bind to photoresponsive peptide (poster), *Gosuke Hayasi, Masaki Hagihara, Kazuhiko Nakatani: Joint Symposium of 18th International Roundtable on Nucleosides, Nucleotides and Nucleic Acids (IRTXVIII) and 35th International Symposium on Nucleic Acids Chemistry.

The Development of The Displacement Assay, Screening Method for Detecting the RNA-ligand Interactions (poster), *Shiori Umemoto, Masaki Hagihara, Kazuhiko Nakatani: 12 th Sanken International Symposium.

Reversible control of DNA hybridization by a small synthetic ligand (poster), *ChikaraDohno, Shinnosuke Uno, Tsuyoshi Yamamoto, Shun Sakai, Kazuhiko Nakatani: The Fifth International Symposium on Integrated Synthesis (ISIS-5).

Publications in Domestic Meetings

Japan Chemical Society Meeting	10 papers
Japanese Society for Chemical Biology Meeting	4 papers
4th Nanotechnology Center Workshop Sponsorship	1 paper
Joint Symposium of Biorelevant Chemistry	5 papers

Academic Degrees

Doctor Degree for Science

G. Hayashi	Studies on PCR with Enantiomeric DNA and Regulation of RNA Structure and Function
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Master Degree for Science

S. Uno	Study of photoswitchable GG mismatch binding ligand
S. Umemoto	The developing a new method to search RNA binding ligands and its' application
T. Doura	Fluorescent properties of malachite green-DNA conjugates
C. Hong	Synthesis of fullerene-DNA conjugate molecules
T. Yamamoto	Synthesis and evaluation of photoresponsive mismatch binding ligands

Sponsorship

Grant-in-Aid for Scientific Research (S)(C)

K. Nakatani	Regulation of DNA Structure and Function	¥17,940,000
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F. Takei	Based on the Stabilization of DNA Duplex Development of SNP detection method with modified PCR primers	¥1,950,000
Grant-in-Aid for Young Scientists (B)		
M. Hagihara	In vivo screening of novel ribozyme	¥2,210,000
Entrusted Research		
K. Nakatani	Japan Science and Technology Agency Development of High throughput screening method of drug compound binding to target RNA	¥6,000,000
K. Nakatani	Japan Science and Technology Agency Investigation of novel functions generated from the biomaterials at interfaces	¥6,370,000
Other Research Fund		
K. Nakatani	NITTO KASEI CO., LTD Synthesis of DNA-binding ligands	¥840,000
M. Hagihara	The International Human Frontier Science Program The biological role of tandem repeats in genomes	¥9,934,000
K. Nakatani	The Asahi Glass Foundation ¥2,000,000	
C. Dohno	The Sumitomo Foundation Synthesis of photoswitchable RNA molecular glue for control of RNA structures and functions	¥720,000

Department of Organic Fine Chemicals

Professor:	Nobuo KATO
Associate Professor:	Junko OHKANDA
Assistant Professors:	Hajime NITTA, Shunro YAMAGUCHI, Kunihiro KAIHATSU
Appointed Researcher:	Masamitsu HIRAOKA
Post Doctoral Fellow:	Shuichi MORI
Graduate Students:	Takatsugu INOUE, Shinnosuke MACHIDA, Yu HARANOSONO, Yusuke HIGUCHI, Shinjiro SAWADA, Kohei FUJII, Yuriko MARUYAMA, Takaaki MONTA, Chihiro KONDO, Tomoya TAKAHASHI, Akie KAWAMURA, Daisuke HAYASHI, Minoru YABU
Under Graduate Student:	Yoshinobu YAMAGUCHI
Technical Assistant:	Hiroyo MATUMURA
Supporting Staff:	Misuzu TANNO

Outlines

The object of this department is to create lead compounds for drug discovery. Based on chemical proteomic approaches, our research interests are focused on the rational design and synthesis of small organic compounds that potentially modulate/inhibit protein-protein interactions. These compounds are also utilized as a tool in our chemical genomic study to elucidate intracellular signalling pathways. The protein surface-directed proteomimetic and peptidomimetic designs are also investigated. The stereoselective synthesis of biologically active compounds and the construction of biomimetic supramolecular systems are also investigated.

Current Research Project

Crystal structure of the association complex of 14-3-3 protein and cotylenin

Cotylenin, a fungal metabolite originally described as a cytokinin-like bioactive substance against plants shows differentiation-inducing and antitumor activity in certain human cancers. We solved the crystal structure of cotylenin acting on a 14-3-3 regulatory protein complex. By comparison with the closely related, but non-anticancer agent fusicoicin, a rationale for the activity of cotylenin in human cancers has been presented.

Design and functional evaluation of dual prenyltransferase inhibitors that recognize common surface structure

Protein prenyltransferases, farnesyltransferase (FTase) and type-I geranylgeranyltransferase (GGTase-I) play a crucial role in the posttranslational modification of oncogenic GTP-binding proteins, and have received intense attention due to their potential to be antitumor agents. Given the characteristic acidic protein surface found in near the active site of both FTase and GGTase-I, a series of bivalent dual inhibitors in which a polyamino-containing gallate motif was linked to a tetrapeptide covalently. One of the agents was found to be extremely potent inhibiting FTase and GGTase-I at

submicromole concentrations.

Synthesis of mix-combinatorial library of metal complexes and screening for proteases inhibition assay

Metal complexes would provide a suitable scaffold for protein surface-directed agents with appropriate molecular size and structural diversity. We evaluated a 6x6 mix library of tris-bipyridine iron complexes, derived from six 2,2'-bipyridine derivatives possessing various functional groups, for inhibition activity against chymotrypsin and thrombin. The combinations of ligands, which were potent for inhibiting each protease, were found to be distinct, suggesting that the selective inhibition is possible based on protein surface recognition, and that selective inhibitors should meet the structural requirements for the specific binding to the targeting surface area.

New synthetic procedure of 4-carbamoylimidazolium 5-olate

4-Carbamoylimidazolium 5-olate (SM-108) has potent anti-tumor activities, especially, has the excellent medicinal properties for myelodysplastic syndromes (MDS). In fact, Phase II clinical trial had been conducted and the results were quite promising. However, further clinical development of SM-108 discontinued because of its instability and the colorants formation during its synthetic process. We have modified the synthetic procedures and, eventually, established the new synthetic procedure, with which pure and stable benzenesulfonic acid salt of SM-108 can be obtained easily.

Synthesis of visible sensitive azobenzene-loaded peptide nucleic acid

In recent years, several research papers reported methods to regulate cellular functions with photosensitive azobenzenes. Establishing these technologies can enable us to regulate cellular functions at a specific site with a desired timing. We succeeded to synthesize a novel visible light sensitive azobenzene (AZO) and introduced it into bis-peptide nucleic acid (bis-PNA), which consists of two homopyrimidine PNA strands, as a linker. Irradiation of visible light irradiation to the bis-PNA-AZO conjugate was found to induce photoisomerization of the azobenzene moiety from *trans* to *cis*.

Inhibition of influenza virus infection by novel tea catechin derivatives

A series of fatty acid derivatives of (–)-epigallocatechin-3-O-gallate (EGCG), a major green tea catechin, were prepared by one-pot lipase-catalyzed transesterification. EGCG-fatty acid esters were found to interfere the virus-cell membrane fusion step that is the early stage of highly pathogenic human and avian influenza A viruses and influenza B virus. The unique anti-influenza fashion can be utilized for the treatment of oseltamivir-resistant viruses.

Publications

Original Papers

Identification of diterpene biosynthetic gene clusters and functional analysis of labdane-related diterpene cyclases in *Phomopsis amygdali*., T. Toyomasu, R. Niida, H. Kenmoku, Y. Kanno, S. Miura, C. Nakano, Y. Shiono, W. Mitsuhashi, H. Toshima, H. Oikawa, T. Hoshino, T. Dairi, N. Kato, T. Sassa: Biosci. Biotechnol. Biochem., 72 (4) (2008) 1038-1047.

Enhanced anti-influenza A virus activity of (-)-epigallocatechin-3-O-gallate fatty acid monoester derivatives: Effect of alkyl chain length, S. Mori, S. Miyake, T. Nakaya, N. Kato, K. Kaihatsu: *Bioorg. Med. Chem. Let.*, 18 (14) (2008) 4249-4252.

Synthesis and mercuriphilic properties of dithiocrown ethers having an azulene pendant., K. Kubo, A. Mori, T. Nishimura, N. Kato: *Heterocycles*, 76 (1) (2008) 209-214.

Enhanced antitumor activities of (-)-epigallocatechin-3-O-gallate fatty acid monoester derivatives in vitro and in vivo, K. Matsumura, K. Kaihatsu, S. Mori, H.H Cho, N. Kato, S.H Hyon: *Biochem. Biophys. Res. Commun.*, 377 (4) (2008) 1118-1122.

Biosynthetic gene-based secondary metabolite screening: A new diterpene, methyl phomopsenonate, from the fungus *Phomopsis amygdali*., T. Toyomasu, A. Kaneko, T. Tokiwano, Y. Kanno, Y. Kanno, R. Niida, T. Kawano, H. Oikawa, N. Kato, T. Sassa: *J. Org. Chem.*, 74 (4) (2009) 1541-1548.

Identification and functional analysis of brassicicene C biosynthetic gene cluster in *Alternaria brassicicola*, A. Minami, N. Tajima, Y. Higuchi, T. Toyomasu, T. Sassa, N. Kato, T. Dairi: *Bioorg. Med. Chem. Let.*, 19 (3) (2009) 870-874.

A structural rationale for selective stabilization of anti-tumor interactions of 14-3-3 proteins by cotylenin A., C. Ottmann, M. Wayand, T. Sassa, T. Inoue, N. Kato, A. Wittinghofer, C. Oecking: *J. Mol. Biol.*, 386 (4) (2009) 913-919.

Review Papers

Regulation of protein-protein interactions by small organic molecules, N. Kato, *Seisan to Gijutsu*, 60 (2008) 43-45.

Patents

Derivatives of 4-carbamoyl-5-hydroxyimidazole and their salts with several sulfonic acids, N. Kato, Y. Higuchi, C. Kondo, and M. Sunagawa, PCT/2008//067050.

Membrane fusion inhibitors, K. Kaihatsu, S. Mori, T. Daidoji, S. Miyake, and N. Kato, PCT/2009/051721.

Development and application of visible sensitive azobenzene, K. Kaihatsu, S. Sawada, N. Kato, JP2008-323606.

Sugar-modified 12-deoxyfusicochin derivatives, N. Kato, T. Inoue, Y. Maruyama, H. Nitta, Y. Honma, T. Sassa, JP2009-02583.

International Conferences

Anti-influenza A virus activity of (-)-epigallocatechin-3-O-gallate fatty acid monoester derivatives (poster), *K. Kaihatsu, S. Mori, S. Miyake, T. Nakaya, N. Kato: 21st International Conference on Antiviral Research, Canada, April 13-17, 2008.

Diterpene Cyclase Responsible for Fusicoccin Biosynthesis (poster), *T. Toyomasu, T. Daiiri, N. Kato, T. Sassa: 7th US-Japan Seminar on the Biosynthesis of Natural Products Enzymology, Structural Biology, and Drug Discovery, La Jolla, California, USA, June 22-27, 2008.

Chemical ligation of epoxide-containing fusicoccins and peptide fragments induced by 14-3-3 protein surface (poster), *J. Ohkanda, T. Maki, A. Kawamura, N. Kato: 9th Tetrahedron Symposium, San Francisco, USA, July 22-23, 2008.

Synthetic Method of 4-Carbamoylimidazolium 5-olate (poster), *C. Kondo, Y. Higuchi, M. Sunagawa, N. Kato: The First International Symposium on Process Chemistry [ISPC 08], Kyoto, Japan, July 28-30, 2008.

Antitumor activity of (-)-epigallocatechin-3-O-gallate fatty acid derivatives (invited), *K. Kaihatsu, K. Matsumura, S. Mori, H.H. Cho, S.H. Hyon, N. Kato: The 8th International Conference of Anticancer Research, Greece, October 17-22, 2008.

Fusicoccin derivative (ISIR-005) suppression anchorage-independent growth of cancer cells through anoikis activation (poster), *Y. Honma, M. Akimoto, T. Sassa, N. Kato: 20th EORTC-NCI-AACR Symposium on Molecular Targets and Cancer Therapeutics, Geneva, Switzerland, October 21-24, 2008.

Module assembly for protein surface recognition (invited), *J. Ohkanda: The IUMRS International Conference in Asia 2008, Nagoya, Japan, December 9-11, 2008.

Design and functional evaluation of prenyltransferase dual inhibitors targeting active site and protein surface (poster), *S. Machida, N. Kato, J. Ohkanda: 12th Sanken International Symposium, Osaka, Japan, January 22, 2009.

Synthesis and evaluation of photochromic properties of heteroatom-substituted azobenzene derivatives (poster), *S. Sawada, K. Kaihatsu, N. Kato: 12th Sanken International Symposium, Osaka, Japan, January 22, 2009.

Synthesis of green tea catechin derivatives and evaluation of their anti-influenza virus activity (poster), *S. Mori, N. Kato, K. Kaihatsu: 12th Sanken International Symposium, Osaka, Japan, January 22, 2009.

Design and synthesis of differentiation Inducers: A new and efficient synthetic approach from natural fusicoccins (poster), *T. Inoue, Y. Higuchi, Y. Maruyama, M. Yabu, H. Nitta, J. Ohkanda, N. Kato: 12th Sanken International Symposium, Osaka, Japan, January 22, 2009.

Synthesis of new MBL inhibitor with hydroxamic acid (poster), *Y. Haranosono, T. Kawano, M. Sunagawa, N. Kato: 12th Sanken International Symposium, Osaka, Japan, January 22, 2009.

Contributions to International Conferences and Journals

N. Kato 27th Conference on Combinatorial Chemistry, Japan (Organizing Committee)

Publications in Domestic Meetings

The Chemical Society of Japan	7 papers
The Pharmaceutical Society of Japan	1 paper
Japan Society for Bioscience, Biotechnology, and Agrochemistry	3 papers
The Japanese Cancer Association	1 paper
Japanese Society for Catechinology	1 paper
The Society of Fiber Science and Technology, Japan	1 paper
Japan Combinatorial Chemistry Symposium	1 paper
The Japanese Society of Virology	1 paper
The Pharmaceutical Society of Japan Kanto-Regional Symposium	1 paper
Others	5 papers

Academic Degrees

Master Degree for Science

S. Sawada	Synthesis of visible sensitive azobenzenes and their physico-chemical properties
K. Fuji	Synthesis of mix-combinatorial library of metal complexes for exploring agents that recognize protein surfaces
Y. Maruyama	Differentiation inducing properties of sugar-altered fusicoccin derivatives
T. Monta	Design and synthesis of antagonists for quorum sensing

Sponsorship

Grant-in-Aid for Scientific Research for Young Scientists (B)

K. Kaihatsu	Construction of artificial DNA bulb structure and regulation of transcription by light controllable antisense molecules	¥1,300,000
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Grant-in-Aid for JSPS Fellows

T. Inoue	Forward and Reverse Chemogenomics on 14-3-3 Proteins	¥900,000
Y. Higuchi	Chemical biology for understanding the functions of 14-3-3 protein	¥600,000

Entrusted Research

N. Kato	Program for Development of new Promotion of anti-cancer agents based on Fundamental the differentiation-inducing Studies in diterpene glycoside Health Sciences	¥24,000,000
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K. Kaihatsu	(NIBIO) NEDO Foundation for Science Researches	Development of Screening Systems for Anti-RNA Virus Drugs Using Novel Tea Catechin Derivatives	¥6,240,000
Other Research Fund			
J. Ohkanda	The Takeda Science Foundation	Design and functional evaluation of dual prenyltransferase inhibitors targeting common structure of protein surfaces	¥2,000,000
J. Ohkanda	Naito Memorial Foundation	Design and functional evaluation of synthetic agents for protein-protein interactions	¥3,000,000
K. Kaihatsu	JST	Construction of artificial DNA bulb structure and regulation of transcription by light controllable antisense molecules	¥2,000,000

Department of Organic Molecular Materials

Professor:	Yoshio ASO
Associate Professor:	Yutaka IE (2009.3.16-)
Assistant Professors:	Yutaka IE (-2009.3.15), Kaori ASANO
Graduate Students:	Masaru ENDOU, Masashi NITANI, Tomoya HIROSE, Toshihiko UTO, Makoto OKABE, Takahiro NOZAWA, Yuuya HAMANO
Under Graduate Students:	Takahiro SAKURAI, Atsuki YOSHIMURA
Supporting Staff:	Misayo IMAI

Outlines

The main subject in the Department of Organic Molecular Materials is the development of novel molecular-based materials with promising electronic and photoelectric properties for organic electronics. The research is based on the elucidation of the relationship between molecular structures and physical properties to control and improve the functions. We have been focusing our research on the design, synthesis, and properties of (1) novel extended conjugation systems as active materials for organic field-effect transistors and photovoltaic devices and (2) nano-scale conjugated molecules for promising functional molecular wires. These nano-scale molecular materials have potential use as a fundamental framework for organic electronic devices.

Current Research Project

Organic Electronics Materials

We have developed organic materials for n-type field-effect transistors. It has been known that the introduction of electron-withdrawing groups into pi-conjugated systems dramatically increases their n-type character. We have designed difluorodioxocyclopentene-annelated thiophene and carbonyl-bridged bithiazole monomer units and have synthesized their based conjugated oligomers. Their electronic absorptions, X-ray analyses, and redox potentials indicated that ring fusion of aromatics not only keeps the planarity between consecutive aromatic rings but also increases n-type character. Some of these electronegative oligomers revealed high field-effect electron mobility, and the oligomer bearing a carbonyl-bridged bithiazole unit showed the highest class of electron mobility and air stability. Solution-processable n-type materials have also been accomplished by introducing difluorodioxocyclopentene-annelated thiophenes and lipophilic 3-hexylthiophene into pi-conjugated oligomeric backbone.

In anticipation of self-association properties, we have synthesized the highly branched oligothiophenes with the juncture of 1,3,5-trisubstituted benzene for the development of high carrier-mobility materials in a film. The branched-oligothiophene/perylenebisimide linkage molecules showed highly efficient photo-induced intra- and intermolecular electron transfer. Their thin films fabricated with spin-coating showed good photovoltaic properties, and the appearance of this character indicates that the self-aggregation of the dendritic oligothiophene parts

effectively contributes the formation of hole- as well as electron-transporting channels. The branched-oligothiophene/naphtalenebisimide linkage molecule has been also exhibited as active materials for organic photovoltaic devices.

Molecular Electronics Materials

The cyclopentathiophene with a spiro-type substituted dioctylfluorene has been designed as a monomer unit for encapsulated molecular wire, and then a series of their oligomers up to 12-mer were synthesized. The electronic absorption maxima of the oligomers were found to be bathochromically shifted with increasing the number of thiophene rings, clearly indicating that the bulky groups have little influence on the effective conjugation. The X-ray analyses also revealed that the oligomeric backbone is completely insulated by the bulky groups. The electronic absorption spectra of oxidized species of these insulated oligothiophenes showed complete blocking of pi-dimer formations unlike usual oligothiophenes. Moreover, it is highly important to connect each molecular wire to the bulk nano-gap electrode. In this context, we have achieved the synthesis of the encapsulated thiophene 6-mers with terminal thiol anchor groups for gold electrodes as well as with terminal ethynyl anchor groups for silicon electrodes.

For certain connection of molecular wires with metal electrodes and efficient carrier injection, we have developed tetraphenylmethane tripodal anchor units with selenium functional groups. Their monolayers on a gold electrode revealed the effectiveness of selenol functional groups as well as the three-armed structure.

Publications

Original Papers

Synthesis, Structure, and Properties of 2,5,8,11,14,17-Hexamethyltriphenylene [2,1-b:3,4-b':6,5-b'':7,8-b''':10,9-b''':11,12-b'''] hexathiophene, M. Endou, Y. Ie, Y. Aso: *Heterocycles*, 76 (2) (2008) 1043-1048.

Dendritic Oligothiophene Bearing Perylene Bis(dicarboximide) Groups as an Active Material for Photovoltaic Device, Y. Ie, T. Uto, N. Yamamoto, Y. Aso: *Chem. Commun.*, 2009 (10) (2009) 1213-1215.

Review Papers

Development of Electron-Transporting Conjugated Oligomers Based on Fluorination Reactions and Their Application to Organic Field-Effect Transistors, Y. Ie and Y. Aso, *J. Syn. Org. Chem. Jpn.*, 66[5] (2008) 504-514.

Development of Novel Organic n-Type Semiconductors Based on Fluoroalkyl Annulation, Y. Aso and Y. Ie, *Manufacturing & Technology*, 60[3] (2008) 73-76.

Books

Molecular Wires (part), Y. Aso and Y. Ie, in *Fundamental Technologies of Molecular Electronics and Prospect*, Supervisor: K. Matsushige, K. Tanaka, and Y. Wada, CMC (2009) 151-158.

Synthesis and Functions of Branched-Conjugation Hierarchical Structures for Controlling Charged-Carrier Transport (part), Y. Aso and Y. Ie, in Control of Super-Hierarchical Structures and Innovative Functions of Next-Generation Conjugated Polymers, Supervisor: K. Akagi, CMC (2009) 51-56.

Patents

Conjugated Compounds and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, Y. Aso, M. Okabe, and M. Ueda, JP2007-311381.

Compounds Consisting of Nitrogen-containing Condensation Ring, Polymers Consisting of Nitrogen-containing Condensation Ring, and Organic Thin Films and Organic Thin-Film Devices, Y. Ie, M. Nitani, Y. Aso, and M. Ueda, JP2008-220031.

Branched Compounds and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, T. Uto, Y. Aso, and M. Ueda, JP2008-221779, PTC/JP2009/050083.

Conjugated Compounds and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, Y. Aso, M. Okabe, and M. Ueda, JP2008-290027.

Conjugated Compounds, Compounds Consisting of Nitrogen-containing Condensation Ring, Polymers Consisting of Nitrogen-containing Condensation Ring, and Organic Thin Films and Organic Thin-Film Devices, Y. Aso, Y. Ie, M. Okabe, M. Nitani, and M. Ueda, PCT/JP2008/071520.

Polymers and Their Organic Thin Films and Organic Thin-Film Devices, M. Karakawa, Y. Aso, and M. Ueda, PCT/JP2009/052156.

Polymers and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, A. Yoshimura, Y. Aso, and M. Ueda, JP2009-058565.

Branched Compounds and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, M. Okabe, Y. Aso, and M. Ueda, JP2009-058664.

Conjugated Compounds and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, M. Okabe, Y. Aso, and M. Ueda, JP2009-058737.

Fluorinated Polymers and Their Organic Thin Films, Y. Ie, M. Nitani, Y. Aso, and M. Ueda, JP2009-058739.

Dendrimers with Low Refraction, Their Synthetic Method, and Their Synthetic Materials, Y. Tanaka, T. Nagai, Y. Aso, and Y. Ie, JP2009-059936.

International Conferences

Synthesis, Properties, and n-Type FET Performances of Difluorodioxocyclopentene-annelated Oligothiophenes, *Yutaka Ie, Yoshikazu Umemoto, Makoto Okabe, Yoshio Aso: The 8th International Symposium on Functional pi-Electron Systems (Fpi8), Graz, Austria, July 21-25 (2008).

Synthesis, Structure, and Properties of 2,5,8,11,14,17-Hexamethyltriphenyleno [2,1-b:3,4-b':6,5-b'':7,8-b''':10,9-b''':11,12-b''']hexathiophene (poster), *Masaru Endou, Yutaka Ie, Yoshio Aso: LXII Yamada Conference 2008 "Topological Molecules", Awaji, Hyogo Japan, September 1-4, 2008.

Synthesis, Properties, and n-Type FET Performances of Difluorodioxocyclopentene-annelated Oligomers (poster), *Yutaka Ie, Makoto Okabe, Yoshikazu Umemoto, Yoshio Aso: LXII Yamada Conference 2008 "Topological Molecules", Awaji, Hyogo Japan, September 1-4, 2008.

Synthesis and Photovoltaic Performance of Branched Oligothiophenes Having Perylene Bis(dicarboximide) (poster), *Toshihiko Uto, Yutaka Ie, Yoshio Aso: The Fifth International Symposium on Integrated Synthesis (ISIS-5), Kobe, Japan, September 5-6, 2008.

Synthesis and Properties of Tripodal Anchor Units Bearing Selenium Functional Groups (poster), *Tomoya Hirose, Yutaka Ie, Yoshio Aso: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, September 29 – October 1, 2008.

Synthesis, Properties, and Photovoltaic Performances of Branched Oligothiophenes Bearing Perylene Bis(dicarboximide) Groups (poster), *Yutaka Ie, Toshihiko Uto, Yoshio Aso: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, September 29 – October 1, 2008.

Difluorodioxocyclopentene-Annelated Thiophenes: Synthesis, Properties, and n-Type FET Performances (poster), *Yutaka Ie, Makoto Okabe, Yoshikazu Umemoto, Yoshio Aso: 18th Iketani Conference, International Conference on Control of Super-Hierarchical Structures and Innovative Functions of Next-Generation Conjugated Polymers, Awaji, Hyogo, Japan, October 21-23, 2008.

Synthesis and Properties of Branched Oligothiophenes Having Perylene Bisimide Groups as an Electron-Accepting Unit (poster), *Toshihiko Uto, Yutaka Ie, Yoshio Aso: 18th Iketani Conference, International Conference on Control of Super-Hierarchical Structures and Innovative Functions of Next-Generation Conjugated Polymers, Awaji, Hyogo, Japan, October 21-23, 2008.

Synthesis of Anchor Compounds Bearing Selenium Functional Groups and Characterization of Their Monolayers (poster), *Tomoya Hirose, Yutaka Ie, Yoshio Aso: The International Workshop on Molecular Information and Dynamics 2008, Taipei, Taiwan, November 10-12, 2008.

Synthesis, Structure, and Properties of 2,5,8,11,14,17-Hexamethyltriphenyleno [2,1-b:3,4-b':6,5-b'':7,8-b''':10,9-b''':11,12-b''']hexathiophene (poster), *Masaru Endou, Yutaka Ie, Yoshio Aso: The International Workshop on Molecular Information and Dynamics 2008, Taipei, Taiwan, November 10-12, 2008.

Synthesis, Properties, and Field-Effect Transistor Characteristics of Conjugated Oligomer Containing Carbonyl-Bridged Bithiazole Unit (poster), *Masashi Nitani, Yutaka Ie, Yoshio Aso: Osaka University Forum 2008 : Bio-Environmental Chemistry, San Francisco, December 8-9, 2008.

Synthesis and Properties of Branched Oligothiophenes Bearing Perylene Bis(dicarboximide) Groups (poster), *Toshihiko. Uto, Yutaka. Ie, Yoshio. Aso: The 12th SANKEN International Symposium, Osaka Univ., January 22, 2009.

Development of Tripodal Anchor Units Bearing Selenium Functional Groups and Characterization of Their Monolayers (poster), *Tomoya Hirose; Yutaka Ie; Yoshio Aso: The 12th SANKEN International Symposium, Osaka Univ., January 22, 2009.

Synthesis, Properties, and Photovoltaic Performances of Branched Oligothiophenes Bearing Naphthalene Bis(dicarboximide) Groups (poster), *Yutaka Ie, Toshihiko Uto, Yoshihito Honsho, Shu Seki, Makoto Karakawa, Yoshio Aso: Fifth International Conference on Molecular Electronics and Bioelectronics (M&BE5), Miyazaki, Japan, March 15-18, 2009.

Publications in Domestic Meetings

The Chemical Society of Japan	5 papers
Symposium on Main Element Chemistry	1 paper
Symposium on Organic pi-Systems	2 papers
Symposium on Fundamental Organic Chemistry	3 papers
Symposium on Fluorine Chemistry	1 paper
The Japan Society of Applied Physics	1 paper

Academic Degrees

Master Degree for Engineering

T. Uto	Synthesis, Properties, and Photovoltaic Performance of Branched Oligothiophenes Having Electron-Accepting Units
M. Okabe	Synthesis, Properties, and n-type FET Characteristics of New Conjugated Oligomers Having Difluorodioxocyclopentene-Annelated Thiophenes

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

Y. Aso	Development of Extended Conjugated Oligomers toward Construction of Charge-Transporting Hierarchical Structure	¥1,500,000
Y. Ie	Development of Insulated Oligothiophene Molecular Wires Bearing Tripodal Anchor Units at Terminal	¥2,100,000

Position

Grant-in-Aid for Scientific Research on Innovative Areas

Y. Aso	Functions of Highly Elaborated pi-Space Based on Synthesis of Extended pi-Electron Systems and Application to Electronics	¥4,420,000
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Research Fellowship for Young Scientists

M. Nitani	Synthesis and Function of Conjugated Oligomers Containing Fluorine Atoms as Novel n-Type Semiconducting Materials	¥600,000
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Entrusted Research

Y. Aso	Japan Science and Technology Agency	Synthesis and Application of Novel Conjugated Oligomers as n-Type Semiconductors for Stable Operation	¥4,999,000
Y. Ie	The New Energy and Industrial Technology Developing Organization (NEDO) of Japan	Development of n-Type and Ambipolar Organic Semiconductors Based on Novel Molecular Design	¥18,850,000

Cooperative Research

Y. Aso	Sumitomo Chemical Co., Ltd.	Development of Materials for Organic Electronics	¥1,012,000
Y. Aso	Daikin Industries, Ltd	Development of Ultra-low Reflection Materials	¥3,300,000

Other Research Fund

Y. Ie	Kinki Regional Invention Center	Development of Solution-Processable n-Type Organic Semiconductors	¥1,200,000
Y. Ie	Foundation Advanced Technology Institute	Development of n-Type Organic Semiconductors Based on Novel Molecular Design	¥1,400,000
Y. Ie	Osaka University Engineering Society	Synthesis, Properties, and n-Type FET Performances of Difluorodioxocyclopentene-related Oligothiophenes	¥150,000

Department of Molecular Excitation Chemistry

Professor: Tetsuro MAJIMA
Associate Professor: Mamoru FUJITSUKA
Assistant Professors: Sachiko TOJO, Takashi TACHIKAWA
Specially Appointed Professor: Akira SUGIMOTO
Research Technical Expert: Takumi KIMURA
Post Doctoral Fellows: Shingo SAMORI
Graduate Students: Yasuko OSAKADA, Kazuya NAITO, Yoshiki MIYAMOTO,
Man Jae PARK, Jun Rye CHOI, Shi-Cong CUI, Yuichiro
TAKEDA, Takeshi NAKATANI, Haruka KODERA,
Haruhiro NISHITERA,
Under Graduate Students: Eri MATSUTANI, Soichiro YAMASHITA
Supporting Staff: Sanae TOMINAGA

Outlines

"Beam-induced molecular chemistry" based on photo- and radiation-induced chemistry of organic compounds has been investigated from both basic and beam-functional points of view. The research topics are underway with respect to developments of new beam-controlled chemistry, new synthetic chemistry, and new molecular devices and functional materials.

1. Formation and reactivities of reactive intermediates in photochemistry and radiation chemistry, and photochemistry of reactive intermediates
2. Multi-beam chemistry with irradiation by two-color laser-laser and electron pulse-laser flash
3. Multiple-photon chemistry of organic compounds using UV, visible, and infrared lasers
4. Beam-controlled chemistry of artificial biomolecules such as modified DNA and proteins

Current Research Project

Multi-beam Chemistry

Multi-beam chemistry has been studied using pulse radiolysis-laser flash photolysis combined method, two-color two-laser photolysis and three-color three-laser photolysis. Photochemistry of reaction intermediates and short-lived chemical species generated from the reaction induced by the first beam excitation of a starting molecule (two-step excitation method), and moreover, photochemistry of other chemical species generated from the reaction of the short-lived intermediate induced by the second beam excitation (three-step excitation method) can be studied. This year, by using the multi-beam irradiation method, we have successfully observed excited state of radical cation of oligothiophenes. Hole transfer process from the excited radical cation was also investigated. In addition, α - and β - bond cleavage of aromatic carbonyl compounds was investigated by two-color two-laser flash photolysis. Furthermore, we have investigated

the electron transfer process of porphycene, a structural isomer of porphyrin, supramolecular dyad. Conformation-dependence of the electron transfer rate in oligothiophene-perylenediimide dyad was also revealed. We also clarified qualitative relation between stabilization energy of delocalized negative charge on stacked chromophores and structure by investigating the charge resonance band of reduced cyclophanes.

Nanophotochemistry

1) Mechanisms of TiO₂ Photocatalytic Reactions: Heterogeneous photocatalysts have both potential and demonstrated applications for use in the water-splitting reaction that produces hydrogen, the degradation of organic pollutants, the surface wettability conversion, etc. We investigated temporal and spatial distributions of various reactive oxygen species (ROS), such as singlet oxygen and the hydroxyl radical, generated by the photoexcitation of TiO₂ nanomaterials using single-molecule fluorescence spectroscopy. In particular, the single-molecule, single-particle observation of emissive fluorescein molecules generated in individual TiO₂ nanotubes under UV light irradiation clearly revealed that the transport of reagents inherent in the porous structures is closely related to the photocatalytic activity. Furthermore, we clarified the defect-mediated PL dynamics of pure and Eu³⁺-doped TiO₂ nanoparticles at the single-particle or single-aggregate level. The quantitative examination of the spectral and kinetic characteristics revealed that the PL bands originating from defects in the bulk and/or on the surface appeared in the visible region with numerous photon bursts by the photoirradiation with a 405-nm laser in an inert gas atmosphere. Our findings provide a significant opportunity to understand the temporal and spatial distributions of ROS generated during the photoirradiation of TiO₂ nanomaterials and directly explore the microscopic world in many fields ranging from fundamental physics and chemistry to practical applications.

2) Electron Transfer in Single Nanoconjugates of Semiconductor Quantum Dots and Organic Compounds: The interfacial electron transfer process from the photoexcited CdTe quantum dots to a pyromellitimide derivative was studied at the single-particle level. On the basis of the experimental and analytical results, it was concluded that the blinking characteristics observed for individual conjugates are due to the intermittent changes in the interfacial ET redox turnover rates.

3) Photoinduced One-Electron Oxidation of Aromatic Compounds on MOF-5 Nanoparticles: The interfacial charge transfer from the photoexcited MOF-5 nanoparticles to various organic compounds was investigated by time-resolved diffuse reflectance spectroscopy. It was found that MOF-5 has a much higher oxidation reaction efficiency than that of P25 TiO₂ powder.

Publications

Original Papers

Intramolecular Excimer Formation and Photoinduced Electron Transfer Process in bis-1,8-Naphthalimide Dyads Depending on the Linker Length, D. W. Cho, M. Fujitsuka, A. Sugimoto, and T. Majima: *J. Phys. Chem. A*, 112 (31) (2008) 7208-7213.

Excitation Energy Dependence of Photoinduced Processes in Pentathiophene-Perylenediimide Dyads with a Flexible Linker, M. Fujitsuka, K. Harada, A. Sugimoto, and T. Majima: *J. Phys. Chem. A*, 112 (41) (2008) 10193-10199.

Photodecomposition Profiles of β -Bond Cleavage of Phenylphenacyl Derivatives in the Higher Triplet Excited States during Stepwise Two-Color Two-Laser Flash Photolysis, M. Yamaji, X. Cai, M. Sakamoto, M. Fujitsuka, and T. Majima: *J. Phys. Chem. A*, 112 (45) (2008) 11306-11311.

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Books

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International Conferences

Development of New TiO₂ Photocatalyst: Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 213th Electrochemical Society meeting, Phoenix, USA, May 20, 2008.

Intramolecular Electron Transfer from Axial Ligands to S₂-Excited Tetraphenyl Porphyrins (invited), T. Tachikawa, M. Fujitsuka, and *T. Majima: 213th Electrochemical Society meeting, Phoenix, USA, May 20, 2008.

Charge Transfer in DNA (invited), T. Majima: 10th International Workshop on Radiation Damage to DNA, Fukushima, Japan, Jun. 8-12, 2008.

Real-Time Single Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species with Fluorescent Probes: Applications to TiO₂ Photocatalysts (poster), *K. Naito, T. Tachikawa, M. Fujitsuka, T. Majima: 21st IUPAC Symposium on Photochemistry, Gothenburg, SW, Jul. 28, 2008.

Single-Molecule Detection of Hole Transfer Through DNA (poster), *T. Tadao, M. Fujitsuka, and T. Majima: 21st IUPAC Symposium on Photochemistry, Gothenburg, SW,

Jul. 28, 2008.

Charge Transfer in DNA (invited), *T. Majima, K. Kawai, and M. Fujitsuka: 236th ACS National Meeting, Philadelphia, PA, Aug. 17-21, 2008.

3-D Writing of metal nanoparticles in a polymer matrix with two-color laser beams (poster), *M. Sakamoto, T. Tachikawa, M. Fujitsuka, and T. Majima: 236th ACS National Meeting, Philadelphia, PA, Aug. 17-21, 2008.

Charge Transfer in DNA, K. Kawai, M. Fujitsuka, and *T. Majima: 2nd Asia-Pacific Symposium on Radiation Chemistry (APSRC-2008), Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Charge Transfer in DNA (invited), T. Majima: 2008 KOREA-JAPAN Symposium on Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

Intermolecular Photoinduced Electron-Transfer of 1,8-Naphthalimides in Protic Polar Solvents (poster), *D. W. Cho, M. Fujitsuka, U. C. Yoon and T. Majima: 2008 KOREA-JAPAN Symposium on Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

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Three-dimensional Fabrication of Metal Nanoparticles in Polymer Matrix (invited), T. Majima: Langmuir Symposium in Beijing, Beijing, China, Oct. 31, 2008.

Photochemical Fabrication of 3D Metal Nanoparticles in Polymer Matrix (invited), T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Solvent Effects on Photoinduced Electron Transfer in 1,8-Naphthalimide Dyads (poster), *D. W. Cho, U. C. Yoon, M. Fujitsuka, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Inter- and/or Intramolecular Excimer and Exciplex Emission in 1,8-Naphthalimide Derivatives (poster), *D. W. Cho, M. Fujitsuka, U. C. Yoon, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Emission Mechanism of Doubly Orth-Linked Quinoxaline/Diphenylfluorene or *cis*-Stilbene/Fluorene Hybrid Compounds Based on the Transient Absorption and Emission Measurements during the Pulse Radiolysis (poster), Y. Wei, S. Samori, S. Tojo,

M. Fujitsuka, J.-S. Lin, *C.-T. Chen, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 9th Int Symp Ceramic Materials and Components for Energy and Environmental Application, Shanghai, China, Nov. 11, 2008.

Single-Molecule Observation of Photocatalytic Reaction in TiO₂ Nanotube: Importance of Molecular Transport through Porous Structures (poster), *K. Naito, T. Tachikawa, M. Fujitsuka, and T. Majima: Osaka University Forum in San Francisco: Grobal COE Program, Bio-Environmental Chemistry, San Francisco, USA, Dec.8-11, 2008.

Bilateral Cooperation between Korea and Japan: To the Future (invited), T. Majima: International Symposium on Core University Program between Japan and Korea -New Processing and Nanostructure/Property Relationship for Multi-functional Materials - (The 21st JSPS-KOSEF CUP Seminar between Japan and Korea), Awajishima, Japan, Dec. 15, 2008.

Design of Cyclic Reaction Driven by the Two-color Two-photon Excitation (poster), M. Sakamoto, *S. S. Kim, M. Fujitsuka, T. Majima: International Symposium on Core University Program between Japan and Korea -New Processing and Nanostructure/Property Relationship for Multi-functional Materials - (The 21st JSPS-KOSEF CUP Seminar between Japan and Korea), Awajishima, Japan, Dec. 15, 2008.

Interfacial Electron Transfer Dynamics in a Single CdTe Quantum Dot-Pyromellitimide Conjugate (poster), *S.-C. Cui, T. Tachikawa, M. Fujitsuka, and T. Majima: International Symposium on Core University Program between Japan and Korea -New Processing and Nanostructure/Property Relationship for Multi-functional Materials - (The 21st JSPS-KOSEF CUP Seminar between Japan and Korea), Awajishima, Japan, Dec. 15, 2008.

Development of TiO₂ Photocatalyst: Real-Time Single Molecule Imaging of TiO₂ Photocatalytic Reactions (invited), T. Majima: The 10th International Symposium on Eco-materials Processing and Design, Xi'an, China, Jan. 13-16, 2009.

Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 2009 Korea-Japan Workshop on Photocatalysis and Solar Conversion, Pohang, Korea, Jan. 20, 2009.

Interfacial Electron Transfer Process in a Single CdTe Quantum Dot-Pyromellitimide Conjugate (poster), S.-C. Cui, *T. Tachikawa, M. Fujitsuka, and T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Defect-Mediated Photoluminescence Dynamics of Eu³⁺-Doped TiO₂ Nanocrystals Revealed at the Single-Particle Level (poster), *T. Tachikawa, T. Ishigaki, J.-G. Li, M.

Fujitsuka, and T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Real-Time Single-Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species Generated on TiO₂ Photocatalysts (poster), K. Naito, T. Tachikawa, M. Fujitsuka, and *T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Single-Molecule Observation of Photocatalytic Reactions in Mesoporous TiO₂ Nanotube (poster), K. Naito, T. Tachikawa, M. Fujitsuka, and *T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Development of New TiO₂ Photocatalyst (invited), T. Majima: The 1st Hanyang-Osaka Symposium on Fusion-Tech based Materials, Seoul, Korea, Feb. 27, 2009.

Approach Toward Efficient Photo-electronic Devices by Supramolecular Chemistry (invited), *M. Fujitsuka, A. Sugimoto, and T. Majima: The 1st Hanyang-Osaka Symposium on Fusion-Tech based Materials, Seoul, Korea, Feb. 27, 2009.

Real-Time Single-Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species Generated on TiO₂ Photocatalysts (invited), T. Majima: Asian Academic Seminar 2008 on "Frontiers in the Photocatalysis and Photochemistry of Advanced Materials" Kawasaki, Japan, Mar. 2-6, 2009.

Charge Transfer in DNA (invited), T. Majima: Kyudai International Symposium on Photo and Supramolecular Chemistry, Fukuoka, Japan, Mar. 7, 2009.

Contributions to International Conferences and Journals

T. Majima	2007 Korea-Japan Symposium on Frontier Photoscience (Conference Chair)
T. Majima	2 nd Asia-Pacific Symposium on Radiation Chemistry (APSRC-2008) (Organizing Committee)
T. Majima	10 th International Symposium on Eco-materials Processing and Design (Organizing Committee)
T. Majima	Langmuir Symposium in Beijing 2008 (Organizing Committee)
T. Majima	2009 Korea-Japan Workshop on Photocatalysis and Solar Conversion (Organizing Committee)
T. Majima	1 st Hanyang-Osaka Symposium on Fusion-Tech based Materials' (Organizing Committee)
T. Majima	Langmuir, American Chemical Society (Senior Editor)

Publications in Domestic Meetings

The 30 th Japan Photobiology and Photomedicine Meeting	1 paper
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Photochemistry Meeting 2008	8 papers
The 23 rd symposium on Biofunctional Chemistry	1 paper
The 51 th Radiation Chemistry Meeting	2 papers
The 89 th Japan Chemical Society Meeting	7 papers

Academic Degrees

Doctor Degree for Engineering

Y. Osakada	Studies on Charge Transfer in DNA and Photosensitized DNA Damage
K. Naito	Studies on the Mechanism of TiO ₂ Photocatalytic Reaction by Single-Molecule Fluorescence Spectroscopy

Master Degree for Engineering

Y. Takeda	Excess Electron Transfer in Benzo-phenothiazine-Modified DNA Hairpins
T. Nakatani	Electron Transfer from Oligothiophene in the Higher Triplet Excited State

Sponsorship

Grand-in-Aid for Scientific Research (S)

T. Majima	Nanoscience of Photofunctionalized DNA	¥8,840,000
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Grand-in-Aid for Basic Scientific Research

T. Majima	Construction of devices for photoelectronic conversion using photochemical control of Tobacco Mosaic Virus supramolecules	¥800,000
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Grand-in-Aid for Scientific Research (B)

M. Fujitsuka	Studies toward molecular device using femtosecond multi-laser	¥6,370,000
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Grant-in-Aid for Scientific Research on Priority Areas

M. Fujitsuka	Kinetics of photochemical ultrafast processes in polymer chains	¥1,700,000
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Grand-in-Aid for Encouragement of Young Scientists

T. Tachikawa	Fabrication and Photocatalytic Activity of Nanostructured TiO ₂ -DNA Composites	¥650,000
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Grand-in-Aid for Scientific Research for Young Scientist

S. Samori	Beam chemical reaction towards high efficient photochemical molecular devices	¥900,000
Y. Osakada	Study on photoinduced DNA damage caused by charge transfer in DNA toward application to	¥900,000

K. Naito	photo dynamic therapy Characterization and application of photo-functionalized carbon nanotube by single molecular fluorescence spectroscopy	¥900,000
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Other Research Fund

T. Majima	Sekisui Chemicals Co.	Super hydrophilicity by TiO ₂ photocatalytic reaction	¥400,000
T. Majima	Matsushita Electric Industrial Co.	Study on highly reactive nanostructured TiO ₂ photocatalysts	¥1,732,500
T. Majima	TOYOTA Co.	Hydrogen absorbing alloys with high surface area produced by photoreduction	¥5,000,000

Department of Synthetic Organic Chemistry

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Assistant Professors:	Junko ICHIHARA, Kazuhiro TAKENAKA (2008.12.16~)
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Research Fellow:	Rashid Nabisaheb NADAF (~2008.9.15)
Graduate Students:	Naohito INOUE, Doss RAJESH, Kazem GHOZATI, Gabr Randa Kassem MOHAMED, Mohanta Suman CHANDRA, Shuichi HIRATA, Noriyuki ITOH, Kimiko KIRIYAMA, Kaori TANAKA, Yugo TANIGAKI, Toyohiro NAGANO Naoya KANBAYASHI, Yutaro HAKOI, Shintaro HASHIMOTO, Keisuke SUGIMOTO
Under Graduate Student:	Yumiko ATSUJI (~2008.7.1)
Supporting Staff:	Miho OHAMA (~2008.5.23), Tomoko KISHI (2008.5.16~)

Outlines

Asymmetric synthesis, a phenomenon fine-tuned to perfection by nature, forms the central theme of our research efforts. We have been interested in the design and syntheses of a novel class of chiral ligands that are unique in promoting new asymmetric reactions. The mechanisms of these organic reactions are also studied by means of physical organic techniques. Novel chiral spiro ionic liquids and organocatalysts have been synthesized with a focus on developing environmentally benign asymmetric processes.

Current Research Project

Dual Activation in Oxidative Coupling of 2-Naphthols Catalyzed by Chiral Dinuclear Vanadium Complexes

The dinuclear vanadium(V) complex **1** was found to be prepared by complexation of VOCl_3 with the Schiff base derived from (*R*)-3,3'-diformyl-2,2'-dihydroxy-1,1'-binaphthyl and (*S*)-tert-leucine. In the catalyst **1**-mediated coupling reactions, the two vanadium atoms in the complex activate two molecules of 2-naphthol simultaneously, resulting in a high reaction rate with high enantioselectivity. The dual activation mechanism in this system was supported by the kinetic analysis.

We also developed a convenient method for preparing the dinuclear vanadium catalyst **1**, which promotes the coupling of 9-phenanthrol to give (*S*)-biphenanthrol in quantitative yield with high enantioselectivity.

Enantioselective Oxidative Cyclization Catalyzed by Pd-SPRIX Complexes

Recently, catalytic reactions via Pd(IV) intermediates generated from a Pd(II) precursor by the action of a powerful oxidant have been accomplished. Compared to the impressive development of enantioselective reactions through the Pd(0)/Pd(II) catalytic

cycle, only minimal attention has been devoted to exploring asymmetric Pd(II)/Pd(IV) catalysis. We have found that spiro bis(isoxazoline) compounds (SPRIXs), which are remarkably stable under oxidative conditions, serve as effective chiral ligands in Pd(II)/Pd(IV) catalytic enantioselective transformations. Thus, cyclization of enyne derivatives proceeds in the presence of the Pd–SPRIX catalyst and a hypervalent iodine oxidant to give lactones bearing a bicyclo[3.1.0]hexane skeleton with up to 95% ee. It is noteworthy that no enantioselectivity is observed with general phosphine or oxazoline containing chiral ligands.

Novel enantioselective Pd(0)/Pd(II) catalysis using SPRIX ligands was also accomplished. Thus, Pd–SPRIX-catalyzed oxidative cyclization of 2-allylphenols afforded optically active chromene derivatives, which were valuable architectural platform for many biologically active substances.

Asymmetric Synthesis of Chiral Hybrid Spiro (Isoxazole–Isoxazoline) Ligands

Preparation of novel chiral spiro (isoxazole–isoxazoline) ligands without a tedious optical resolution was examined. Diastereoselective intramolecular double nitrile oxide cycloaddition of the key dioxime derived from bis(2,2,2-trifluoroethyl) malonate and the enantiomerically pure alcohol gave the desired ligands.

Development of Novel Chiral Molecules Based on Spirobilactams

New functional chiral molecules were prepared from spirobilactams which were readily available via an enantioselective palladium-catalyzed intramolecular double N-arylation. Optically pure spirobilactams were converted into diammonium salts as a novel chiral phase transfer catalyst and bis(amine-phosphine) as an effective chiral ligand by conventional synthetic methods.

Solvent-free Catalytic Oxidation Using Green Solid Dispersant

We have developed a green solid-phase oxidation reaction system for an organic compound, which has such advantages that the system does not require any organic solvent which may adversely affect the global environment, has a high product yield, enables to reuse a catalyst and the like, and therefore which is industrially valuable. The solid-phase oxidation reaction system comprises a mixture of a powder of a solid dispersant and a powder of a solid catalyst for the oxidation reaction, the organic compound and aqueous hydrogen peroxide, wherein the organic compound, the solid catalyst and the aqueous hydrogen peroxide are dispersed in the mixture so that these components contact with one another.

Publications

Original Papers

Divergent Synthesis of Chiral Spiro (Isoxazole-isoxazoline) Hybrid Ligands, K. Takenaka, S. Nakatsuka, T. Tsujihara, P. S. Koranne, H. Sasai: *Tetrahedron: Asymmetry*, 19 (21) (2008) 2492-2496.

Dicationic Palladium(II)–Spiro Bis(isoxazoline) Complex for Highly Enantioselective Isotactic Copolymerization of CO with Styrene Derivatives, G. B. Bajracharya, P. S. Koranne, T. Tsujihara, S. Takizawa, K. Onitsuka, H. Sasai: *Synlett*, (2) (2009) 310-314.

Pd^{II}/Pd^{IV} Catalytic Enantioselective Synthesis of Bicyclo[3.1.0]hexanes via Oxidative Cyclization of Enynes, T. Tsujihara, K. Takenaka, K. Onitsuka, M. Hatanaka, H. Sasai: J. Am. Chem. Soc., 131 (10) (2009) 3452-3453.

Enantioselective Synthesis of C₂-symmetric Spiro lactams via Pd-catalyzed Intramolecular Double N-Arylation, K. Takenaka, N. Itoh, H. Sasai: Org. Lett., 11 (7) (2009) 1483-1486.

Regio- and Enantioselective Allylation of Indole Catalyzed by a Planar-chiral Cyclopentadienyl-Ruthenium Complex, K. Onitsuka, C. Kameyama, H. Sasai: Chem. Lett., 38 (5) (2009) 444-445.

Review Papers

Development of Chiral Spiro Ligands for Metal-catalyzed Asymmetric Reactions, G. B. Bajracharya, M. A. Arai, P. S. Koranne, T. Suzuki, S. Takizawa, and H. Sasai, Bull. Chem. Soc. Jpn., 82 [3] (2009) 285-302.

Development of Novel Immobilization Methods for Multicomponent Asymmetric Catalyst (MAC), S. Takizawa, T. Arai, and H. Sasai, J. Synth. Org. Chem. Jpn. 67 [3] (2009) 194-207.

Dinuclear Chiral Vanadium Catalysts for Oxidative Coupling of 2-Naphthols via a Dual Activation Mechanism, S. Takizawa, T. Katayama, and H. Sasai, Chem. Commun., [35] (2008) 4113-4122.

Patents

Vanadium-containing Heterocyclic Compounds and Preparation of 1,1'-Binaphthols by Oxidative Coupling of 2-Naphthols Using Them as Catalysts, S. Takizawa, H. Sasai, T. Katayama, JP2008-063250.

Synthetic Method of Epoxides, J. Ichihara, JP2008-162155.

Solid-phase Oxidation Reaction System, J. Ichihara, S. Yamaguchi, WO 2008/093711.

International Conferences

Catalytic Enantioselective Synthesis of Spiro lactams via an Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, H. Sasai: Third International Conference on Advanced Organic Synthesis Directed toward the Ultimate Efficiency and Practicability, Shiga, Japan, May 26-27, 2008.

Novel Enantioselective Reactions Catalyzed by Palladium(II)-Spiro Bis(isoxazoline) Complex (poster), *H. Sasai, S. Takizawa, K. Takenaka, T. Tsujihara, R. N. Nadaf, G. B. Bajracharya, P. S. Koranne, K. Onitsuka: International Symposium on Homogeneous Catalysis (ISHC-16), Florence, Italy, July 6-11, 2008.

Chiral Dinuclear Vanadium(V) Catalyst for Dual Activation of 2-Naphthols in Oxidative

Couplings, *H. Sasai, S. Takizawa, T. Katayama: 6th International Vanadium Symposium, Lisbon, Portugal, July 17-19, 2008.

Enantioselective Synthesis of Spiro lactams via the Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, H. Sasai: The First International Symposium on Process Chemistry (ISPC 08), Kyoto, Japan, July 28-30, 2008.

Novel Catalytic Enantioselective Reactions Promoted by a Pd-SPRIX Complex (invited), *H. Sasai: 3rd International Conference on Cutting-Edge Organic Chemistry in Asia, Hangzhou, China, October 19-23, 2008.

Novel Catalytic Enantioselective Reactions Promoted by Palladium(II)-Spiro Bis(isoxazoline) Complex (invited), *H. Sasai: 11th International Symposium on Natural Product Chemistry, Karachi, Pakistan, October 29-November 1, 2008.

Enantioselective Synthesis of Spiro lactams via the Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, K. Sugimoto, H. Sasai: UK/Japan Joint Symposium on Asymmetric Catalysis, Kyoto, Japan, December 8-9, 2008.

Novel Catalytic Enantioselective Reactions Promoted by Pd-SPRIX Complexes (invited), *H. Sasai: UK/Japan Joint Symposium on Asymmetric Catalysis, Kyoto, Japan, December 8-9, 2008.

Iridium-catalyzed Oxidative Dimerization, Tishchenko Reaction and Oxidative Desymmetrization (poster), *T. Suzuki, G. Kazem, N. K. Mangu, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Novel Enantioselective Reactions Catalyzed by Palladium(II)-Spiro Bis(isoxazoline) Complex (poster), T. Tsujihara, G. B. Bajracharya, P. S. Koranne, R. N. Nadaf, *K. Takenaka, S. Takizawa, K. Onitsuka, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Enantioselective Synthesis of Spiro lactams via the Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, K. Sugimoto, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Development of Dinuclear Vanadium Catalysts and Acid-Base Organocatalysts for Enantioselective Reactions via Dual Activation Mechanism (poster), *S. Takizawa, K. Matsui, T. Katayama, N. Inoue, D. Rajesh, S. Hirata, K. Kiriya, T. Suzuki, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

An Eco-Process; Selective Oxidation of Sulfide (poster), *J. Ichihara, K. Sakamoto, I. Fujihara: 2nd International Symposium on the Manipulation of Advanced Smart Materials (ISMASM2008), Hyogo, Japan, May 28-29, 2008.

Oxidative Dehydration of Terpene by Eco-Process (poster), *J. Ichihara: 2nd International Symposium on the Manipulation of Advanced Smart Materials (ISMASM2008), Hyogo, Japan, May 28-29, 2008.

Publications in Domestic Meetings

Annual Meeting of The Chemical Society of Japan	12 papers
Symposium on Organic Reaction	2 papers
Symposium on Organometallic Chemistry	2 papers
Symposium on Organic Synthesis	1 paper
Annual Meeting of The Pharmaceutical Society of Japan	1 paper
Conference on Combinatorial Chemistry	1 paper
Symposium on Molecular Chirality	1 paper

Academic Degrees

Doctor Degree for Science

T. Tsujihara	Catalytic Oxidative Cyclization Utilizing Chiral Spiro Bis(isoxazoline) Ligand
Rashid Nabisaheb Nadaf	The Realization of Copper Catalyzed Enzymatic Reactions and Palladium Catalyzed 5-Endo-Trig Type Cyclizations

Master Degree for Science

N. Itoh	Enantioselective Synthesis of Chiral Spirobilactams via Pd-Catalyzed N-Arylation
K. Kiriyaama	Development of Novel Acid-Base Organocatalysts
K. Tanaka	Development of Novel Quaternary Ammonium Salts Based on a Chiral Spiro Framework
Y. Tanigaki	Development of Novel Asymmetric Intramolecular Wacker-type Cyclization Utilizing Pd-SPRIX
T. Nagano	Asymmetric Synthesis of Chiral Spiro-type Ligands

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

H. Sasai	Development of Chiral Organocatalyst with Synergistic Effect	¥2,300,000
K. Onitsuka	Synthesis and Properties of Hybrid-type of Organometallic Conjugated Polymers	¥1,400,000
K. Onitsuka	Development of Enantioselective Reactions Catalyzed by Planar-Chiral Organometallic Complexes	¥1,900,000

Other Research Fund

H. Sasai	Meiji Kaisha	¥1,000,000
H. Sasai	Daiso Co.	¥1,200,000

H. Sasai	Nissan Chemical Industries		¥400,000
H. Sasai	Nagase ChemteX Co.		¥1,000,000
K. Onitsuka	Iketani Science and Technology Foundation	Development of Enantioselective Reactions Catalyzed by Planar-Chiral Ruthenium Complexes	¥1,500,000
S. Takizawa	The Ogasawara Foundation for the Promotion of Science & Engineering	Development and Application of Immobilized Chiral Catalyst with Dual Activation Mechanism	¥3,000,000
J. Ichihara	Kyodo Printing Co.		¥800,000
J. Ichihara	Adeka Co.		¥600,000

Division of Intelligent Systems Science

Outline

The advent of the digital society where tremendous amount of information is electronically accessible has brought the intelligent information processing technologies indispensable. This division, consisting of four departments, challenges the task of computerizing the intelligent human information processing capability to help solve difficult engineering problems and assist intellectual activities. The major research targets include ontology engineering and knowledge reuse/sharing (Knowledge Systems Dept.), use of multi-dimensional information sources and their multi-purpose processing (Intelligent Media Dept.), human-computer interfaces and agents (Architecture for Intelligence Dept.) and data mining, knowledge discovery and machine learning (Reasoning for Intelligence Dept.). While pursuing its own research target, each department works closely together to similar problems from different perspectives. The division as a whole collaborates with other divisions in the institute by providing the tools we have developed to help them solve their problems and also is benefited by the feedback to open up new research frontiers.

Achievement

- Enhancement of theory of role and distributed ontology development environment
- Systematization of functional knowledge using ontological engineering and its deployment
- Release of OMNIBUS: Ontology of learning/instructional theories and theory- and standards-aware authoring system
- Development of clinical ontology, sustainability science ontology and upper ontology
- Development of a theory-aware authoring tool for collaborative learning and meta-cognitive skill modeling
- Development and evaluation of a task-oriented mobile service navigation
- Creation of novel sensors
- 3D modeling and visualization
- Medical image analysis
- Omnidirectional surveillance system and human behavior analysis
- Predicate Invention
- Introducing sensors to constructive adaptive user interfaces
- Adaptive agents
- Adaptive Intelligent Tutoring Systems
- Web summarization
- Construction of sensor networks
- Knowledge discovery from extremely high dimensional dynamics data
- Development of basic principles to derive large scale and frequent substructure co-occurrences
- Development of basic principle to derive frequent graph sequences
- Knowledge discovery from large scale similarity data
- Development of OLAP database technique for event sequences

Department of Knowledge Systems

Professor:	Riichiro MIZOGUCHI
Associate Professor:	Yoshinobu KITAMURA
Assistant Professor:	Munehiko SASAJIMA
Specially Appointed	
Assistant Professors:	Yusuke HAYASHI, Hiroko KOU, Jun ZHOU
Graduate Students:	Shinya TARUMI, Seiji ISOTANI, Mamoru OHTA, Satoshi ENDO, Koichiro FURUTANI, Kohei SUMITA, Sho SEGAWA, Takeru HIROTA
Research Student:	Meng SHUAI
Under Graduate Students:	Jun NAKAYAMADA, Shunsaku SATO, Satoshi NISHIMURA
Supporting Staff:	Naomi BANO

Outlines

Information science has developed into knowledge science which is expected to play critical roles in the advanced information processing in this new century. In the real world, tiny computers of the higher performance have been used by ordinary people in their homes where they also enjoy access to vast amount of information sources scattered all over the world thanks to the internet. In academic society, on the other hand, the research on artificial intelligence is changing from building stand-alone machines which try to solve problems by themselves to building intelligent partners which augment human capability of problem solving. This division has been run under the philosophy that it contributes not only to the promotion of knowledge science but also to prosperity of the real world by the feedback of the research results to it in the information era. The major topic here is to investigate Ontological Engineering to establish basic theories and technologies for the next-generation knowledge science. The current research projects include: methodology for ontology development and its support environment based on basic theories of ontological engineering, creative design work bench and advanced diagnostic systems based on knowledge systematization, knowledge sharing and reuse, intelligent educational/training systems, and ontology-aware authoring systems.

Current Research Project

1. Ontology: Theoretical Foundation of Knowledge Engineering

The research on knowledge-based systems aims at making computer systems more intelligent by mimicking intellectual capability of human. The key to achievement of this goal is the fluent knowledge-level communication between humans and computers. The current state of the art of knowledge engineering, however, has not been matured enough to realize it. Considerable amount of meaning of the concepts in human mind is lost in most of the existing knowledge-based systems. This is the major cause of the difficulty of knowledge reuse and sharing and the too strict behavior of the systems for users to feel comfortable. Thus, new theoretical foundation for knowledge engineering

is badly needed in knowledge engineering fields. The research on ontology engineering is one of the most promising approaches to establishment of the foundation. We theorized about the fundamental issues on ontology from both scientific and engineering viewpoints. As a result, we published three enlightening papers which describe drawbacks of the current research, importance of ontological engineering, definitions of an ontology, its functions and roles, its classification and research topics. We further published some research results based on ontological engineering to show concrete examples of a new research direction. One of the most remarkable achievements is a book on “Ontological Engineering” has been published from Ohm-sha Ltd. In January, 2005 which is the first book on the topic in Japan. HOZO, an environment for ontology building/utilization, has been augmented to make it a usable tool by revising its GUI and reimplementation of some functions. It has been extended to cope with distributed development of a large ontology and to improve the compliance with the WWW standards. In 2007, we developed a mapping tool for enabling viewpoint-specific overview of ontologies to help domain experts better understand the target world across domains. We have started building comprehensive ontologies for medicine and genomics in the collaboration with experts of the respective domains. Concerning theoretical issues, further refinement of Role theory and reconsideration on the ontological theory of objects, processes and events have been done aiming at fundamental contribution of ontology theory. We have started research on an innovative theory of roles by employing the notion of meta-role and on a new theory of parts based on the in-depth analyses of roles. In addition, we released an upper ontology named YATO, which we have been investigating for years, on the home page of HOZO.

2. Systematization of Functional Design Knowledge

In the engineering domain, the importance of knowledge sharing among designers has been widely recognized. Although advancement of computer technologies has enabled easy access to objective information such as structural information using CAD without designer's intention, it is difficult to share conceptual engineering knowledge about functionality that can represent designer's intention so-called design rationales, because there is neither rich common vocabulary for representing functionality of devices nor well-established ontological commitment for capturing such knowledge. The main goal of this research is to promote sharing of the conceptual engineering knowledge about functionality by providing a conceptual framework enabling systematic description of the functional knowledge. We have developed an ontological framework for its modeling including layered ontologies, which provides rich concepts for describing consistent and reusable knowledge. The framework has been deployed successfully in a manufacturing company. Moreover, based on extensions of the ontological framework, a semantic search system for technical documents has been developed and integration of fault knowledge has been realized. In 2008, we developed the two-way mappings between functional taxonomies based on a reference ontology of function and then extensively analyzed the mapping results. The interoperability of functional meta-data has been realized based on the mappings. Next, aiming at clearer understanding of the notion of function, we investigated ontological distinctions of function and then developed a macroscopic temporal model of function in a product life-cycle. Furthermore, we developed a functional knowledge externalization and sharing tool named OntoGear based on an advanced XML technology in the collaborative research

with the Materials Science and Technology Research Center. Especially, semi-automatic extraction of fault knowledge from text data has been investigated and implemented.

3. Methodology for Building Learning Support Systems

The goal of research on intelligent educational systems is to implement the intellectual capability of human teachers on computer systems. Huge efforts have been devoted to the research for the last two decades. However, the research field has not been growing methodologically because of lack of theoretical foundation. Ontology is expected to be a firm basis for knowledge engineering, on top of which we can accumulate our knowledge about the principled methodologies to build sharable and reusable knowledge bases. Especially, task ontology, which captures the inherent conceptual structure of problem solving, works as a bridge to fill the conceptual gap between humans and computers during the process of building and using knowledge-based systems. It keeps up the correspondence between the conceptual structure in human mind and the functional structure of knowledge-based systems. In this research project, we have investigated the essential structure of a variety of educational tasks in detail and built educational task ontology. Furthermore, with the aid of the task ontology built, we have developed a sophisticated authoring tool (intelligent educational system development environment) for substation operator training. The recent results include a proposal of Ontology-Awareness aiming at marriage of learning and educational theories and technology. Based on the proposal, we have realized an ontology-aware authoring environment. We have developed authoring task ontology and an architecture of an evolving authoring tool based on the task ontology together with an authoring system for the collaborative learning and an innovative model of meta-cognitive skills with a framework based on the model. The latest achievements include the following; 1) update of a learning and instructional theory ontology named OMNIBUS and analysis the existing learning/instructional theories in order to consider the functionalities for promoting a better understanding of them, 2) association of OMNIBUS and a comprehensive ontology of Education of Informatics in high school and development of a prototype of theoretical analysis system of learning contents, 3) development of group formation support system based on investigation of the effectiveness of our collaborative learning theory ontology and 4) analysis of debating based on our innovative model of meta-cognitive skills and a proposal of debating support method whose effectiveness is investigated through its practical use.

4. Task Ontology-based Framework for Mobile Internet Services

We can get many kinds of mobile services via mobile handsets today. On the other hand, a large number of services cause difficulties in searching, finding and selecting suitable services for consumer's needs. Users have to learn the menu system to access the services; hierarchical structure of the menu, relation between name of the category and services in the category. To solve this problem this project aims at realization of task-oriented menu which is more efficient for retrieving information. By task, we mean users' problem solving activity in the real world. In the task oriented menu, the users seek for services by the name of the directory which represents a task they are involved in rather than the name of category which might be unfamiliar to them. Users select a menu that is most resemble to what they want to do; "get on the train", "draw cash", for example. It has potential of providing useful information for mobile service users

quicker than that of a domain-oriented menu today. Value of information depends on the quality of contextual information that contains. You seek for information when you face a trouble, which is difficult to get over with knowledge at hand, on your way of achieving a task. Such a situation is the context and origin of the necessity for the information. In this research project, we have been developing a task ontology-based modeling framework for mobile service navigation. We applied our modeling framework for prototyping a task-oriented menu system with real-scale mobile internet services. With the prototype software, we carried out the first experiment in the real field to find that our method works even with real scale; especially effective for novice mobile users.

Publications

Original Papers

Technical Knowledge Management Platform Based on Ontology Engineering and XML Technology-Embodiment of Foundation of Externalization, Sharing, and Co-creation Support of Functional Knowledge of Artifacts-, Sunao Takafuji, Yoshinobu Kitamura, Riichiro Mizoguchi: Journal of the Japanese Society for Artificial Intelligence, 23 (6) (2008) 424-436.

Obstacles Reveal the Needs of Mobile Internet Services -OOPS:Ontology-Based Obstacle, Prevention And Solution Modeling Framework-, Munehiko Sasajima, Yoshinobu Kitamura, Takefumi Naganuma, Kunihiro Fujii, Shoji Kurakake and Riichiro Mizoguchi: Journal of Web Engineering, 7 (2) (2008) 133-157.

Toward Task-oriented Mobile Internet Service Navigation - Ontology-based User Modeling Method with Obstacles in Daily Life -, Munehiko Sasajima, Yoshinobu Kitamura, Takefumi Naganuma, Shoji Kurakake, Riichiro Mizoguchi: Journal of Japan Society for Fuzzy Theory and Intelligent Informatics, 20 (2) (2008) 171-189.

A Framework of Difficulty in Metacognitive Activity, Michiko Kayashima, Akiko Inaba, Riichiro Mizoguchi: Transaction of Japanese Society of Information and Systems in Education, 25 (1) (2008) 19-31.

Research Directions on Semantic Web and Education, Ig Ibert Bittencourt, Seiji Isotani, Evandro Costa and Riichiro Mizoguchi: Journal Scientia - Interdisciplinary Studies in Computer Science, 19 (1) (2008) 59-66.

Toward Knowledge Structuring of Sustainability Science Based on Ontology Engineering, Terukazu Kumazawa, Osamu Saito, Kouji Kozaki, Takanori Matsui and Riichiro Mizoguchi: Sustainability Science, 4 (1) (2009) 99-116.

An Ontology-based Framework and Its Application to Effective Collaboration, Seiji Isotani and Riichiro Mizoguchi: CLEI electronic Journal, 11 (1) (2008) 1-9.

Review Papers

Overview of Academic Roadmap on Robotics, Tomomasa Sato, Riichiro Mizoguchi,

Yutaka Tomita and Takashi Uchiyama, Journal of the Robotics Society of Japan, Vol. 26 No. 7(2008) 722-727

Resources for Building and Applying Ontologies (My Bookmark), Munehiko Sasajima, Journal of Japanese Society for Artificial Intelligence, Vol.23(4) (2008) 572-576

Books

A Device-oriented Definition of Functions of Artifacts and Its Perspectives, Yoshinobu Kitamura, Riichiro Mizoguchi, Functions in Biological and Artificial Worlds: Comparative Philosophical Perspectives, Ulrich Krohs, Peter Kroes (eds.), MIT Press, (2009).

International Conferences

Semantics of the Integrated BioMedical Database Project -A Japanese National Project-, Jun Nakaya, Saburo Sakota, Riichiro Mizoguchi, Kouji Kozaki, Kaei Hiroi, Keisuke Ido, Michio Kimura, Hiroshi Tanaka: 9th International HL7 Interoperability Conference (IHIC2008), Crere, Greece, Oct.8-11, (2008).

Multi-Entry System for Supporting Teachers in Designing Instruction, Toshinobu Kasai, Kazuo Nagano and Riichiro Mizoguchi: 16th International Conference of Computers in Education (ICCE'08), Taipei, Taiwan, Nov. 27-31, (2008) 79-86.

Toward Accumulation of Learning/Instructional Design Knowledge for Authoring Systems, Yusuke Hayashi, Jacqueline Bourdeau and Riichiro Mizoguchi: 16th International Conference of Computers in Education (ICCE'08), Taipei, Taiwan, Nov. 27-31, (2008) 19-26.

Adventure in the Boundary between Domain-Independent Ontologies and Domain-Specific Content for CSCL, Seiji Isotani and Riichiro Mizoguchi: 12th International Conference on Knowledge-Based and Intelligent Information & Engineering Systems (KES'08), Zagreb, Croatia, Sep. 3-5, (2008) 523-532.

Theory-Driven Group Formation through Ontologies, Seiji Isotani and Riichiro Mizoguchi: 9th International Conference on Intelligent Tutoring Systems (ITS'08), Montreal, Canada, June 23-27, (2008) 646-655.

Structurization of Learning/Instructional Design Knowledge for Theory-aware Authoring systems, Yusuke Hayashi, Jacqueline Bourdeau and Riichiro Mizoguchi: 9th International Conference on Intelligent Tutoring Systems (ITS'08), Montreal, Canada, June 23-27, (2008) 573-582.

Toward Establishing an Ontological Structure for the Accumulation of Learning/Instructional Design Knowledge, Yusuke Hayashi, Jacqueline Bourdeau and Riichiro Mizoguchi: 6th International Workshop on Ontologies and Semantic Web for E-Learning (SWEL'08), Montreal, Canada, June 22, (2008) 1-10.

Yet Another Top-level Ontology: YATO, Riichiro Mizoguchi: Second Interdisciplinary

Ontology Meeting, Tokyo, Japan, February 28 - March 1, (2009) 91-101.

Toward Integration of Mouse Phenotype Information, Hiroshi Masuya and Riichiro Mizoguchi: Second Interdisciplinary Ontology Meeting, Tokyo , Japan , February 28 - March 1, (2009) 35-44.

Understanding Semantic Web Applications, Kouji Kozaki, Yusuke Hayashi, Munehiko Sasajima, Shinya Tarumi and Riichiro Mizoguchi: 3rd Asian Semantic Web Conference (ASWC 2008), LNCS 5367, Bangkok, Thailand, February 2-5, (2009) 524-539,.

Instance Management Problems in the Role Model of Hozo, Kouji Kozaki, Satoshi Endo and Riichiro Mizoguchi: 10th Pacific Rim International Conference on Artificial Intelligence (PRICAI-08), LNAI 5351, Hanoi, Vietnam, December 15-19, (2008) 614-625.

Deep Semantic Mapping between Functional Taxonomies for Interoperable Semantic Search, Yoshinobu Kitamura, Sho Segawa, Munehiko Sasajima, Shinya Tarumi and Riichiro Mizoguchi: 3rd Asian Semantic Web Conference (ASWC 2008), LNCS 5367, Bangkok, Thailand, February 2-5, (2009) 137-151.

Prototyping of Task-Oriented Mobile Navigation System with Real Scale Mobile Services, Munehiko Sasajima, Koichiro Furutani, Yoshinobu Kitamura, Takefumi Naganuma, Shoji Kurakake and Riichiro Mizoguchi,: Advances in Computer Science and Engineering (ACSE 2009), Phuket, Thailand, Mar.16-18,(2009) 205-210.

Knowledge Structuring Process of Sustainability Science based on Ontology Engineering, Terukazu Kumazawa, Takanori Matsui, Keishiro Hara, Michinori Uwasu, Yohei Yamaguchi, Yugo Yamamoto, Kouji Kozaki, Osamu Saito and Riichiro Mizoguchi: 8th International Conference on Eco Balance, Tokyo, Japan, December 10-12, (2008).

Knowledge Structuring Tool for Sustainability Science Based on Ontology Engineering, Terukazu Kumazawa, Osamu Saito, Kouji Kozaki, Takanori Matsui and Riichiro Mizoguchi: 1st International Workshop on Intelligent Systems for Environmental (Knowledge) Engineering and EcoInformatics (i-SEEK' 09) , Fukuoka, Japan, March 16-19, (2009) 1138-1143.

Knowledge Structuring and an Exploration System for Global Sustainability and its Application to the Biofuel Issue, Osamu Saito, Kouji Kozaki, Takeru Hirota, Riichiro Mizoguchi: Climate Change: Global Risks, Challenges and Decisions, Copenhagen, Denmark, March 10-12, (2009).

Towards a Reference Model to Semantic Web-based Educational Systems, Ig Ibert Bittencourt, Evandro Costa, Seiji Isotani, Riichiro Mizoguchi, Ibsen Mateus Bittencourt: Workshop on Semantic Web and Education, Fortaleza, Brazil, November 12-14, (2008) 1-10.

HOZO: An ontology building environment (poster), Riichiro Mizoguchi and Kouji Kozaki: Demonstrations Program of 9th International Conference of Intelligent Tutoring Systems (ITS'08), Motreal, Canada, June 23-27, (2008) 35-36.

Tying Ontologies to Domain Contents for CSCL (poster), Seiji Isotani and Riichiro Mizoguchi: 9th International Conference on Intelligent Tutoring Systems (ITS'08), Montreal, Canada, June 23-27, (2008) 752-754.

CHOCOLATO: A Concrete and Hepful Ontology-Aware Collaborative Learning Authoring Tool (poster), Seiji Isotani and Riichiro Mizoguchi: Demonstrations Program of 9th International Conference of Intelligent Tutoring Systems (ITS'08), Montreal, Canada, June 23-27, (2008) 21-24.

SMARTIES: a Theory-aware and Standard-compliant Authoring System (poster), Yusuke Hayashi, Jacqueline Bourdeau and Riichiro Mizoguchi: Demonstrations Program of 9th International Conference of Intelligent Tutoring Systems (ITS'08), Montreal, Canada, June 23-27, (2008), 65-67.

Development of a Conceptual Map Generation Tool for Exploring Ontologies (poster), Kouji Kozaki, Takeru Hirota and Riichiro Mizoguchi: Poster Noets of the 5th European Semantic Web Conference (ESWC 2008), Tenerife, Spain, Jun. 1-5th, (2008).

Divergent Exploration of an Ontology (poster), Takeru Hirota, Kouji Kozaki and Riichiro Mizoguchi: Poster & Demo Notes of the 7th International Semantic Web Conference (ISWC 2008), Karlsruhe, Germany, October 26-30, (2008).

Contributions to International Conferences and Journals

R. Mizoguchi	Semantic Web Science Association (Vice-president)
R. Mizoguchi	International Journal of Web Semantics (Editors-in-Chief)
R. Mizoguchi	International Artificial Intelligence in Education Society (Executive Committee)
R. Mizoguchi	Asia-Pacific Society for Computers in Education(APSCE) (Board member)
R. Mizoguchi	The 16 th International Conference on Computers in Education (ICCE2008) Conf. on AIED/ITS & Adaptive Learning (Program Co-Chair)
R. Mizoguchi	The Tenth Pacific Rim International Conference on Artificial Intelligence (PRICAI-08) (PC Vice-Chair)
R. Mizoguchi	The 3 rd European Conference on Technology Enhanced Learning (EC-TEL 2008) (PC member)
R. Mizoguchi	The 9 th International Conference on Intelligent Tutoring System (ITS2008) (PC member)
R. Mizoguchi	The 9 th International Conference on Intelligent Tutoring System (ITS2008) (Panel Chair)
R. Mizoguchi	The 5 th European Semantic Web Conference (ESWC2008) (PC member)

R. Mizoguchi	The 2008 IEEE International Conference on Information Reuse and Integration (IEEE IRI-08) (PC member)
R. Mizoguchi	The 17 th International World Wide Web Conference Semantic Web Track (PC Chair)
R. Mizoguchi	ODBASE 08 : Intl. Conf. on Ontologies, DataBases, and Applications of Semantics (PC member)
R. Mizoguchi	The 3 rd Asian Semantic Web Conference (ASWC2008) (PC member)
R. Mizoguchi	The 7 th international semantic web conference (ISWC2008) (Vice Chair)
R. Mizoguchi	EKAUW 2008 - 16th International Conference on Knowledge Engineering and Knowledge Management Knowledge Patterns (PC member)
R. Mizoguchi	Formal Ontologies Meet Industry: FOMI 2008 (PC member)
R. Mizoguchi	IIP2008 - 5th International Conference on Intelligent Information Processing (PC member)
R. Mizoguchi	14th Collaboration Researchers' International Workshop on Groupware (PC member)
R. Mizoguchi	The 6 th International Workshop on Applications of Semantic Web Technologies for E-Learning (SWEL'08) (Workshop Organizers)
R. Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
R. Mizoguchi	International Journal of Applied Ontology (Editorial board)
R. Mizoguchi	Research and Practice in Technology Enhanced Learning (Editorial board)
R. Mizoguchi	International Journal of Artificial Intelligence in Education (Editorial board)
R. Mizoguchi	Frontiers in AI and Application (Editorial board)
R. Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)
R. Mizoguchi	Asian Semantic Web Conference (Steering committee chair)
Y. Kitamura	The 3 rd Asian Semantic Web Conference (ASWC2008) (PC member)
Y. Kitamura	International Journal of Advanced Engineering Informatics (Editorial board)
Y. Hayashi	The 16 th International Conference on Computers in Education (ICCE2008) Conf. on AIED/ITS & Adaptive Learning (PC member)
Y. Hayashi	The 16 th International Conference on Computers in Education (ICCE2008) Conf. on Advanced Learning Technologies, Open Contents, & Standards (PC member)
Y. Hayashi	The 7 th International Conference on Practical Aspects of Knowledge Management (PAKM2008) (PC member)
Y. Hayashi	The 1st International Workshop on Distributed Knowledge

M. Sasajima	Management (DKM 2008) (PC member) The 5 th International Conference on Autonomic and Autonomous Systems(ICAS 2009) (PC member)
M.Sasajima	International conference on Internet and Multimedia Systems and Applications (IMSA 2009) (PC member)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	18 papers
The institute of Electronics, information and communication engineers	1 paper
Japanese Society for the Science of Design	1 paper
Japan Society of Mechanical Engineers	1 paper
Japanese Society for Information and Systems in Education	1 paper
Japanese Society for Educational Technology	1 paper
Japanese Association for Medical Informatics	1 paper

Academic Degrees

Master Degree in Engineering

S. Endo	Consideration of Role Theory and Identity in Instance Management Problem
K. Furutani	Development and Evaluation of Task-oriented Menu System with Real Scale Mobile Internet Services

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

R. Mizoguchi	Technical documents integration based on an artifact ontology	¥5,000,000
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Grant-in-Aid for Scientific Research (A)

R. Mizoguchi	Building a Theory-aware and Standard-compliant Knowledge Server	¥15,340,000
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Grant-in-Aid for Young Scientists (B)

M. Sasajima	Research on modeling users' daily activities for improvement of mobile internet services	¥1,430,000
Y. Hayashi	Building a practical-knowledge repository for good circulation of knowledge between theory and practice in learning contents design	¥1,430,000

Entrusted Research

R. Mizoguchi	The University of Tokyo	Research on development of a medical knowledge database for medical information systems; Design of a semantic relational model	¥15,000,000
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R. Mizoguchi	The University of Tokyo	Biofuel Use Strategies for Sustainable Development; Restructuring problems of biofuel use by using Ontology and developing policy-making supporting tools.	¥2,401,000
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Donation

R. Mizoguchi	Justsystem Corporation		¥2,500,000
R. Mizoguchi	Y.M.P-International Corporation		¥650,000
R. Mizoguchi	Niigata Machine Techno Co., Ltd.		¥650,000
R. Mizoguchi	Y.M.P-International Corporation		¥650,000
R. Mizoguchi	Okidata Corporation		¥1,000,000

Cooperative Research

R. Mizoguchi	NTT DoCoMo, Inc.	Research on an ontology for users in mobile environment to understand the real world context	¥3,000,000
R. Mizoguchi	Justsystem Corporation	Information sharing for safety-first manufacturing based on the unification of ontological engineering and natural language processing	¥20,000,000
R. Mizoguchi	Idemitsu Kosan Co., Ltd.	Development of knowledge base systems for nano-materials	¥3,300,000
R. Mizoguchi	TOYOTA Info Technology Center Co., Ltd.	Research on ontological techniques for automobiles	¥3,000,000

Department of Intelligent Media

Professor: Yasushi YAGI
Associate Professor: Yasuhiro MUKAIGAWA
Assistant Professor: Ryusuke SAGAWA, Yasushi MAKIHARA
Postdoctoral Researcher: Junqiu WANG, Md. Altab HOSSAIN, Kazuaki KONDO,
Chunsheng HUA
Graduate Students: Nobuya AOKI, Hai VU, Hidetoshi MANNAMI,
Ngo Thanh TRUNG, Takashi ANEZAKI,
Kazushige SUGIURA, Haruka AZUMA,
Kiyotaka AKASAKA, Akira TUJI,
Seiichi TAGAWA, Nguyen Da TAN, Yuya OHTA,
Yusuke NISHIDE, Atsushi MORI
Under Graduate Students: Mayu OKUMURA, Yoko BABA, Seiichiro KABASHIMA,
Tomoya TAKEUCHI
Research Student (FrontiaLab@OsakaU): Xiang XIANG(2008.10.1-2009.2.16)

Outlines

The studies in this laboratory focus on computer vision and media processing including basic technologies such as sensor design and camera calibration, and applications such as an intelligent system with visual processing functions. Some of our major research projects are development of a novel vision sensor, including an omnidirectional mirror, calibration of an omnidirectional vision system, video analysis for endoscopic diagnosis assistance, measurement of detailed reflectance properties, gait identification, modeling of environments.

Current Research Project

Video Capsule Endoscopy Analysis For Diagnostic Assistance

Video capsule endoscopy (VCE) represents a significant advance in examinations of digestive diseases by providing a non-invasive method to view the small bowel. In addition, VCE provides a valuable source for visualizing the intestinal contractions, which are mainly events for intestinal motility assessment. However, the advantages of VCE diagnosis technique are facing with the time consuming for reading video sequence as well as challenging to detect the intestinal contractions. In this thesis, computer-assisted applications are motivated from these drawbacks through techniques of VCE analysis.

Because of non-scene, non-object characteristics of VCE, and natural movement of the capsule device, VCE interpretations could be implemented by analyzing spatial and temporal features. First, several image features such as color, edges, and motion displacement are extracted. Then their temporal analyses are presented in several ways to adapt with different tasks. Two applications utilizing this framework are developed. In the first application, we propose a new method to reduce diagnostic time under the constraint that all original images should be displayed to an examining doctor without skipping frames. To realize such a system, delay time for drawing images between

frames is controlled in adaptive rate, according to the states of capturing images. Several techniques for the state classification, delay time calculation, and log-based analysis are deployed in this application. In the second application, we develop a three-stage procedure for the intestinal contraction detections. Based on the characteristics of contractile patterns, the possible contractions can be investigated using essential images features extracted from VCE such as changes in edge of the intestinal folds and by evaluating similarities features in consecutive frames. Then true contractions are determined through spatial analysis of directional information. To exclude as many non-contractions as possible, we consider about information of contractions frequencies along capsule transit time. Both the quality and quantity indices are analyzed in experiments for performance evaluations.

Research on Adaptive Dynamic Range Camera with Liquid Crystal

Wide Dynamic Range Images (WDRIs) are needed for capturing scenes which include drastic lighting changes. This paper presents a method to widen the dynamic range of a camera by using a liquid crystal. The system consists of a camera and a reflective liquid crystal placed in front of the camera. By controlling the attenuation ratio of the liquid crystal, scene radiance of each pixel is controlled adaptively. After applying the control, the original scene radiance is derived from the attenuation ratio of the liquid crystal and the radiance obtained by the camera. We have implemented a prototype system and conducted experiments in a scene that includes drastic lighting changes. We confirmed that the radiance of each pixel could be independently controlled, and that WDRIs could be obtained by calculating the original scene radiance from these results.

Gait Identification based on Multi-view Matching using an Omnidirectional Camera and View Transformation Models

Gait identification is a promising method of individual identification at a distance from a camera, and it is known that a performance is improved integrating multi-view gait features. However, the improvement can not be hoped for when an overlapped view range between a gallery and a probe sequence is narrow. So, we propose a method of gait identification based on multi-view matching using an omnidirectional camera and a View Transformation Model (VTM). Gait sequences contain changes of observed tilt and azimuth views provided by an omnidirectional, and a range of observed azimuth view change is much wider than that of observed tilt view change. So, an appropriate VTM considering each view changes are decided for observed tilt and azimuth views transformation. First, we apply perspective projection of sagittal plane for the tilt transformation, and create gait silhouette images which are normalized in 0 degree. Then, observed azimuth view is transformed based on a factorization method, and missing-view gait features for each gallery and probe sequence is synthesized in matching phase. Experiments of gait identification including 22 subjects from different view ranges demonstrate the effectiveness of the proposed method.

Spatio-Temporal Lifelog Using a Wearable Compound Omnidirectional Sensor

In this paper, we propose a spatio-temporal lifelog, that enables us intuitively to understand both the spatial and temporal aspects of a situation. We have designed a new wearable compound omnidirectional sensor comprising a hyperboloidal mirror and multiple paraboloidal mirrors. Using this sensor, visual information is recorded in all

directions around the user. Objects are classified as foreground or background according to their distance. The stored log can be viewed using a browser that supports two different views, a spatial view and temporal view, which allow an effective visualization of the situation based on the classification. The user can switch between views depending on the purpose.

A Sensor for Simultaneously Capturing Texture and Shape by Projecting Structured Infrared Light

Simultaneous capture of the texture and shape of a moving object in real time is expected to be applicable to various fields including virtual reality and object recognition. Two difficulties must be overcome to develop a sensor able to achieve this feature: fast capturing of shape and the simultaneous capture of texture and shape. One-shot capturing methods based on projecting colored structured lights have already been proposed to obtain shape at a high frame rate. However, since these methods used visible lights, it is impossible to capture texture and shape simultaneously. In this paper, we propose a method that uses projected infrared structured light. Since the proposed method uses visible light for texture and infrared light for shape, simultaneous capturing can be achieved. In addition, a system was developed that maps texture on to the captured shape without occlusion by placing the cameras for visible and infrared lights coaxially.

Silhouette Transformation based on Walking Speed for Gait Identification

We propose a method of gait silhouette transformation from one speed to another to cope with walking speed changes in gait identification. Firstly, static and dynamic features are divided from gait silhouettes using a human model. Secondly, a speed transformation model is created using a training set of dynamic features for multiple persons on multiple speeds. This model can transform dynamic features from a reference speed to another arbitrary speed. Finally, silhouettes are restored by combining the divided static features and the transformed dynamic features. Evaluation by gait identification using frequency-domain features shows the effectiveness of the proposed method.

Publications

Original Papers

Omnidirectional Vision Attachment for Medical Endoscope, Takurou SAKAI, Ryusuke SAGAWA, Tomio ECHIGO, Keiko YAGI, Masatsugu SHIBA, Kazuhide HIGUCHI, Tetsuo ARAKAWA, Yasushi YAGI: IEICE Transactions on Information and Systems, J91-D (7) (2008) 1778-1787.

Gait Identification Based on Multi-view Observations Using Omnidirectional Camera, Kazushige Sugiura, Yasushi Makihara, Yasushi Yagi: IPSJ Transactions on Computer Vision and Image Media, 49 (2) (2008) 76-85.

Detection of Contractions in Adaptive Transit Time of the Small Bowel from Wireless Capsule Endoscopy Videos, H. Vu, T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, Y. Yagi: Computers in Biology and Medicine, 39 (1) (2009) 16-26.

Rapid BRDF Measurement using an Ellipsoidal Mirror and a Projector, Y.Mukaigawa, K.Sumino, Y.Yagi: IPSJ Transactions on Computer Vision and Applications, 1 (2009) 21-32.

Controlling the Display of Capsule Endoscopy Video for Diagnostic Assistance, H. Vu, T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, Y. Yagi: IEICE Transactions on Information and Systems, E92-D (3) (2009) 512-528.

International Conferences

Accurate Calibration of Intrinsic Camera Parameters by Observing Parallel Light Pairs, *Ryusuke Sagawa, Yasushi Yagi: 2008 IEEE International Conference on Robotics and Automation, Pasadena, California, May, 2008.

Robust and Real-Time Egomotion Estimation Using a Compound Omnidirectional Sensor, *Thanh Trung Ngo, Hajime Nagahara, Ryusuke Sagawa, Yasuhiro Mukaigawa, Masahiko Yachida, Yasushi Yagi: 2009 IEEE International Conference on Robotics and Automation, Pasadena, California, May, 2008.

Human Tracking and Segmentation Supported by Silhouette-based Gait Recognition, *Junqiu Wang, Yasushi Makihara, Yasushi Yagi: 2010 IEEE International Conference on Robotics and Automation, Pasadena, California, May, 2008.

Dynamic scene shape reconstruction using a single structured light pattern (poster), *H. Kawasaki, R. Furukawa, R. Sagawa, Y. Yagi: IEEE Conference on Computer Vision and Pattern Recognition, Anchorage, Alaska, USA, Jun., 2008.

3D Scanning Method for Fast Motion using Single Grid Pattern with Coarse-to-fine Technique (poster), *R. Furukawa, H. Kawasaki, R. Sagawa, Y. Yagi: British Machine Vision Conference 2008. Leeds, UK, Sep., 2008.

Free-form Mirror Designing based on Integrability of its Gradient Field (poster), *Kazuaki Kondo, Yasuhiro Mukaigawa, Yasushi Yagi: MIRU International Workshop on Computer Vision 2008, Karuizawa, Japan, Jul., 2008.

Analysis of Subsurface Scattering under Generic Illumination (poster), *Y.Mukaigawa, K.Suzuki, Y.Yagi: MIRU International Workshop on Computer Vision 2008, Karuizawa, Japan, Jul., 2008.

Free-Form Mirror Design Inspired by Photometric Stereo (poster), *Kazuaki Kondo, Yasuhiro Mukaigawa, Yasushi Yagi: the IEEE Workshop on OMNIVIS, Marseille, France, Oct. 2008.

Spatio-Temporal Lifelog Using a Wearable Compound Omnidirectional Sensor, *Haruka Azuma, Yasuhiro Mukaigawa, Yasushi Yagi: the IEEE Workshop on OMNIVIS, Marseille, France, Oct. 2008.

Omnidirectional Gait Identification by Tilt Normalization and Azimuth View Transformation, *Kazushige Sugiura, Yasushi Makihara, Yasushi Yagi: the IEEE Workshop on OMNIVIS, Marseille, France, Oct. 2008.

One-Shot Range Scanner Using Coplanarity Constraints (poster), *Ryo Furukawa, Huynh Quang Huy Viet, Hiroshi Kawasaki, Ryusuke Sagawa, Yasushi Yagi: IEEE Int'l. Conf. on Image Processing 2008, San Diego, California, USA, Oct., 2008.

Patch-based adaptive tracking using spatial and appearance information (poster), *Junqiu Wang, Yasushi Yagi: IEEE Int'l. Conf. on Image Processing 2008, San Diego, California, USA, Oct., 2008.

People Tracking and Segmentation Using Spatiotemporal Shape Constraints, Junqiu Wang, Yasushi Makihara, *Yasushi Yagi: 1st ACM International Workshop on Vision Networks for Behaviour Analysis, Vancouver, Canada, Oct., 2008.

Silhouette Extraction Based on Iterative Spatio-Temporal Local Color Transformation and Graph-Cut Segmentation, *Yasushi Makihara, Yasushi Yagi: the 19th Int. Conf. on Pattern Recognition, Tampa, Florida USA, Dec., 2008.

Clothes-Invariant Gait Identification Using Part-Based Adaptive Weight Control, *Md. Altab Hossain, Yasushi Makihara, Junqiu Wang, Yasushi Yagi: the 19th Int. Conf. on Pattern Recognition, Tampa, Florida USA, Dec., 2008.

Switching Local and Covariance Matching for Efficient Object Tracking, Junqiu Wang, *Yasushi Yagi: the 19th Int. Conf. on Pattern Recognition, Tampa, Florida USA, Dec., 2008.

Scale-Invariant Density-Based Clustering Initialization Algorithm and Its Application (poster), *Chunsheng Hua, Ryusuke Sagawa, Yasushi Yagi: the 19th Int. Conf. on Pattern Recognition, Tampa, Florida USA, Dec., 2008.

Analysis of Subsurface Scattering under Generic Illumination, *Yasuhiro Mukaigawa, Kazuya Suzuki, Yasushi Yagi: the 19th Int. Conf. on Pattern Recognition, Tampa, Florida USA, Dec., 2008.

Evaluating the Control of the Adaptive Display Rate for Video Capsule Endoscopy Diagnosis, *H. Vu, T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, Y. Yagi: the 2008 IEEE International Conference on Robotics and Biomimetics, Bangkok, Thailand, Feb., 2009.

Towards an Interpretation of Intestinal Motility Using Capsule Endoscopy Image Sequences (poster), *H. Vu, T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, Y. Yagi: the 2nd Pacific-Rim Symposium on Image and Video Technology, Tokyo, Japan, Jan., 2009.

Computer-Assisted Intestinal Contraction Detections In Small Bowel From Wireless

Capsule Endoscopy Image Sequence, *H. Vu, T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, Y. Yagi: the 2nd International Gastrointestinal Consensus Symposium (IGICS), Tokyo, Japan, Jan., 2009.

Image Stabilization Algorithm for Video with Large Image Fluctuation, *H.Yamada, M.Kimura, J.Ohmiya, J.Tagawa, T.N.Thanh, Y.Mukaigawa, Y.Yagi: IEEE International Conference on Consumer Electronics, Las Vegas, Nevada, USA, Jan., 2009.

Contributions to International Conferences and Journals

Y. Yagi	International Journal of Automation and Computing International Journal of Automation and Computing(Editorial Board Member)
Y. Yagi	Bentham Science Publishers. Ltd(Editorial Board Member)
Y. Yagi	IEEE Robotics and Automation Society ICRA2008(Editorial Board Member)
Y. Yagi	IEEE Computer Society CVPR2008(Program Committee Member)
Y. Yagi	OMNIVIS '2008(Program Committee Member)
Y. Yagi	IPSJ Trans. on Computer Vision and Applications(Associate Editor in Chief)
Y. Yagi	Workshop on Omnidirectional Robot Vision(Program Committee Member)
Y. Yagi	IEEE Robotics and Automation Society ICRA2009(Technical Visit Chair)
Y. Yagi	IEEE Robotics and Automation Society ICRA2009(Editorial Board Member)
Y. Yagi	IEEE Computer Society CVPR2009(Program Committee Member)
Y. Mukaigawa	The 19th Int'l Conference on Pattern Recognition(Technical Committee Member)
Y. Mukaigawa	IEEE Computer Society CVPR2009(Program Committee Member)
Y. Mukaigawa	ICCV2009(Review Committee Member)
R. Sagawa	IPSJ Trans. on Computer Vision and Applications(Editorial Board Member)
R. Sagawa	IEEE Computer Society CVPR2009(Associate Editor in Chief)
R. Sagawa	PSIVT 2009 WCVIMM(Program Committee Member)

Publications in Domestic Meetings

Information Processing Society of Japan	2 papers
Forum for Image Informatics in Japan	4 papers

Academic Degrees

Doctor Degree for Information Science

H. VU	Video Capsule Endoscopy Analysis For Diagnostic Assistance
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H. Mannami	Research on Adaptive Dynamic Range Camera with Liquid Crystal
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Master Degree for Information Science

K. Sugiura	Gait Identification based on Multi-view Matching using an Omnidirectional Camera and View Transformation Models
H. Azuma	Spatio-Temporal Lifelog Using a Wearable Compound Omnidirectional Sensor
K. Akasaka	Shape Matching of Non-rigid Objects using Textured Range Images
A. Tuji	Silhouette Transformation based on Walking Speed for Gait Image Analysis

Sponsorship

Grant-in-Aid for Scientific Research (S)

T. Yagi	Wearable Omnidirectional Stereo Surveillance System	¥21,370,000
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Grant-in-Aid for Young Scientists (B)

Y. Makihara	Research on Gait Identification based on Multi-view Matching using an Omnidirectional Camera	¥ 1,560,000
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Research Fellowship for Young Scientists

H. Mannami	Research on Gait Identification based on Gait Pattern Analysis among Wide Range Generation	¥780,000
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Entrusted Research

Y. Yagi	Matsushita Electric Industrial Co., Ltd.	Research on image stabilization using exposure control imaging technology	¥500,000
Y. Yagi	Matsushita Electric Industrial Co., Ltd.	Research on super-wide view camera and video stabilization technologies	¥16,590,000
Y. Yagi	Matsushita Electric Industrial Co., Ltd.	Research on super-wide view stereo camera system	¥21,966,000

Other Research Fund

Y. Yagi	Japan Science and Technology Agency, Special	Dive into the Movie Project	¥62,000,000
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	Coordination Funds for Promoting Science and Technology	
Y. Yagi	Fujinon Corporation	¥ 960,000
Y. Mukaigawa	Artificial Intelligence Research Promotion Foundation	¥700,000

Department of Architecture for Intelligence

Professor: Masayuki NUMAO
Associate Professor: Satoshi KURIHARA
Assistant Professor: Koichi MORIYAMA
Specially Appointed Assistant Professor: Ken-ichi FUKUI
Post Doctoral Fellow: Roberto LEGASPI
Graduate Students: Ryoza KIYOHARA(-2008.9.30), Nagayoshi YAMASHITA,
Kazushi NAKAMURA, Minoru KAWANO,
Mitsuhiro MATSUMOTO, Toshihito SUGIMOTO,
Hiroshi TAMAKI, Takayuki NISHIKAWA,
Kazuhisa SATOH, Ryo NAGAOKA
Under Graduate Students: Kohei IWAO, Akinobu UEDA
Exchange Student: Lin, Tsung Han (2007.10.1-2008.7.31)
Supporting Staff: Fumie NAKAO

Outlines

The main research objective is to explore basic technology for computer systems, which support human learning and understanding, beyond conventional artificial intelligence. We particularly focus on the process of human-computer interaction to discover and create architecture of intelligence for such systems. We try to produce highly original research with findings from cognitive science, psychology, education, and computer science. Principal issues addressed are as follows: 1. Constructive Adaptive User Interfaces, 2. Intelligent Tutoring System, and 3. Intelligent Ubiquitous Sensor-Networks.

Current Research Project

Constructive Adaptive User Interfaces

This department is developing a computer with learning ability, for which it researches efficient learning algorithms, acquisition of background knowledge for learning, application to Intelligent Tutoring Systems. These are applied to adaptive user interfaces. The conventional adaptive user interfaces only select a good response out of some previously given ones. Although this helps to use interfaces, such as a navigation system, it is not sufficient to stimulate human intelligence or creativity. The department has developed a method to compose a new content adaptively. This technology enables automatic acquisition of human feelings, and automatic music composition system adapted to personality and emotion of its user.

Intelligent Tutoring System

To have an instructional plan guide the learning process is significant to various teaching styles and an important task in an ITS. Though various approaches have been used to tackle this task, the compelling need is for an ITS to improve on its own the plans established in a dynamic way. We hypothesize that the use of knowledge derived from student categories can significantly support the improvement of plans on the part

of the ITS. This means that category knowledge can become effectors of effective plans. We have conceived a Category-based Self-improving Planning Module (CSPM) for an ITS tutor agent that utilizes the knowledge learned from learner categories to support self-improvement. The learning framework of CSPM employs unsupervised machine learning and knowledge acquisition heuristics for learning from experience. We have experimented on the feasibility of CSPM using recorded teaching scenarios.

Intelligent Ubiquitous Sensor-Networks

In recent years, progress in computer technology, the appearance of IPv6, the development of various radio technology including IEEE802.11, and the practical use of radio-tags like RFID have greatly activated studies of ubiquitous computing like sensor-networks. But, the purpose of many proposed ubiquitous systems is to present information of the virtual-world like the Internet to humans living in the real-world by using physical properties like monitors and loudspeakers, etc. On the other hand, our purpose is to construct a framework to enable flexible and real-time interaction between humans and the real-world. Keyword is resonance. Each human has his own natural frequency, which is a metaphor for personality or daily habitual behaviors. In the proposed framework, each human behavior reacts with the environment and the environment performs sensor-data mining and extracts each human's natural frequency. The real-world that we assume in this study is homes and offices, etc., where daily habitual behaviors of humans are easy to extract. So, we call the real-world "the environment." The environment learns the daily habitual behaviors of each human, and performs the most suitable interaction to whoever should receive it. To embody this interaction framework, the environment must be an autonomous action entity, and it is necessary to construct this entity as a massively multi-agent system to enable management and control of various broadly dispersed sensors and physical properties for interaction and to enable real-time interaction with humans. To begin with, we have set up several interaction devices between humans and the environment as well as various kinds of many sensors.

Publications

Original Papers

Modelling affective-based music compositional intelligence with the aid of ANS analyses, Toshihito Sugimoto, Roberto Legaspi, Akihiro Ota, Koichi Moriyama, Satoshi Kurihara, Masayuki Numao: Knowledge-Based Systems, 21 (3) (2008) 200-208.

Reinforcement Learning on a Futures Market Simulator, Koichi Moriyama, Mitsuhiro Matsumoto, Ken-ichi Fukui, Satoshi Kurihara, Masayuki Numao: Journal of Universal Computer Science, 14 (7) (2008) 1136-1153.

How does Q-learning Maintain Cooperation in Prisoner's Dilemma Games?, Koichi Moriyama: Computer Software, 25 (4) (2008) 145-153.

Topic Detection from WWW Based on Link Structure, Nagayoshi Yamashita, Koichi Moriyama, Masayuki Numao, Satoshi Kurihara: IPSJ Transactions on Mathematical Modeling and its Applications, 2 (1) (2009) 133-144.

Design and Implementation of Network Defense System Using Address Migration, Hiroaki Kuroda, Toshio Hirotsu, Kensuke Fukuda, Satoshi Kurihara, Osamu Akashi, Toshiharu Sugawara: IPSJ Transaction on Advanced Computing Systems, 2 (1) (2009) 223-32.

Migration of the IP Routing Points for Distributed Virtual Routing, Toshio Hirotsu, Kensuke Fukuda, Satoshi Kurihara, Osamu Akashi, Toshiharu Sugawara: IPSJ Transaction on Advanced Computing Systems, 2 (1) (2009) 123-132.

Review Papers

Human Behavior Mining Using Sensing Network (in Japanese), Satoshi Kurihara, Journal of the Japanese Society for Artificial Intelligence, 23 [5] (2008) 611-616

Books

Digital Encyclopedia in Artificial Intelligence (in Japanese), Masayuki Numao (Editor and Author), Japanese Society of Artificial Intelligence, (2008)

(Book Chapter) Indirect Coordination Mechanism of MAS, Satoshi Kurihara, Kensuke Fukuda, Shinya Sato and Toshiharu Sugawara, Multiagent Systems, Edited by Salman Ahmed and Mohd Noh Karsiti, Publisher: IN-TECH (2009) 221-232.

International Conferences

An Empathy Learning Problem for HSI: To Be Empathic, Self-improving and Ambient, *Roberto Legaspi, Satoshi Kurihara, Ken-ichi Fukui, Koichi Moriyama, Masayuki Numao: Conference on Human System Interaction (HSI), Krakow, Poland, May 25-27, 2008.

Self-improving Empathy Learning, *Roberto Legaspi, Satoshi Kurihara, Ken-ichi Fukui, Koichi Moriyama, Masayuki Numao: 5th International Conference on Information Technology and Applications (ICITA), Cairns, Australia, June 23-26, 2008.

Web Page Classification Based on Structural Equivalence, *Nagayoshi Yamashita, Koichi Moriyama, Masayuki Numao, Satoshi Kurihara: 5th International Conference on Information Technology and Applications (ICITA), Cairns, Australia, June 23-26, 2008.

Proposition of The Context-Aware Interface for Cellular Phone Operations (poster), *Mitsuhiro Matsumoto, Ryoza Kiyohara, Hidenori Fukui, Masayuki Numao, Satoshi Kurihara: Fifth International Conference on Networked Sensing Systems(INSS 2008), Kanazawa, Japan, June 17-19, 2008.

Elucidating Relationships among Research Subjects from Grant Application Data, *Ryutaro Ichise, Kazuhiro Satoh, Masayuki Numao: 12th International Conference on Information Visualization.

Learning-Rate Adjusting Q-learning for Prisoner's Dilemma Games, *Koichi Moriyama: 2008 IEEE/WIC/ACM International Conference on Intelligent Agent

Technology (IAT'08), Sydney, Australia, Dec. 9-12, 2008.

Pheromone Approach to the Adaptive Discovery of Sensor-Network Topology, *Hiroshi Tamaki, Ken-ichi Fukui, Masayuki Numao, and Satoshi Kurihara: 2008 IEEE/WIC/ACM International Conference on Intelligent Agent Technology (IAT'08), Sydney, Australia, Dec. 9-12, 2008.

Analysis on Grant Application Data (poster), *Kazuhiro Satoh, Ryutaro Ichise, Satoshi Kurihara, Masayuki Numao: The 12th SANKEN International Symposium, Osaka, Japan, Jan. 22, 2009.

Web Page Classification Based on Structural Equivalence (poster), *Nagayoshi Yamashita, Koichi Moriyama, Satoshi Kurihara, Masayuki Numao: The 12th SANKEN International Symposium, Osaka, Japan, Jan. 22, 2009.

Constructive Adaptive User Interfaces and Empathic Computing (invited), *Masayuki Numao: 9th Philippine Computing Science Congress (PCSC 2009), Dumaguete City, Philippines, Mar. 2-3, 2009.

Co-occurrence Analysis Focused on Blogger Communities, *Shin-ya Sato, Kensuke Fukuda, Toshio Hirotsu, Satoshi Kurihara, Toshiharu Sugawara: the 2008 IEEE/WIC/ACM International Conference on Web Intelligence, , Sydney, Australia, Dec. 9-12, 2008.

Controlling Contract Net Protocol by Local Observation for Large-Scale Multi-Agent Systems, *Toshiharu Sugawara, Toshio Hirotsu, Satoshi Kurihara, Kensuke Fukuda: 12th International Workshop on Cooperative Information Agents (CIA2008), Prague, Czech Republic, Sep. 10-12, 2008.

Adaptive Manager-side Control Policy in Contract Net Protocol for Massively Multi-Agent Systems, *Toshiharu Sugawara, Toshio Hirotsu, Satoshi Kurihara, Kensuke Fukuda: 6th International Joint Conference on Autonomous Agents and Multiagent Systems (AAMAS2008), Estoril, Portugal, May 12-16, 2008.

Controlling Contract Net Protocol by Local Observation for Large-Scale Multi-Agent Systems, *Satoshi Kurihara: The First International Workshop on Content Creation Activity Support by Networked Sensing(CCASNS08), Kanazawa, Japan, June 16, 2008.

Contributions to International Conferences and Journals

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|----------|---|
| M. Numao | The Twelfth International Conference on Discovery Science (DS09) (Program Committee) |
| M. Numao | The Ninth ACIS International Conference on Software Engineering, Artificial Intelligence, Networking, and Parallel/Distributed Computing (SNPD2008) (Program Committee) |
| M. Numao | Pacific Rim Knowledge Acquisition Workshop (PKAW'08) |

	(Program Committee)
S. Kurihara	The First International Workshop on Contents Creation Activity Support by Networked Sensing (CCASNS2008) (Organizer)
S. Kurihara	5th International Workshop on Networked Sensing Systems (INSS2008) (Program Committee)
S. Kurihara	6th International Workshop on Networked Sensing Systems (INSS2009) (Program Committee)
S. Kurihara	The Second International Workshop on Coordination and Control in Massively Multi-Agent Systems (CCMMS 2008) (Program Committee)
S. Kurihara	The Tenth Pacific Rim International Conference on Artificial Intelligence (PRICAI-08) (Program Committee)
S. Kurihara	2008 Winter Workshop on Economics with Heterogeneous Interacting Agents (WEHIA) (Program Committee)
S. Kurihara	Autonomic and Trusted Computing (ATC-08) (Program Committee)
S. Kurihara	IEEE 8th International Conference on Computer and Information Technology (CIT2008) (Program Committee)
S. Kurihara	IEEE/WIC/ACM International Conference on Intelligence Agent Technology (IAT'08) (Program Committee)
S. Kurihara	IEEE/WIC/ACM International Conference on Intelligence Agent Technology (IAT'09) (Program Committee)
S. Kurihara	The 1st International Symposium on u- and e- Service, Science and Technology (UNESST) (Program Committee)
S. Kurihara	The Fifth International Conference on Autonomic and Autonomous Systems (ICAS 2009) (Program Committee)
S. Kurihara	The 12th Pacific Rim International Conference on Multi-Agents, Industrial Track (Program Committee Chair)
S. Kurihara	The Third International Workshop on Emergent Intelligence on Networked Agents (WEIN'09) (Workshop Chair)
S. Kurihara	The 1 st IJCAI Workshop on Social Simulation (Program Committee)
K. Moriyama	The 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008) (Local Arrangement Member)

Publications in Domestic Meetings

The Japanese Society for Artificial Intelligence	13 papers
Information Processing Society of Japan	8 papers
Japanese Society for Software Science and Technology	2 papers
Publications in Domestic Meetings	4 papers
The Institute of Electronics, Information and Communication Engineers	2 papers

Academic Degrees

Doctor Degree for Information Science

R. Kiyohara	Study on Mobile Phone Software Add-in
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N. Yamashita	Study on WWW Analysis based on Structure Equivalence
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Master Degree for Information Science

K. Satoh	Time-Series Prediction of Research Subjects Using Collaborative Research Relationship
T. Sugimoto	Music Recommendation System that Predicts Affective Changes Based on Brain Wave Analysis
H. Tamaki	Constructing a Traffic Information Providing System Utilizing Multi-Source Information
R. Nagaoka	Identifying location mentioned on weblog utilizing related terms
T. Nishikawa	Automatic composition system considering both partial and overall music structure

Sponsorship

Grant-in-Aid for Scientific Research (C)

S. Kurihara	Proposal of top-down controllable multi-agent coordination algorithm	¥1,950,000
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Grant-in-Aid for Young Scientists (B)

K. Moriyama	Deriving Appropriate Utility in Agent Learning	¥910,000
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Entrusted Research

M. Numao	Japanese Society for the Promotion of Science	Investigation on science trend in artificial intelligence field	¥14,500,000
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Other Research Fund

S. Kurihara	Ministry of Internal Affairs and Communications Science Researches, SCOPE	Study on inter-ubiquitous network information infrastructure	¥14,741,000
S. Kurihara	Sumitomo Electric Industries, Ltd.	Research on constructing the safe and secure next generation traffic control and information security systems by multi-agent approach	¥1,950,000

Department of Reasoning for Intelligence

Professor: Takashi WASHIO
Assistant Professor: Kouzou OHARA, Akihiro INOKUCHI
Post Doctoral Fellow: Shohei SHIMIZU (2008.04.01-2008.07.31)
Graduate Students: HADIYANTO, Viet Phuong NGUYEN, Noriyuki OHNISHI,
Ha Hong NGUYEN, Vinh Duy NGUYEN
Research Student: Hongping LI (2008.09.01-)
Under Graduate Students: Yasuhiro SOGAWA, Takanori INAZUMI
Supporting Staff: Hiroko OKADA

Outlines

We, humans, can extract variety of knowledge from given data by the full use of our reasoning. However, such reasoning ability of humans is so limited that most of the massive and complex data acquired through computer network are wasted without any humans' inspection. To provide efficient remedies to this difficulty, our department studies novel reasoning approaches to extract knowledge from the massive and complex data by using computers. These techniques are named data mining and knowledge discovery. We also study the application of these techniques to variety of fields such as science, information network, quality/risk management, medicine, security, marketing and finance. In this year, we obtained significant outcomes in the research topics of knowledge discovery from massively high dimensional dynamics data, knowledge discovery from graph structured data and knowledge discovery from massively high dimensional similarity data.

Current Research Projects

Knowledge discovery from extremely high dimensional data

Measurement data consisting of massive variables (extremely high dimensional data), which represent many events simultaneously occurred, became available by the development of computer network, ubiquitous sensing and scientific measurement technologies. Examples are the sensing data obtained from a large scale urban traffic system or a large scale process plant for power generation and manufacturing, and the profile data of thousands of gene expressions in biological systems. Our department further promoted a research project to estimate temporal dynamics and state of an objective system from the data acquired from such large scale and complex systems. Concretely speaking, we extended a state identification method "particle filter" to estimate the state and the dynamics of a large and complex system from high dimensional data observed from the system. This approach enables modeling and state identification of such large scale systems.

Knowledge discovery from graph structured data

Data mining approaches on graph structured data which cannot be captured by popular relational data bases attract many researchers in recent data mining field. Our

department has been working on this research topic as a worldwide pioneer. We recognize the generic and strong ability of the graphs to represent complex knowledge and concept since more than 10 year ago. The task of finding frequently appearing subgraphs (subgraph isomorphism) in a set of graph data is known to be computationally hard, and our study address this hard computational complexity. In this year, we worked on the following two novel studies to overcome the limitations of the state of the art.

1) Development basic principles to derive large scale and frequent substructure co-occurrences

The size of the frequently co-occurred sub-graph structures which can be derived in the current graph mining techniques is limited to the structures consisting of a few dozens of vertices. Under the aim to overcome this limitation, we analyzed the properties of graph spectra to characterize the graph structures. We could clarify the mechanism that the graph spectra reflect their underlying graph structures, and confirmed the high feasibility to efficiently derive the frequently co-occurred sub-graph structures having large scale.

2) Development of basic principle to derive frequent graph sequences

The conventional framework of the graph mining remains to derive the frequently co-occurred sub-graph structures shared by many data graphs. In this year, we extended our research scope to efficiently derive frequently co-occurred sequence patterns embedded in graph series data. Upon the extensive explorations, we are almost establishing a practical mining approach to derive frequent graph subsequences.

Knowledge discovery from large scale similarity data

In the last two years, we have been working on the development of a fast estimation method of correlations between variables and Euclidean distance between objects from the data consisting of massive number of variables and objects. In this year, we further extended our research scope to efficiently estimate probability distribution of the relations between the variables or the objects from their partial relations. This new extended approach enables highly practical data estimation for the element complement of tables and matrices obtained in various scientific experiments and for the estimation of missing values in many engineering and social data.

OLAP database system for complex temporal intervals

The current OLAP database systems are incapable of supporting to analyze event time series with temporal intervals. In the last two years, we have been working on the development of an OLAP database system to interactively analyze medical data whose classes include temporal intervals. It is to analyze the medical data in a multidimensional manner by storing the data in tables of vertical layout and by designing OLAP operations for temporal intervals. In addition, we achieved a linear speedup by partitioning the data into multiple computers and by parallelizing the operations with these computers, and we confirmed the practicality of our system to huge databases.

Publications

Original Papers

A Range Query Approach for High Dimensional Euclidean Space Based on EDM Estimation, Kentarou Kido, Hiroshi Kuwajima, Takashi Washio: The Eighth SIAM International Conference on Data Mining (SDM08), (2008) 387-398.

Modeling Dynamic Substate Chains among Massive States, Nguyen Viet Phuong, Takashi Washio: Intelligent Data Analysis, 2 (3) (2008) 271-291.

A Bank Run Model in Financial Crises, Katsutoshi Yada, Takashi Washio, Yasuharu Ukai, Hisao Nagaoka: KES 2008(The 12th International Conference on Knowledge-Based and Intelligent Information & Engineering Systems), LNAI 5178 (2008) 703-710.

A Fast Method to Mine Frequent Subsequences from Graph Sequence Data, Akihiro Inokuchi, Takashi Washio: 2008 Eighth IEEE International Conference on Data Mining, (2008) 303-312.

Causal discovery of linear acyclic models with arbitrary distributions, Patrik O. Hoyer, Aapo Hyvarinen, Richard Scheines, Peter Spirtes, Joseph Ramsey, Gustavo Lacerda, Shohei Shimizu: The 24th Conference on Uncertainty in Artificial Intelligence, (2008) 282-289.

Causal modelling combining instantaneous and lagged effects: an identifiable model based on non-Gaussianity, Aapo Hyvarinen, Shohei Shimizu, Patrik O. Hoyer: The 25th International Conference on Machine Learning (ICML2008), (2008) 424-431.

Review Papers

A Strategy to Present Your Paper in Prestige International Conferences, Takashi Washio, Journal of The Japanese Society for Artificial Intelligence, Vol.23, No.3 (2008) 362-366.

Featured section on data mining and statistical science, Tomoyuki Higuchi and Takashi Washio, Anals of the Institute of Statistical Mathematics, Vol.60, No.4 (2008).

Special Issue on Data Mining and Statistical Mathematics, Tomoyuki Higuchi and Takashi Washio, Statistical Mathematics, Vol.56, No.2, (2008) 167-168.

Learning linear acyclic models using independent component analysis, Shohei Shimizu, Journal of the Japan Statistical Society (Japanese Issue) , Vol. 37, No. 2 (2008) 223-237.

Books

Statistics in 21st Century –Statistics for Nature, Biology and Health-, Chapter 10: Graph Mining and Its Application to Statistical Modeling, Takashi Wasiho, et al., Tokyo University Press., (2008) 291-314.

Applications of Data Mining in E-Business and Finance, Carlos Soares, Younghong

Peng, Jun Meng, Takashi Washio and Zhi-Hua Zhou (Eds.), *Frontiers in Artificial Intelligence and Applications*, No.177, IOS Press (2008).

Advances in Knowledge Discovery and Data Mining, Takashi Washio, Einoshin Suzuki, Kai Ming Ting and Akihiro Inokuchi (Eds.), *Proc. of 12th Pacific-Asia Conference of Knowledge Discovery and Data Mining, PAKDD 2008*, *Lecture Notes in Computer Science (LNCS) Vol.5012*, Springer (2008).

A Method to Search ARX Model Orders and Its Application to Sales Dynamics Analysis, Data Mining for Design and Marketing, Kenta Fukata, Takashi Washio, Katsuyoshi Yada and Hiroshi Motoda, CRC Press, Taylor & Francis Corp., Chapter 5 (2008) 81-94.

PAKDD 2008 International Workshops, Osaka, Japan, May 20-23, 2008, Revised Selected Papers, LNCS: *Lecture Notes in Computer Science*, LNAI: *Lecture Notes in Artificial Intelligence*, S. Chawla, T. Washio, S. Minato, S. Tsumoto, T. Onoda, S. Yamada, A. Inokuchi, Vol. 5433 (2008).

Patents

Instrument to Extract Frequent Change Pattern, A. Inokuchi, T. Washio,
PCT No. PCT/JP2009/000092

Multidimensional Data Analysis Method, Multidimensional Data Analysis System, and Their Programs, A. Inokuchi, T. Washio, and K. Takabayashi: PCT No. PCT/JP2008/003366

International Conferences

Feasibility of Graph Sequence Mining based on Admissibility Constraints, *Akihiro Inokuchi, Takashi Washio: *The 3rd International Workshop on Data Mining and Statistical Science (DMSS2008)*, Tokyo, Japan, September, 25-26, 2008.

On Feasibility of Graph Spectrum-based Frequent Sub-graph Mining, *Kouzou Ohara, Takashi Washio, Vinh Duy Nguyen: *The 3rd International Workshop on Data Mining and Statistical Science (DMSS2008)*, Tokyo, Japan, September, 25-26, 2008.

Isomorphism Identification by Using Graph Spectra and Its Application to Graph Mining (invited), Kouzou Ohara, *Takashi Washio: *The Joint Meeting of 4th World Conference of the IASC and 6th Conference of the Asian Regional Section of the IASC on Computational Statistics & Data Analysis*, Kanagawa, Japan, December 5-8, 2008.

Regression with interval output values, *Hisashi Kashima, Kazutaka Yamasaki, Akihiro Inokuchi, Hiroto Saigo: *The 19th International Conference on Pattern Recognition (ICPR 2008)*, Florida, USA, December 8-11, 2008.

Linear non-Gaussian structural equation models (invited), *Shohei Shimizu, Patrik O. Hoyer, Aapo Hyvarinen: *IMPS 2008, the 73rd Annual Meeting of the Psychometric Society*, University of New Hampshire, U.S.A., June 29-July 2.

Contributions to International Conferences and Journals

T. Washio	The 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008)(Program Chair)
T. Washio	The First Asian Conference on Machine Learning (ACML-2009)(Program Chair)
T. Washio	The 10th Pacific Rim International Conference on Artificial Intelligence (PRICAI-08)(Workshop Chair)
T. Washio	The 9th SIAM International Conference on Data Mining (SDM09): Program Committee Member and Area Chair(Area Program Chair)
T. Washio	Pacific-Asia Conference on Knowledge Discovery and Data Mining(Steering Committee)
T. Washio	The Eleventh International Conference on Discovery Science (DS-2008)(Program Committee)
T. Washio	Algorithms for Large-Scale Information Processing in Knowledge Discovery (ALSIP 2008)(Program Committee)
T. Washio	ACM 17th Conference on Information and Knowledge Management (CIKM2008)(Program Committee)
T. Washio	The 10th Pacific Rim International Conference on Artificial Intelligence (PRICAI-08) (Program Committee)
T. Washio	The 2nd International Conference on Mining and Learning with Graphs (MLG-08)(Program Committee)
T. Washio	International Conference on Large-scale Knowledge Resources (ILKR2008)(Program Committee)
T. Washio	The 8th SIAM International Conference on Data Mining (SDM)(Program Committee)
T. Washio	The 2008 edition of the IEEE International Conference on Data Mining series (ICDM 2008)(Program Committee)
T. Washio	The Fourteenth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (SIG-KDD08)(Program Committee)
T. Washio	2008 IEEE/WIC/ACM International Conference on Web Intelligence (WI'08)(Program Committee)
T. Washio	The fifteenth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (SIG-KDD09)(Program Committee)
T. Washio	The 7th International Workshop on Mining and Learning with Graphs (MLG-2009)(Program Committee)
T. Washio	The 18th ACM Conference on Information and Knowledge Management (CIKM 2009)(Program Committee)
T. Washio	2009 IEEE International Conference on Data Mining (ICDM09)(Program Committee)
T. Washio	The Twelfth International Conference on Discovery Science (DS09)(Program Committee)
T. Washio	The First International Workshop on LEarning and Mining for Robotics (LEMIR 2009) (Program Committee)

T. Washio	Knowledge and Information Systems: Special Issue on Selected Papers of The 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008)(Guest Editorial Chair)
T. Washio	New Generation Computing: Special Issue on Selected Papers of The 3 rd International Workshop on Data Mining and Statistical Science (DMSS2008)(Guest Editorial Chair)
K. Ohara	Local Arrangement Committee Co-Chair of the 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008)(Local Arrangement Co-Chair)
K. Ohara	Program Committee of the 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008)(Program Committee)
K. Ohara	Program Committee of the 2008 International Symposium on Ubiquitous Multimedia Computing (UMC2008)(Program Committee)
K. Ohara	Program Committee of the 2008 Pacific Rim Knowledge Acquisition Workshop (PKAW'08)(Program Committee)
K. Ohara	Program Committee of the 22nd Australasian Joint Conference on Artificial Intelligence (AI'08)(Program Committee)
K. Ohara	Program Committee of the 22nd Australasian Joint Conference on Artificial Intelligence (AI'09)(Program Committee)
A. Akihiro	The 12 th Program Committee of Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD 2008) (Publication Chair)
A. Akihiro	IADIS European Conference on Data Mining (ECDM 2008) (Program Committee)
A. Akihiro	Editorial Review Board of International Journal of Applied Evolutionary Computation (IJAEC) (Editorial Review Board)
A. Akihiro	International Workshop on Data-Mining and Statistical Science (DMSS2008) (Program Committee)
A. Akihiro	The 13 th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2009) (Program Committee)
A. Akihiro	The 9 th SIAM International Conference on Data Mining (SDM2009) (Program Committee)
A. Akihiro	International Workshop on Data-Mining and Statistical Science (DMSS2009) (Workshop Chair)
A. Akihiro	The 1 st Asian Conference on Machine Learning (ACML2009) (Program Committee)
A. Akihiro	IADIS European Conference on Data Mining (ECDM 2009) (Program Committee)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	8 papers
Japan Association for Medical Informatics	1 paper

Academic Degrees

Master Degree for Engineering

N. Ohnishi A Study on Discovery of Optimal Investment Portfolio from Data

Bachelor Degree for Engineering

Y. Sogawa A Study on Identification of Exogenous Gene Expression Based on Independent Component Analysis

Sponsorships

Grant-in Aid for Scientific Research (A)

T. Washio Development of Causal Structure Mining Method for Large Scale Dimensional Data and Construction of Knowledge Base on Gene Functional Relations ¥12,350,000

Grant-in Aid for Scientific Research on Priority Area

T. Washio Establishment of Knowledge Mining and Modeling Principles for Large Scale Dimensional Time Series and Its Application to Commercial Ubiquitous Data ¥3,000,000

Grant-in-Aid for Young Scientists (B)

K. Ohara Development of Graph Mining Method Using Domain Knowledge as Constraints ¥2,080,000

Grant-in-Aid for Young Scientists (B)

A. Inokuchi Development of Method for Mining Local and Characteristic Patterns from Changing Graph Structured Data ¥2,210,000

Grant-in-Aid for JSPS Fellows

S. Shimizu Development of new multivariate statistical methods combining independent component analysis and structural equation modelling ¥1,100,000

Entrusted Research

T. Washio	Fujitsu Research Institute	Consulting on Advanced Technology Development to Improve Trouble Analysis Service	¥348,621
A. Inokuchi	Japan Airline International	Technology Survey on New Integrated Safety Operational Supporting System (Information Grand	¥6,090,916

Voyage)

Other Research Fund

T. Washio	Kyoto Technica, Inc.		¥1,000,000
A. Inokuchi	Japan Science and Technology Agency	Development of Knowledge Organization and Understanding Support of Massive Graph Sequence Data	¥3,315,000
A. Inokuchi	Japan Science and Technology Agency	Development and Validation of Multidimensional Database System for Complex Sequence Data of Medicine	¥2,000,000

Division of Biological Science

Outline

The Division of Biological Sciences is composed of three departments: Dept. of Single-Molecule Biophysics, Dept. of Cell Membrane Biology, and Dept. of Structural Molecular Biology. These departments are engaged in researches in various fields of biological sciences including molecular enzymology, signal transduction, energy transformation, membrane transport, and mechanism of gene expression. The research projects covered by this division are as follows:

1. Single-molecule studies on the mechanochemical coupling of F- and V-type H⁺ ATPases.
2. Development of FRET-based ATP sensor.
3. Water/Oil droplet micro array for highly sensitive bioassay system.
4. The molecular structures and the molecular mechanisms of xenobiotic extruding pumps functioning as a host-defense mechanism in cellular level
5. Comprehensive studies on bacterial xenobiotic exporter genes and the regulation of the expression by two-component signal transduction systems
6. Physiological roles of efflux transporters in signal transduction and mammalian development
7. The mechanisms of biogenesis of the topa quinone cofactor in copper amine oxidase and other novel “built-in” cofactors in quinohemoproteins
8. Identification of novel protein kinase C-interacting proteins and elucidation of their roles in signal transduction
9. Development of a new method of the gene delivery system using hepatitis B virus surface antigen particles

Achievement

- Identification of ubiquitin ligase activity of RBCK1 and its inhibition by splice variant RBCK2 and protein kinase C β
- In vivo delivery of bio-nanocapsules displaying L4-PHA isolectin to malignant tumors overexpressing N-acetylglucosaminyltransferase V
- Expression of squamous cell carcinoma antigen-1 in liver enhances the uptake of HBV envelope-derived bio-nanocapsules in transgenic rats
- Response regulator YycF essential for bacterial growth: X-ray crystal structure of the DNA-binding domain and its PhoB-like DNA recognition motif
- Development of femtoliter chamber made of water-in-oil emulsion
- Development of fluorescent protein sensor for live-cell ATP imaging
- Kinetic analysis of COPII vesicle by single molecule imaging
- Regulatory mechanism of the epsilon subunit of ATP synthase
- Study on the correlation between crystal structure of F1 and substeps of F1 found in the single-molecule rotation assay
- Development of a high-speed laser dark-field microscopy for 105 frame/sec imaging

- Studies on regulatory networks of xenobiotic exporters in *Salmonella enterica*
- Characterization of the lipophilic signal transducing molecules export system in the mammalian cells.
- Identification of the membrane exporter that mediates secretion of sphingosine-1-phosphate
- Identification of a physiologically functional S1P transporter, *spns2*
- Characterization of the enzymatic properties of erythrocyte S1P transporter

Department of Structural Molecular Biology

Professor:	Katsuyuki TANIZAWA
Associate Professor:	Shun'ichi KURODA
Assistant Professor:	Kenji TATEMATSU (2008.9.1-Long term study leave)
Specially Appointed Assistant Professor:	Takashi MATSUZAKI
Part-time Researchers:	Nobuo YOSHIMOTO, Noriko SHIKAKU, Yoko MATSUSHITA, Masumi IJIMA
Graduate Students:	Takeshi KASUYA, Mitsuo YAMADA, Yuko IKEDA, Akio HAMAGUCHI, Yukari MATSUI, Akihito MOTOYAMA, Noriko NAKAGAWA, Hidenori NONOMURA, Atsuro TADA, Yasuyuki TAKAISHI, Azusa TANIMURA, Hiromichi YONEKURA
Supporting Staffs:	Mayuko MURAI, Ai OKUBO

Outlines

The research of this laboratory is focused on the biochemical and molecular biological studies on various enzymes. Their active-site structures and catalytic mechanisms are being investigated by site-directed mutagenesis, various spectroscopies, and X-ray crystallography. A previous conspicuous finding is the copper ion-dependent, post-translational modification mechanism for the biogenesis of the topa quinone cofactor in copper amine oxidase. Furthermore, we investigate the intracellular mechanisms involving protein kinase C family, which play important roles in the cell proliferation, differentiation, oncogenesis, and apoptosis by cross talking with other molecules. Recently, we have succeeded to identify several protein kinase C-interacting proteins and characterized them as regulatory proteins for the protein kinase activities and/or their subcellular localization and also as effectors of kinase signaling. In addition, we have developed bio-nanocapsules displaying various biorecognition molecules, which are expected to be an ideal vector for the tissue- and cell type-specific gene and drug delivery system.

Current Research Project

Identification of Ubiquitin Ligase Activity of RBCK1 and Its Inhibition by Splice Variant RBCK2 and Protein Kinase C β

We previously identified a RING-IBR protein, RBCK1, as a protein kinase C (PKC) β and ζ -interacting protein, and its splice variant, RBCK2, lacking the C-terminal half including the RING-IBR domain. RBCK1 has been shown to function as a transcriptional activator, whose nuclear translocation is prevented by interaction with the cytoplasmic RBCK2. We here demonstrate that RBCK1, like many other RING proteins, also possesses a ubiquitin ligase (E3) activity and that its E3 activity is inhibited by interaction with RBCK2. Moreover, RBCK1 has been found to undergo efficient phosphorylation by PKC β . The phosphorylated RBCK1 shows no self-ubiquitination activity *in vitro*. Overexpression of PKC β leads to significant

increases in the amounts of intracellular RBCK1, presumably suppressing the proteasomal degradation of RBCK1 through self-ubiquitination, while coexpression with PKC α , PKC ϵ , and PKC ζ shows no or little effect on the intracellular amount of RBCK1. Taken together, the E3 activity of RBCK1 is controlled by two distinct manners, interaction with RBCK2 and phosphorylation by PKC β . It is possible that other RING proteins, such as Parkin, BRCA1, and RNF8, having the E3 activity, are also down-regulated by interaction with their RING-lacking splice variants and/or phosphorylation by protein kinases.

In Vivo Delivery of Bio-nanocapsules Displaying L4-PHA Isolectin to Malignant Tumors Overexpressing N-Acetylglucosaminyltransferase V

Metastasis is a key aspect of tumor malignancy, and several malignant tumors show expression of various mature N-type glycans. In particular, beta1-6 branching N-acetylglucosamine (GlcNAc) is abundantly expressed as a part of high-mannose glycans in various highly metastatic cancers. Phaseolus vulgaris agglutinin-L(4) isolectin (L(4)-PHA), which adheres to beta1-6 GlcNAc specifically, has been used for in situ cancer diagnosis. Bionanocapsules (BNCs), hollow particles with a diameter of approximately 80 nm and composed of hepatitis B surface antigen (HBsAg) and a lipid bilayer, have been developed as human liver-specific nanocapsules for in vivo drug delivery system. In this study, we have generated L(4)-PHA-displaying BNCs (PHA-BNCs) and examined whether L(4)-PHA could retarget the BNCs to malignant tumors as a “biosensor” distinguishing tumor metastaticity. Fluorescence-labeled PHA-BNCs injected systemically into a mouse xenograft model were found to accumulate in beta1-6 GlcNAc-expressing malignant tumors. The PHA-BNCs were able to deliver DNA to the malignant cancer cells. These results open up the possibility of using L(4)-PHA lectin as a targeting molecule in a drug delivery system, and of using PHA-BNCs as a novel nanodevice for malignant tumor-specific bioimaging and drug delivery.

Expression of Squamous Cell Carcinoma Antigen-1 in Liver Enhances the Uptake of HBV Envelope-derived Bio-nanocapsules in Transgenic Rats

We previously developed the bio-nanocapsule, which consists of hepatitis B virus envelope L proteins. The bio-nanocapsule can be used to deliver genes and drugs specifically to the human liver-derived tissues in xenograft models, presumably by utilizing the human liver-specific mechanism of hepatitis B virus infection. The hepatitis B virus tropism is highly restricted to humans and higher primates. Thus, to evaluate the in vivo therapeutic effects of forthcoming bio-nanocapsule-based medicines, it will be crucial to develop an animal model whose liver is susceptible to both bio-nanocapsule and hepatitis B virus. In the present study, we aimed to establish a bio-nanocapsule-susceptible animal model using transgenic rats expressing squamous cell carcinoma antigen-1 (SCCA1), which has been proposed to be a receptor for hepatitis B virus, interacting with the hepatitis B virus envelope protein and enhancing the cellular uptake of hepatitis B virus. We show that the recombinant SCCA1 protein interacts directly with bio-nanocapsule and inhibits its attachment to the cultured human liver-derived cells. Furthermore, we have established a transgenic rat that specifically expresses SCCA1 in the liver and also demonstrate that the amount of bio-nanocapsule accumulated in the liver is significantly increased by the SCCA1 expression.

Histological analysis suggests that bio-nanocapsule is preferentially incorporated into the SCCA1-expressing hepatocytes but not into macrophages, such as Küppfer cells, nor into endothelial cells. Therefore, this animal model is expected to be useful for the development of bio-nanocapsule-based medicines.

Response Regulator YycF Essential for Bacterial Growth: X-ray Crystal Structure of the DNA-binding Domain and its PhoB-like DNA Recognition Motif

A response regulator YycF and its cognate sensor kinase YycG constitute the two-component signal transduction system essential for growth of Gram-positive bacteria with a low GC content. We have determined the X-ray crystal structure of the effector domain of *Bacillus subtilis* YycF involved in DNA binding. The structure, containing a winged helix-turn-helix motif, was found to be very similar to that of the response regulator PhoB from *Escherichia coli*. Specific binding of YycF to the PhoB-regulated alkaline phosphatase promoter was also demonstrated.

Publications

Original Papers

Efficient bacterial production of functional antibody fragments using a phagemid vector, H. Kuba, A. Furukawa, T. Okajima and K. Furukawa: *Protein Expr. Purif.*, 58 (2) (2008) 292-300.

Identification of ubiquitin ligase activity of RBCK1 and its inhibition by splice variant RBCK2 and protein kinase C β , K. Tatematsu, N. Yoshimoto, T. Okajima, K. Tanizawa and S. Kuroda: *J. Biol. Chem.*, 283 (17) (2008) 11575-11585.

Yeast-based fluorescence reporter assay of G protein-coupled receptor signaling for flow cytometric screening: FAR1-disruption recovers loss of episomal plasmid caused by signaling in yeast, J. Ishii, T. Tanaka, S. Matsumura, K. Tatematsu, S. Kuroda, C. Ogino, H. Fukuda and A. Kondo: *J. Biochem.*, 143 (5) (2008) 667-674.

Enigma homolog 1 scaffolds protein kinase D1 to regulate the activity of the cardiac L-type voltage-gated calcium channel, A.D. Maturana, S. Wälchli, M. Iwata, S. Ryser, J. Van Lint, M. Hoshijima, W. Schlegel, Y. Ikeda, K. Tanizawa and S. Kuroda: *Cardiovascular Res.*, 78 (3) (2008) 458-465.

Crystal structures of *Lymnaea stagnalis* AChBP in complex with neonicotinoid insecticides imidacloprid and clothianidin, T. Okajima, M. Ihara, A. Yamashita, T. Oda, K. Hirata, H. Nishiwaki, T. Morimoto, M. Akamatsu, Y. Ashikawa, S. Kuroda, R. Mega, S. Kuramitsu, D.B. Sattelle and K. Matsuda: *Invert. Neurosci.*, 8 (2) (2008) 71-81.

Further insight into the mechanism of stereoselective proton abstraction by bacterial copper amine oxidase, M. Taki, T. Murakawa, T. Nakamoto, M. Uchida, H. Hayashi, K. Tanizawa, Y. Yamamoto and T. Okajima: *Biochemistry*, 47 (29) (2008) 7726-7733.

In vivo protein delivery to human liver-derived cells using hepatitis B virus envelope

pre-S region, T. Kasuya, T. Yamada, A. Uyeda, T. Matsuzaki, T. Okajima, K. Tatematsu, K. Tanizawa and S. Kuroda: *J. Biosci. Bioeng.*, 106 (1) (2008) 99-102.

In vivo delivery of bio-nanocapsules displaying L4-PHA isolectin to malignant tumors overexpressing N-acetylglucosaminyltransferase V, T. Kasuya, J. Jung, H. Kadoya, T. Matsuzaki, K. Tatematsu, T. Okajima, E. Miyoshi, K. Tanizawa and S. Kuroda: *Hum. Gene Ther.*, 19 (9) (2008) 887-895.

Response regulator YycF essential for bacterial growth: X-ray crystal structure of the DNA-binding domain and its PhoB-like DNA recognition motif, T. Okajima, A. Doi, A. Okada, Y. Gotoh, K. Tanizawa and R. Utsumi: *FEBS Lett.*, 252 (23, 24) (2008) 3434-3438.

Expression of squamous cell carcinoma antigen-1 in liver enhances the uptake of HBV envelope-derived bio-nanocapsules in transgenic rats, T. Kasuya, S. Nomura, T. Matsuzaki, J. Jung, T. Yamada, K. Tatematsu, T. Okajima, K. Tanizawa and S. Kuroda: *FEBS J.*, 275 (22) (2008) 5714-572.

The peroxisomal membrane protein import receptor Pex3p is directly transported to peroxisomes by a novel Pex19p- and Pex16p-dependent pathway, T. Matsuzaki and Y. Fujiki: *J. Cell Biol.*, 183 (7) (2008) 1275-1286.

Review Papers

“Nanoparticles for Human Liver-specific Drug and Gene Delivery Systems: In Vitro and In Vivo Advances”, T. Kasuya, and S. Kuroda, *Expert Opinion Drug Delivery* 6 (2009) 1-14.

Books

“Copper Amine Oxidases: Structure, Catalytic Mechanism and Role in Physiopathology” (G. Floris and B. Mondovi, Eds.), Chapter 3: Cofactors of Amine Oxidases: Copper Ion and Its Substitution and the 2,4,5-Trihydroxyphenylalanine Quinone, S. Suzuki, T. Okajima, K. Tanizawa, and M. Mure, CRC Press, New York (2009) 19-37.

“Copper Amine Oxidases: Structure, Catalytic Mechanism and Role in Physiopathology” (G. Floris and B. Mondovi, Eds.), Chapter 8: Mechanism of TPQ Biogenesis in Prokaryotic Copper Amine Oxidase, T. Okajima and K. Tanizawa, CRC Press, New York (2009) 103-118.

“Drug delivery using functional DDS carriers” (T. Okada, Ed.), *Bio-nanocapsules*, S. Kuroda, CMC Press, Tokyo, Japan (2008) 360.

International Conferences

In vivo delivery of bio-nanocapsules displaying L4-PHA isolectin to malignant tumors overexpressing N-acetylglucosaminyl-transferase V (poster), *T. Kasuya, J. Jung, H. Kadoya, T. Matsuzaki, K. Tatematsu, T. Okajima, E. Miyoshi, K. Tanizawa and S. Kuroda: 35th Annual Meeting & Exposition of the Controlled Release Society, New

York, USA, July 12-16, 2008.

Direct observation of cell entry of hepatitis B virus envelope L-derived bio-nanocapsules (poster), *M. Yamada, T. Kasuya, T. Matsuzaki, K. Tanizawa and S. Kuroda: The Molecular Biology of Hepatitis B Viruses, San Diego, USA, August 17-21, 2008.

Enhancement of cellular uptake of HBV envelope L-derived bio-nanocapsules by liver-specific expression of SCCA1 in transgenic rat model (poster), *T. Kasuya, T. Matsuzaki, M. Yamada, K. Tanizawa and S. Kuroda: The Molecular Biology of Hepatitis B Viruses, San Diego, USA, August 17-21, 2008.

Analysis of the fusogenic activity of the HBV L protein utilizing bio-nanocapsule (poster), *T. Matsuzaki, Y. Sasaki, T. Kasuya, K. Tanizawa and S. Kuroda: The Molecular Biology of Hepatitis B Viruses, San Diego, USA, August 17-21, 2008.

Involvement of an iron sulfur protein and a subtilisin-like protease in the biogenesis of quinoxinoprotein amine dehydrogenase (invited), T. Okajima, K. Ono and *K. Tanizawa: Japan-Holland Joint Seminar on New Aspects in Enzyme Science and Biotechnology, Fukuoka, Japan, September 28-30, 2008.

X-ray crystal structure of Streptococcus mutans response regulator involved in biofilm formation (poster), *A. Tada, S. Nomura, Y. Eguchi, R. Utsumi, S. Kuroda, K. Tanizawa and T. Okajima: 4th Handai Nanoscience and Nanotechnology International Symposium, Suita, Osaka, Japan, Sept. 29-Oct. 1, 2008.

In vivo pinpoint gene/drug delivery system using bio-nanocapsules (invited), *S. Kuroda: 1st International Symposium on Innovative-Cancer Therapy, Seoul, Korea, October 24-25, 2008.

Conformational flexibility of the TPQ cofactor in bacterial copper amine oxidase (poster), *T. Okajima, S. Nakanishi, T. Murakawa, H. Hayashi and K. Tanizawa: The Second International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Athens, Georgia, USA, October 26-31, 2008.

Involvement of an iron sulfur protein and a subtilisin-like protease in the posttranslational modification of quinoxinoprotein amine dehydrogenase (invited), *K. Tanizawa, K. Ono and T. Okajima: The Second International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Athens, Georgia, USA, October 26-31, 2008.

Conformational Flexibility of the TPQ Cofactor in Bacterial Copper Amine Oxidase (poster), *T. Okajima, S. Nakanishi, and K. Tanizawa: 12th SANKEN International Symposium /Joint Meeting of The 7th SANKEN Nanotechnology Center Symposium/The 2nd SANKEN MSTeC Symposium/The 1st SANKEN Alliance Symposium, Suita, Osaka, Japan, January 22, 2009.

Contributions to International Conferences and Journals

K. Tanizawa	Federation of Asian and Oceanian Biochemists and Molecular Biologists (Delegate of Japan)
K. Tanizawa	The Journal of Biochemistry (Associate Editor)
K. Tanizawa	Journal of Nutritional Science and Vitaminology (Associate Editor)
S. Kuroda	The Open Veterinary Science Journal, Bentham Science Publishers Ltd. (Editorial Board Member)
S. Kuroda	The Open Nanomedicine Journal, Bentham Science Publishers Ltd. (Editorial Board Member)

Publications in Domestic Meetings

Joint Annual Meeting of the Molecular Biology Society of Japan and the Japanese Biochemical Society (BMB2008)	12 papers
Annual Meeting of the Japanese DDS Society	5 papers

Academic Degrees

Doctor Degree for Engineering

T. Kasuya	<i>In Vivo</i> Targeting Mechanism of Hepatitis B Virus <i>Env</i> Protein-Derived Bionanocapsule and Its Application
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Master Degree for Science

N. Nakagawa	Development and Functional Assessment of Bionanocapsules Displaying Membrane-permeable Peptides
Y. Ikeda	Reconstitution of Cytokine Signal Transduction System in <i>Saccharomyces cerevisiae</i>
H. Yonekura	Role of Hemes Bound in the α -Subunit of Quinohemoprotein Amine Dehydrogenase in the Cofactor Biogenesis
A. Tada	X-ray Crystal Structure of a Signal Transduction Protein Involved in the Bio-film Formation by <i>Streptococcus mutans</i>
H. Nonomura	Identification of Signaling Molecule Involved in the NELL1-induced Osteoblastic Differentiation and Development of Assay System for Serum NELL1

Master Degree for Engineering

A. Motoyama	Conformational Flexibility and Control of Topa Quinone Cofactor and Its Precursor in Copper Amine Oxidase
Y. Matsui	Optimization of Gene-delivering Capacity of Cationic Liposome and Bionanocapsule Complex

Sponsorship

Grant-in-Aid for Scientific Research (B)

K. Tanizawa	Mechanisms of Biosynthesis and Catalysis of	¥2,600,000
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S. Kuroda	Built-in Type Quinone Cofactor Sonodynamic Diagnosis and Therapy of Cancer Using Molecular Target-directed Nanoparticles	¥2,000,000
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Health and Labour Sciences Research Grants

S. Kuroda	Development of Therapy for Acute Myocardial Infarction Using Nano-sized Liposome	¥200,000
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Entrusted Research

S. Kuroda	Japan Science and Technology Agency (Promotion Program of Utilization of Regional Research and Development)	Development of Bio-nanoparticles for Pinpoint Drug Delivery System in Medical Field	¥109,920,000
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Cooperative Research

S. Kuroda	AsOne Corp.	Development of Ultrafast Screening System for Various Bioactive Compounds Using One Cell Pick-Up Apparatus	¥10,010,000
S. Kuroda	GenoLac BL Corp.	Development of Oral Vaccines Using Lactic Bacteria	¥1,000,000

Other Research Fund

K. Tanizawa	Vitamin B Committee	¥250,000
K. Tanizawa	Japan Foundation for Applied Enzymology	¥1,000,000
T. Matsuzaki	Japan Foundation for Type-1 Diabetes Mellitus	¥1,000,000

Department of Single Molecule Biophysics

Professor: Hiroyuki NOJI
Associate Professor: Yoh WADA
Assistant Professor: Kazuhito TABATA, Ryota IINO
PREST Researcher: Hiromi IMAMURA
Post Doctoral Fellows: Daichi OKUNO, Hiromi IMAMURA, Hiroshi UENO, Sawako ENOKI, Masahiro NAKANO
Graduate Students: Rikiya WATANABE, You HUIJUAN, Mizue TANIGAWARA, Yoshito KOMORIYA, Mariko NAKAMURA, Yoshihiro NISHIKAWA, Uner Nacite ESMA, Kumiko ARATA, Yuki MATSUKAGE, Peng JIZHOU, Huynh Nhat Phuong KIM,
Under Graduate Students: Suguru ARAKI, Takuya OOSAKA, Keisuke TOMIYAMA
Supporting Staff: Kazuyo SAKAI, Lisa DATE, Rie HASEGAWA, Kohei HAYAMA, Kunihito YOSHIKAWA, Miki FUKAZAWA

Outlines

Our main research objective is to reveal energy-conversion mechanism of biomolecular motors using single-molecule imaging and single-molecule manipulation techniques. Currently, we launched research projects of micro- and bio-devices to realize high sensitive and high throughput detection of biological reactions using micro/nano technology. We conduct quite interdisciplinary researches crossing biophysics, biochemistry, nanotechnology, and micro/nano fabrication.

Current Research Project

1. Single-molecule studies on a rotary molecular motor, F_1 -ATPase

The crystal structures of F_1 , which provide the structural basis for the catalysis mechanism, have shown essentially one stable conformational state. In contrast, single-molecule studies have revealed that F_1 has two stable conformational states: ATP-binding dwell state and catalytic dwell state. We revealed the correlation between the conformations observed in the crystal structure and single molecule study, and indicated that the crystal structure represents the catalytic dwell state.

2. The role of the epsilon subunit of *Escherichia coli* F_0F_1

The epsilon subunit of bacterial F_0F_1 -ATP synthase, a rotary motor protein, is known to inhibit the ATP hydrolysis reaction of this enzyme. We revealed that the C-terminal domain of the epsilon subunit of *Escherichia coli* F_0F_1 slows multiple elementary steps in both the ATP synthesis/hydrolysis reactions by restricting the rotation of the gamma subunit.

3. Development of offset printing microdroplet chamber array

By applying the offset printing technology, novel microdroplet chamber array was developed. Since oil was used to isolate each chamber containing water, direct access to individual chamber became possible.

Publications

Original Papers

Correlation between the conformational states of F1-ATPase as determined from its crystal structure and single-molecule rotation, D. Okuno, R. Fujisawa, R. Iino, Y. Hirono-Hara, H. Imamura, H. Noji.: Proc. Natl. Acad. Soc. U.S.A., 105 (2008) 20722-20727.

Loop-mediated isothermal amplification of a single DNA molecule in polyacrylamide gel-based microchamber, L. Lam, S. Sakakihara, K. Ishizuka, S. Takeuchi, H.F. Arata, H. Fujita, H. Noji: Biomed Microdevices, 10 (2008) 539-546.

Books

Two rotary motors in ATP-synthase. Iino, R., and Noji H. In "Single Molecule Dynamics in Life Science" Toshio Yanagida and Yoshiharu Ishii Editors. (2008) WILEY-VCH (Germany).

Patents

Polarized total internal reflection illumination optical system by rotary annulus light. Yoshida, M., Suzuki, T., Shio, M., and Iino, R. US 7,486,440 (Feb. 3, 2009).

International Conferences

Femtoliter chamber for single-molecule and single-cell analysis (invited), H.Noji: 4th IEEE-NEMS09.

Single molecule biophysics of F1-ATPase: Mechanical modulation of reaction rate constants and equilibrium constants by F1-ATPase (invited), H.Noji: 6th Asian Biophysics Association Symposium.

Mechanical modulation of ATP-binding and hydrolysis by single F1-ATPase molecule (invited), H.Noji: MPSA2008.

Single-molecule Imaging of the transport-vesicle formation mediated by COPII system reconstituted on a planner bilayer system. (invited), H.Noji: The 17th CDB Meeting - Towards Synthesis of Cells.

Single molecule studies on F1-ATPase molecular motor (invited), H.Noji: 16th International Colloquium on Scanning Probe Microscopy.

Single-molecule study on the rotation of FoF1-ATPase (invited), R.Iino: 5th NSF-MEXT Young Researcher Exchange Program.

Single-molecule studies on the rotation of F₀F₁-ATPase (invited), R.Iino: 4th HANDAI Nanoscience and Nanotechnology Symposium.

Correlation among mechanical steps in rotation, chemical reaction, and crystal structure

of F₁-ATPase unraveled by single-molecule studies (invited), R.Iino: The Fourth Workshop of the UK-Japan Bionanotechnology Collaboration.

Contributions to International Conferences and Journals

H. Noji 4th HANDAI Nanoscience and Nanotechnology Symposium.
(Organizing committee)
H. Noji The 17th CDB Meeting - Towards Synthesis of Cells (Organizer)

Publications in Domestic Meetings

Biophysical Society of Japan	12 papers
Protein Science Society of Japan	1 paper
Molecular Biology Society of Japan	4 papers
Institute of Electrical Engineers of Japan	1 paper

Academic Degrees

Master Degree for Engineering

M. TANIGAWARA	Effect of ion transport on the rotation of ATP synthase
Y. HUIJUAN	Development of a force-clamping system to study the torque generation mechanism of F ₁ -ATPase
Y. KOMORIYA	Role of the Arg-finger in F ₁ -ATPase
Y. NISHIKAWA	Single-molecule measurement of active-inactive states of V ₁ -ATPase
M. NAKAMURA	Reaction intermediate of F ₁ -ATPase probed by inter-subunit cross-linking

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

H. Noji	Rotational mechanism of F ₀ F ₁ -ATP synthase	¥59,700,000
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Grant-in-Aid for Scientific Research (A)

H. Noji	Development of novel single molecule measurement method using ultra-small reaction chamber array	¥7,800,000
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Grant-in-Aid for Young Scientist (B)

R. Iino	Single molecule measurement of rotation of ATP synthase driven by proton motive force	¥800,000
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Grant-in-Aid for JSPS Fellows

H. Ueno	Single molecule rotational observation of F ₀ -motor reconstituted into planar membrane	¥1,100,000
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Entrusted Research

H. Imamura	Japan Science Analysis of ATP metabolism	¥17,920,000
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and Technology by fluorescent probes
Agency

Department of Cell Membrane Biology

Professor:	Akihito YAMAGUCHI
Associate Professor:	Tsuyoshi NISHI
Assistant Professor:	Kunihiko NISHINO(2008.4.1-2009.1.15)
Specially Appointed Assistant Professor:	Mitsuko NISHINO(2008.4.1-2008.8.31)
Post Doctoral Fellow:	Naoki KOBAYASHI
Graduate Students:	Ayumi IWATA, Megumi OHIGASHI, Yu HISANO, Eiji NIKAIDO, Hiroki SAKATA, Tomoyuki NAKANO, Tamami UEDA, Ikue SHIROSAKA, Manami TANAKA, Maki MURATA
Supporting Staff:	Aiko FUKUSHIMA, Chiho MAEDA(2008.11.16-), Sumie MATSUOKA

Outlines

Xenobiotic extruding pumps have recently been known to be widely distributed in living organisms from mammalian to bacteria as a host-defense mechanism in cellular level. These pumps not only confer multidrug resistance of cancer cells and pathogenic bacteria but also cause hereditary diseases through the mutation. The purposes of our laboratory are to elucidate the molecular structures and the molecular mechanisms of these xenobiotic exporters and the roles of these exporters in cell functions. In addition, the exporters having xenobiotic exporter-like molecular structures are identified in brain and platelets in order to elucidate the possible roles of exporters in intercellular signal transduction.

We first determined the crystal structure of bacterial major xenobiotic exporter AcrB in 2002 and elucidated the molecular mechanism of xenobiotic export and the structural basis of multidrug recognition by determining the crystal structure of the drug-binding form of AcrB. In 2008, we continued to analyze crystal structures of the substrate-binding form of AcrB. In addition, we challenged to crystallize the other drug exporter.

As for the regulation of xenobiotic exporter genes and the intrinsic physiological roles of bacterial xenobiotic exporters are also strictly studied as described below.

In addition, studies on the exporters for lipophilic signal transducers in mammalian cells have also been advanced as described below.

Current Research Project

Crystallographic and protein engineering analysis of xenobiotic exporters.

We have succeeded to determine the first crystal structure of bacterial multidrug efflux transporter AcrB in 2002. This is the first crystal structure for transporter proteins. Then we solved the structure of AcrB in complex with its substrates in 2006. The AcrB-substrate complex consists of three protomers, each of which represents one functional state of transport cycle. Bound substrate was found in the periplasmic domain of one of the three protomers. The structure clearly revealed that drugs are exported by

three-step functionally rotating order binding change mechanism. The multidrug recognition is revealed to be based on the multi-site binding of drugs. In 2008, we continued to solve the substrate-binding form of AcrB with different substrates. In addition, we tried to crystallize the other type of exporters such as TetA.

AcrS/EnvR represses expression of the *acrAB* multidrug efflux genes in *Escherichia coli*.

The *acrS* regulatory gene is located upstream of the *acrEF* multidrug efflux system genes. However, the roles of AcrS in regulation of drug efflux pumps have not been clearly understood. We discovered that AcrS represses other multidrug efflux genes, *acrAB*, which encode a major efflux system in *Escherichia coli*.

AcrAB multidrug efflux pump regulation in *Salmonella enterica* serovar Typhimurium by RamA in response to environmental signals.

Salmonella enterica serovar Typhimurium has at least nine multidrug efflux pumps. Among these pumps, AcrAB is effective in generating drug resistance and has wide substrate specificity. We discovered that indole, bile, and an *Escherichia coli* conditioned medium induced the AcrAB pump in *Salmonella* through a specific regulator, RamA. The RamA-binding sites were located in the upstream regions of *acrAB* and *tolC*. RamA was required for indole induction of *acrAB*. Other regulators of *acrAB* such as MarA, SoxS, Rob, SdiA, and AcrR did not contribute to *acrAB* induction by indole in *Salmonella*. Indole activated *ramA* transcription, and overproduction of RamA caused increased *acrAB* expression. In contrast, induction of *ramA* was not required for induction of *acrAB* by bile. Cholic acid binds to RamA, and we suggest that bile acts by altering pre-existing RamA. This points to two different AcrAB regulatory modes through RamA. Our results suggest that RamA controls the *Salmonella* AcrAB-TolC multidrug efflux system through dual regulatory modes in response to environmental signals.

Role of the AraC-XylS family regulator YdeO in multi-drug resistance of *Escherichia coli*.

Multi-drug efflux pumps contribute to the resistance of *Escherichia coli* to many antibiotics and biocides. We discovered that the AraC-XylS family regulator YdeO increases the multi-drug resistance of *E. coli* through activation of the MdtEF efflux pump. Screening of random fragments of genomic DNA for their ability to increase beta-lactam resistance led to the isolation of a plasmid containing *ydeO*, which codes for the regulator of acid resistance. When overexpressed, *ydeO* significantly increased the resistance of the *E. coli* strain to oxacillin, cloxacillin, nafcillin, erythromycin, rhodamine 6G and sodium dodecyl sulfate. The increase in drug resistance caused by *ydeO* overexpression was completely suppressed by deleting the multifunctional outer membrane channel gene *tolC*. TolC interacts with different drug efflux pumps. Quantitative real-time PCR showed that YdeO activated only *mdtEF* expression and none of the other drug efflux pumps in *E. coli*. Deletion of *mdtEF* completely suppressed the YdeO-mediated multi-drug resistance. YdeO enhances the MdtEF-dependent drug efflux activity in *E. coli*. Our results indicate that the YdeO regulator, in addition to its role in acid resistance, increases the multi-drug resistance of *E. coli* by activating the MdtEF multi-drug efflux pump.

Identification of the sphingosine 1-phosphate transporter.

We have been trying to identify the physiologically functional sphingosine 1-phosphate transporter in mammalian cells. We demonstrated that stimuli-dependent and independent sphingosine 1-phosphate (S1P) secretion from platelet and erythrocyte, respectively. However, we could not determine which transporter is contributing to this S1P secretion. Recently, Dr. Kawahara's group isolated the zebrafish mutant that shows cardiac bifida (two heart) as observed in S1P receptor-2 mutant. Novel zebrafish mutant was due to the single nucleotide change, that altered the amino acid sequence at arginine - 153 to serine residue (R153S), in the spinster like protein 2 (*spns2*) gene. Predicted protein encoded with this gene has ten to twelve membrane spanning regions and has significant similarities to a member of the MFS-type transporter. This encouraged us to test the function of this protein as a S1P transporter. When we expressed *spns2* in the CHO cells that over-expressed the sphingosine kinase and enriched the S1P inside the cells, time dependent S1P export activity was observed. This S1P export was not shown in R153S-mutated *spns2* expressing cells. Moreover, *spns2* expression did not alter the cellular sphingolipid contents and did not induce cell death and leakage of sphingosine kinase from the cells. These results are indicating that *spns2* is a S1P transporter essential for the S1P signaling in heart development *in vivo*. We also identified that human and mouse orthologues of the *spns2* have S1P export activity as similar extent to zebrafish *spns2*. Because the *spns2* constitutively exports the S1P from the cells without any stimuli, it should be a candidate for erythrocyte S1P transporter. Recently, it was reported that erythrocyte derived S1P plays an essential role in maintaining the blood S1P level that is necessary for lymphocyte egress from the lymphoid organs. Thus, *spns2* may be a strong target for development of a new transporter oriented immunosuppressant.

Publications

Original Papers

Secreted indole serves as a signal for expression of type III secretion system translocators in enterohaemorrhagic *Escherichia coli* O157:H7, H. Hirakawa, T. Kodama, A. Takumi-Kobayashi, T. Honda and A. Yamaguchi: Microbiology, 155 (pt2) (2009) 541-550.

The Sphingolipid Transporter Spns2 Functions in Migration of Zebrafish Myocardial Precursors, A. Kawahara, T. Nishi, Y. Hisano, H. Fukui, A. Yamaguchi and N. Mochizuki: Science, 323 (5913) (2008) 524-527.

An Atg4B mutant hampers the lipidation of LC3 paralogues and causes defects in autophagosome closure, N. Fujita, M. Hayashi-Nishino, H. Fukumoto, H. Omori, A. Yamamoto, T. Noda and Y. Tamotsu: Mol Biol Cell., 19 (11) (2008) 6451-6459.

Physiological functions of drug efflux systems in Gram-negative bacteria: Their roles in bacterial drug resistance and virulence, K. Nishino and A. Yamaguchi: Jpn. J. Chemother., 56 (4) (2008) 443-452.

Virulence and Drug Resistance Roles of Multidrug Efflux Pumps in *Escherichia coli* and *Salmonella*, K. Nishino and A. Yamaguchi: Bioscience and Microflora, 27 (3) (2008) 75-85.

AcrS/EnvR Represses the Expression of the *acrAB* Multidrug Efflux Genes in *Escherichia coli*, H. Hirakawa, A. Takumi-Kobayashi, U. Theisen, T. Hirata, K. Nishino and A. Yamaguchi: J. Bacteriol., 190 (18) (2008) 6276-6279.

AcrAB Multidrug Efflux Pump Regulation in *Salmonella enterica* serovar Typhimurium by RamA in Response to Environmental Signals, E. Nikaido, K. Nishino and A. Yamaguchi: J. Biol. Chem., 283 (35) (2008) 24245-24253.

Role of Xenobiotic Transporters in Bacterial Drug Resistance and Virulence, K. Nishino and A. Yamaguchi: IUBMB Life, 60 (9) (2008) 569-574.

Review Papers

Structural basis of multidrug recognition by bacterial transporter, A. Yamaguchi, R. Nakashima, Gene & Medicine MOOK The latest studies on transporters 2009, 12 (2009) 61-66

A selective role of dynamin 1 in synaptic vesicle endocytosis, M. Nishino-Hayashi, Pietro De Camilli, Protein, Nucleic Acid and Enzyme, 53 [16] (2008) 2225-2230

Physiological functions of drug efflux systems in Gram-negative bacteria: Their roles in bacterial drug resistance and virulence, K. Nishino, A. Yamaguchi, Japanese Journal Chemotherapy, 56 (2008) 443-452

Roles of Multidrug Efflux Pumps in *Escherichia coli* and *Salmonella*, K. Nishino, Journal of Intestinal Microbiology, 22 (2008) 64

Virulence and Drug Resistance Roles of Multidrug Efflux Pumps in *Escherichia coli* and *Salmonella*, K. Nishino and A. Yamaguchi, Bioscience and Microflora, 27 (2008) 75-85

3D image analysis of inner membrane of synaptic terminal, M. Nishino-Hayashi, A. Yamaguchi, Cell technology, (2008) 107-113

The molecular mechanism of multidrug recognition and active transport by the multidrug transporter, A. Yamaguchi, Transporter Science, (2008) 305-320

Patents

The novel Sphingosine-1-phosphate transporter, N. Mochizuki, A. Kawahara, T. Nishi, A. Yamaguchi, tokugan2008-245177

International Conferences

Physiological functions of multi-drug efflux systems in *S. enterica* (invited), *K. Nishino: Gordon Research Conference on Multi-Drug Efflux Systems (22-27 Mar. 2009,

Texas, USA).

Roles of drug efflux pumps in bacterial multidrug resistance and virulence (invited), *K. Nishino: 3rd Annual Japanese-French Frontiers of Science Symposium (24-26 Jan. 2009, Kanagawa, Japan).

AcrAB multidrug efflux pump regulation in *Salmonella enterica* serovar Typhimurium in response to indole (poster), *I. Shirosaka, E. Nikaido, K. Nishino and A. Yamaguchi: 12th Sanken International Symposium/7th nanotechnology center international symposium/2nd MSTEC international symposium/1st Sanken Alliance Symposium(22 Jan. 2009, Osaka).

Sphingosine-1-phosphate (S1P) Release From Erythrocytes Mediated By ATP-dependent Transporter (poster), *N. Kobayashi, N. Kobayashi, T. Nishi and A. Yamaguchi: 12th Sanken International Symposium/7th nanotechnology center international symposium/2nd MSTEC international symposium/1st Sanken Alliance Symposium(22 Jan. 2009, Osaka).

Electron Tomography Revealed the Endoplasmic Reticulum as a Cradle for Autophagosome Formation (poster), *M. Hayashi-Nishino, N. Fujita, T. Noda, A. Yamaguchi, T. Yoshimori and A. Yamamoto: The American Society for Cell Biology 48th Annual Meeting, San Francisco, 2008.13-17 December.

AcrAB multidrug efflux pump regulation in *Salmonella enterica* serovar Typhimurium by RamA in response to environmental signals, *K. Nishino, E. Nikaido and A. Yamaguchi: The Awaji International Forum on Infection and Immunity, Awaji Island(10 Sep. 2008, Hyogo).

Regulatory network of multidrug efflux pumps reveals their physiological role in *Salmonella* virulence, *K. Nishino and A. Yamaguchi: Gordon Research Conference (6-11 Jul. 2008, MA, USA).

Molecular Design of the Carbenicillin Hyper-Resistance AcrB Multidrug Exporter in *Escherichia coli* (poster), *A. Iwata, N. Kobayashi, S. Murakami and A. Yamaguchi: 22nd Annual Symposium of The Protein Society (July 19-23, 2008, San Diego, California USA).

Structure and Mechanism of the Tripartite Multidrug Exporter, *A. Yamaguchi: The Joint 4th AOHUPO(Asian Oceania Human Proteome Organisation) and 2nd PRICPS(Pacific Rim International Conference on Protein Science) (22-26 Jun. 2008, Carins Convention Center, Australia).

Zebrafish spinster2 involved in the migration of myocardial precursors is a novel regulator in sphingosine-1-phosphate (S1P) signaling (poster), *A. Kawahara, T. Nishi, A. Yamaguchi and N. Mochizuki: 8th International Meeting on Zebrafish development & Genetics (Jun 25-29, 2008, Madison, USA).

Regulatory Network of Multidrug Transporters Reveals their Physiological Role in *Salmonella* Virulence, *K. Nishino and A. Yamaguchi: American Society for Microbiology 108th General Meeting (1-5 Jun. 2008, Boston Convention and Exhibition Center, Boston, Massachusetts).

Regulation of the AcrAB Multidrug Efflux Pump in *Salmonella enterica* by RamA in Response to Environmental Signals, *E. Nikaido, K. Nishino and A. Yamaguchi: American Society for Microbiology 108th General Meeting (1-5 Jun. 2008, Boston Convention and Exhibition Center, Boston, Massachusetts).

Contributions to International Conferences and Journals

A. Yamaguchi Journal of Bacteriology (Editorial Board Member)

Publications in Domestic Meetings

82 th Japanese Society for Bacteriology	5 papers
Biochemistry and Molecular Biology 2008	7 papers
The 56 th Japanese Society of Chemotherapy, Western Japan Division	1 paper
46 th The Biophysical Society of Japan	1 paper
61 th Japanese Society for Bacteriology, the Kansai Division	1 paper
12 th Spring-8 Symposium	1 paper
30 th Membrane-Drug Interaction Symposium	7 papers
The 60 th Annual Meeting of the Japan Society for Cell Biology	1 paper
The 12 th Scientific Meeting for INTESTINAL MICROBIOLOGY	1 paper
The 56 th Japanese Society of Chemotherapy	1 paper
The 82 th Japanese Association for Infectious Diseases	1 paper

Academic Degrees

Doctor Degree for Pharmaceutical Sciences

A. Iwata	Functional analysis of AcrAB-TolC complex based on crystal structures
M. Ohigashi	Cell-specific expression and function of ABC transporter, ABCA5

Master Degree for Pharmaceutical Sciences

H. Sakata	Physiological functions of xenobiotic transporters in bacterial virulence
T. Nakano	Roles of xenobiotic transporters in polymyxin B resistance

Sponsorship

Grant-in-Aid for Scientific Research (S)

A. Yamaguchi	Structures, functions, regulations and physiological roles of xenobiotic exporters	¥21,580,000
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Grant-in-Aid for Young Scientists (S)

K. Nishino	Roles of orphan transporters in multidrug-resistant bacteria and development of therapeutic strategies to control infectious diseases	¥12,740,000
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Grant-in-Aid for Scientific Research on the Priority Area

K. Nishino	Resistome analysis of bacterial genome	¥4,700,000
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Grant-in-Aid for JSPS Fellows

S. Nishi	Elucidation of control mechanisms of proton pump activity responding to environmental signals	¥800,000
E. Nikaido	Regulatory network of multidrug transporters reveals their physiological role in <i>Salmonella</i> virulence	¥600,000
Y. Hisano	Identification and physiological role of the sphingosine-1-phosphate export system in mouse platelets	¥600,000
M. Ohigashi	Functional analysis of ABCA transporters for identification of the export system that mediates secretion of lipophilic signal transducing molecules	¥900,000

Entrusted Research

A. Yamaguchi	National Institute of Biomedical Innovation	Development of novel inhibitors that counteract infectious diseases by drug resistant bacteria	¥93,000,000
K. Nishino	Japan Science and Technology Agency • PRESTO	Roles of xenobiotic transporters in cellular physiology	¥15,600,000

Other Research Fund

A. Yamaguchi	Takeda science foundation	Analysis of signal transduction system regulated by efflux transporters	¥10,000,000
K. Nishino	Inamori foundation	Regulatory mechanisms of gene expression of drug efflux systems	¥1,000,000
K. Nishino	Kanae foundation for the promotion of medical science	Structure, function and physiological roles of drug efflux systems	¥1,000,000
K. Nishino	Mochida memorial foundation for medical and pharmaceutical research	Roles of xenobiotic transporters in multidrug-resistant bacteria and development of therapeutic strategies to control infectious diseases	¥2,000,000
K. Nishino	Astellas foundation for research on metabolic disorders	Protection principles of pathogenic bacteria and host cell on bacterial infection	¥1,000,000
K. Nishino	The Uehara memorial foundation	Roles of efflux transporters and development of therapeutic strategies to control infectious diseases	¥3,000,000

Division of Quantum Beam Science & Technology

Outline

The quantum beam is the general term for all kinds of radiation beams producing quantum mechanical effects on materials. It includes photon beams and charged particle beams such as lasers, X-rays, synchrotron radiation, γ -rays and free electron lasers, electrons, positrons, muons and ions, as well as neutron beams. Quantum beam science has developed from radiation science and its research fields are classified into two groups. One of them is study on production, control and measurement of new high-brightness and high quality quantum beams, which are remarkably developing recently. The other is study on processes induced by quantum beams in materials, as well as on applications to materials science based on accurate understanding of these phenomena induced by a quantum beam.

The division of Quantum Beam Science and Technology is composed of the department of Accelerator Science and the department of Beam Materials Science. In the department of Accelerator Science, studies are conducted on accelerators, which are main apparatuses for producing quantum beams, and on production, control and measurement of quantum beams using accelerators. In the department of Beam Materials Science, basic studies are conducted to investigate phenomena induced by quantum beams and to apply them to materials science; that is, production and application of new materials such as functional materials and materials working under extreme conditions. Both departments closely work together with different points of view; generation of new quantum beams and applications of them to materials science. This division also cooperates with the Radiation Laboratory, attached to the Nanotechnology center, in order to promote advanced studies with a different point of view from that of national laboratories. Furthermore we plan to actively promote researches to develop and use high-performance accelerators suitable for producing new kinds of high-brilliant and high-quality beams and for applying to materials science, which are being developed or under construction in this country as well as abroad.

Achievements

- In order to upgrade the L-band electron linac, new RF couplers of the loop-type for the magnetic coupling are introduced to monitor ports of the RF cavities for the SHB system, a new method is developed to control the phase and the amplitude of the RF power fast and precisely, and development of a new grid pulse generator has begun to improve performance of the electron gun.
- A new instrument is being developed to directly measure the electron distribution of the electron beam in the phase space consisting of energy and time.
- The wavelength region of the far-infrared FEL is extended between 40 and 110 μm and FEL dynamics in the high power region is studied.
- Development of an L-band RF electron gun has begun to enhance brilliance of the electron beam significantly.
- Study on upgrade of the accelerator system for synchrotron radiation source has

begun in collaboration with the Synchrotron Research Institute of Thailand.

- Analysis of primary process in interactions between beams and molecular/polymer materials.
- Development of ultrafast measurement system using electron and photon pulse.
- Electronic structure and physical properties of π -conjugated polymer materials.
- Reaction mechanisms in polymeric materials for microelectronics.
- Electrodeless measurement of conductivity in organic semiconductors by microwave technique.
- Ionizing radiation induced damages in DNA.

Department of Accelerator Science

Professor: Goro ISOYAMA
Associate Professor: Ryukou KATO
Assistant Professors: Toshiji IKEDA, Shigeru KASHIWAGI
Graduate Students: Yutaka MORIO, Yoshikazu TERASAWA,
Kenichiro FURUHASHI

Outline

Particle accelerators are widely used from basic science to industrial applications. In this department, we conduct research on accelerators and quantum beams such as a free electron laser (FEL). Although accelerators are artificial things, fundamental aspects of physics such as non-linearity and the collective effect become apparent when extreme performance is pursued. Because new kinds of quantum beams extend the world we can see with, they are expected to be used in a large variety of fields extending from basic research to applications. To put it concretely, we conduct researches on production of a highly brilliant electron beam with a linear accelerator and related beam dynamics, development of an infrared FEL for user experiments and SASE (Self-Amplified Spontaneous Emission) in the infrared region.

Current Research Projects

Upgrade of the L-band Linac

Three RF cavities of the Sub-Harmonic Buncher (SHB) system, fabricated last year, have been working well. RF monitors of the antenna type for electric coupling were adopted in these cavities at first. A strange phenomenon was found that the ground level of the pulse waveform shifted when Helmholtz coils for beam focusing were excited. This kind of phenomenon had not been observed in the previous RF cavities, in which loop-type monitors for magnetic coupling were used, so that the antenna-type monitors were replaced with the loop-type monitors with coupling factors of $10^{-3} \sim 10^{-2}$.

In the multi-bunch mode operation used for FEL, it is necessary to accelerate a long-pulse electron-beam with a small energy spread. The amplitude and the phase of the pulsed RF power provided to the linac have to be constant over the pulse duration of 8 μ s. Variations of the input RF power in the pulse are currently reduced to 0.3 degrees in phase and 0.89 % in amplitude with the feed forward control of the low-level input RF. A phase shifter used in this system has a relatively slow response time of $\sim 1 \mu$ s and owing to the response time accuracy of the control is limited. We are, therefore, investigating to use an IQ modulator, with which the RF phase and the amplitude can be fast and simultaneously controlled. An ideal IQ modulator can generate an RF signal with specified phase and amplitude, once the output power of each channel is measured and calibrated for each control voltage, but a real IQ modulator has large errors in phase and amplitude from specified values owing to a coupling between I and Q channels and non-linear responses. We are measuring characteristics of the IQ modulator and studying how to control it.

We are developing an FET grid pulse generator for the thermionic electron gun to be

used for the L-band linac in order to generate a series of bunches with the time duration of 5 ns and intervals of 37 ns. We have set up a test bench for the electron gun and the grid pulse generator and have begun preparation for measurement of its performance. We have confirmed that the electron gun can produce an electron pulse with the peak current of 2.4 A, which meets our specifications, though the pulse duration used for the experiment is a few μ s long.

Production and Measurement of Highly Brilliant Electron Beams

We are conducting research and development of a phase space monitor, with which the electron distribution can be directly measured in the phase space defined by the accelerating energy of the L-band linac and time. Cherenkov light is measured with a streak camera, which is emitted in hydrophobic silica-aerogel (refractive index $n = 1.050$) by the electron beam with the energy dispersion produced by a bending magnet. We are commissioning the phase space monitor fabricated last year. Since the optical transport system from the monitor installed on the FEL beam line to the streak camera in the measurement room has not been completed, we set up a tentative optical line with standard optical components. It is difficult to gather all the Cherenkov light emitted in a large angular cone by means of a mirror placed in the air, so that a part of the light is sliced out with the mirror. Because a phase space distribution with the energy width of only 1.1 % can be obtained in a single measurement, the total phase space distribution over the wide energy range is reconstructed from many data measured by changing the excitation current of the bending magnet. We measured and derived phase space distributions of single bunch electron beams accelerated at three different RF phases around the RF crest. The measured phase space distributions can be qualitatively understood by taking into account the sinusoidal RF field and the wake field produced by the single bunch beam. It has been experimentally demonstrated that the phase space distribution can be measured with the present system.

Development of the Far-Infrared Free Electron Laser

Since the success in the first high power operation of the FEL at wavelengths $\sim 70 \mu\text{m}$ in 2007, we are conducting research to measure characteristics of the FEL and to expand the wavelength region. We have obtained FEL operation in the wavelength region from 40 to 110 μm by changing the electron beam energy and the magnetic field of the wiggler. We measured time spectra of the FEL light of a 105 μm wavelength with the pulse duration of 3~4 μs using a fast Ge:Ga semiconductor detector as a function the length of the optical cavity. The measured time spectra show various features reflecting the FEL dynamics. The FEL gain and the loss of the optical cavity derived from the slopes of the leading edge and the trailing edge are 45 % at the maximum and 8~9.5 %, respectively. Parallel to this measurement, wavelength spectra of FEL light are measured with a grating monochromator as a function of the cavity length. The peak intensity and its width of the measured wavelength spectra change significantly with the cavity length and the behaviors are similar to those observed in near-infrared and mid-infrared FELs.

When the FEL power becomes saturated in the pulse, the sinusoidal oscillation of light intensity is observed on the top of the square pulse. The oscillation period we observed gradually becomes longer as the cavity length increases. Analysis based on the latest FEL theory explains the measured dependence of the oscillation period on the

cavity length more precisely, so that we conclude that the behaviors are generated by the limit cycle FEL lasing.

Development of an L-Band RF Electron Gun

We have begun research and development of the L-band RF electron gun in collaboration with the High Energy Accelerator Research Organization (KEK). We take part in development of an L-band RF electron gun for the Superconducting RF Test Facility (STF) of KEK and prepare for commissioning of the RF cavity in production at the Fermi National Accelerator Laboratory (FNAL). We have investigated methods for tuning the resonance frequency and the electric field distribution of the RF cavity using a computer code. We have also made physical and mechanical design of an RF cavity and an input coupler for Osaka University. We altered the design of the input coupled made by FNAL to have more reasonable structure. The RF cavity and the input coupler were made of aluminum at the Mechanical Engineering Center of KEK and their RF characteristics and performance were measured and evaluated. The input coupler was used for tuning the RF cavity made by FNAL. We have also studied structures and arrangement of solenoid coils for emittance compensation and find a more appropriate solution. The RF cavity made by FNAL was temporally sent to KEK for tuning the resonance frequency and the field distribution, and after completing these adjustments it was sent back to FNAL for final brazing of cooling pipes.

Upgrade of the Synchrotron Radiation Source

We have begun research on upgrading of the accelerator system for the synchrotron radiation source in collaboration with the Synchrotron Light Research Institute in Thailand. It is essential to make performance and stability higher of the injector system consisting of a 40 MeV electron linac and a 1 GeV electron synchrotron in order to make the performance of the light source higher, so that we have begun development of a beam monitor system for the electron linac. A project is in progress to install a superconducting wiggler on the 1.2 GeV storage ring and to set up a beam line for protein crystallography. A vacuum duct for the quadrupole magnets downstream of the wiggler has to be replaced with a new one with higher cooling performance, so that we are designing the vacuum duct.

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Publications in Domestic Meetings

Annual Meeting of Particle Accelerator Society of Japan and the Linear Accelerator Meeting	9 papers
Annual Meeting of the Japanese Society for Synchrotron Radiation Research	1 paper
Annual Meeting of the Physical Society of Japan	3 papers

Academic Degree

Master Degree for Science

Y. Morio	Fast phase and amplitude control of the pulsed RF for acceleration of the L-band electron linac and its application to generation of the highly brilliant electron beam.
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Sponsorships

Grant-in-Aid for Scientific Research (C)

R. Kato	Development of the longitudinal phase-space monitor for high-brightness electron beams	¥780,000
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Grant-in-Aid for Young Scientists (B)

S. Kashiwagi	Development of coherent light source based on the interaction between electron beam and laser undulator field	¥1,950,000
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Other Research Fund

G. Isoyama	Collaboration and supporting program for universities of the High Energy Accelerator Research Organization	Advancement of the electron source with the L-band RF electron gun	¥1,000,000
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Department of Beam Materials Science

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Outline

Main subjects of the present department are utilization of quantum beams for molecular science, research on mechanisms of phenomena induced by quantum beams, and analysis of microscopic structure of materials. Quantum beams mean both beams such as photons and beams inducing interactions with materials in the microscopic level of quantum mechanics. The beams cause completely different physico-chemical reactions in condensed matters from conventional chemical reactions. Features of beams are highly developed for electrons, ions, positrons, as well as photons (synchrotron radiation, gamma-rays, and lasers).

Current Research Projects

1. Analysis of Primary Process in Interactions between Beams and Molecular Materials

Physico-chemical reactions, which occur within nano- and pico- second region, are considered to dominate followed reactions and products in molecular materials. High-accuracy spectrum acquisition system was developed using CCD camera, highly-stable femtosecond white light continuum, and double pulse detection technique, resulting in approximately two orders of magnitude higher performance than conventional system. The direct observation of reactive intermediates is carried out to elucidate the mechanisms and to control the reaction. Aromatics have high radiation resistance. The characteristic has been used in electron beam lithography. Especially, the radiation-induced reaction of aromatics is important to improve and understand the resist materials. Primary process of irradiated aromatics from nano- to picosecond time scale is investigated by electron beam pulse radiolysis.

2. Development of Ultrafast Measurement System Using Electron and Photon Pulses

The measurement system was developed to trace ultrafast phenomena by ultra short

pulses of electrons and photons in the current program. Transient spectroscopy is done within 0.8 psec approaching to shorter time region. Dynamics of short-lived intermediates have been observed for several molecular materials.

3. Electronic Structure and Physical Properties of σ -and π -Conjugated Polymers

Polysilanes and polygermanes containing only silicon and germanium in the backbone are attached considerable attention because of their interesting electro-optical properties which are due to conjugated bondings in the main chain. The electronic structure of conjugated skeleton is investigated in the present program, which leads to improve the physical properties of the conjugated polymers.

4. Reaction Mechanisms in Polymeric Materials for Microelectronics

Line edge roughness (LER) of patterned features in chemically amplified (CA) resists is formed in the acid generation stage and expected to be moderated by the acid diffusion and development process. It is essential to obtain information on the limit of LER in order to realize next-generation lithographies such as electron beam or extreme ultraviolet. We report a process simulator based on physical and physico-chemical reaction mechanisms. The LER of a positive-tone CA resist after development is investigated by the Monte Carlo simulation and Mack's dissolution model. We found that a LER (high frequency) of less than 1.2 nm is achievable, although the process conditions for achieving such a small LER are strict.

5. Electrodeless measurement of conductivity in organic semiconductors by microwave technique

Using time-resolved microwave conductivity (TRMC) which enables us to measure nano-scale electric conductivity in organic semiconductors, we investigated electric and optical properties of super-molecular nanotubes, pentacene thin films, and sigma-conjugated polymer: polysilane. We report the charge carrier dynamics in single-crystal rubrene studied by time-resolved microwave conductivity and transient photoabsorption/emission spectroscopies upon exposure to 355 nm. Based on the comparison of the kinetics and extinction coefficients of radical cation/anion estimated by pulse radiolysis, the minimum alternating-current mobility of $(5.2 \pm 0.7) \times 10^{-2} \text{ cm}^2/\text{V s}$ was obtained without electrodes and resolved into hole and electron components, i.e. exhibition of ambipolar nature. The dynamics and optoelectronic property are discussed in terms of second-order reaction, exciton-exciton annihilation, quantum efficiency, triplet contribution, and density functional theory. Anisotropic mobility is also measured by utilizing defined direction of microwave electric field, suggesting the band-like motion on the nanometer-scale conduction. Time-resolved conductivity and photoabsorption studies of single-crystal rubrene provide important information on the intrinsic nature of charge carrier transport.

6. Ionizing Radiation Induced Damage in DNA

The dynamics of electron adducts of oligonucleotides (ODNs) were measured spectroscopically by nanoseconds pulse radiolysis. The radical anions of the nucleotides were produced by the reaction of hydrated electrons and were protonated to form the

corresponding neutral radicals. The transient spectra of excess electrons of the double-stranded ODNs (**AT**) and (**GC**) differed from those of pyrimidine radicals (C and T) and their composite. In contrast, the spectra of the electron adducts of the single-stranded ODNs **GC** and **AT** exhibited characteristics of C and T, respectively. These results suggest that, in duplex ODNs, the spectral intermediates of G-C and A-T anions complex. On microseconds time scale, the subsequent changes in absorbance of the ODN **AT** had a first-order rate constant reflecting the protonation of T.

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Fluorine Atom on Acid Generation in Chemically Amplified EUV Resists (poster), *T. Fukuyama, T. Kozawa, K. Okamoto, S. Tagawa, M. Irie, T. Mimura, T. Iwai, J. Onodera, I. Hirose, T. Koganesawa, and K. Horie: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Effect of molecular structures of acid generators on acid generation in chemically amplified resists upon exposure to 75 keV electron beam (poster), *K. Natsuda, T. Kozawa, K. Okamoto, and S. Tagawa: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Dynamics of Radical Cation of Poly(4-Hydroxystyrene) and its Complex (poster), *K. Okamoto, M. Tanaka, T. Kozawa, and S. Tagawa: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Effects of Polymer Interference in Acid Generation on Latent Image Quality of Extreme Ultraviolet Resists (poster), *T. Kozawa, and S. Tagawa: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Latent image formation in chemically amplified extreme ultraviolet resists with low activation energy for deprotection reaction (poster), T. Kozawa, S. Tagawa, J. J. Santillan, and T. Itani: 52nd International Conf. Electron, Ion, and Photon Beam Technology & Nanofabrication, Portland, Oregon, USA.

Multispur in chemically amplified electron beam resists (poster), T. Kozawa, K. Okamoto, and S. Tagawa: 52nd International Conf. Electron, Ion, and Photon Beam Technology & Nanofabrication, Portland, Oregon, USA.

Study on acid generation of acid generators in chemically amplified resists for electron beam Reactivity of Halogenated Resist Polymer with Low-energy Electrons (poster), *K. Natuda, T. Kozawa, K. Okamoto, and S. Tagawa: International Workshop on Molecular Information and Dynamics 2008, Taipei, Taiwan.

Nano-fabrication of Fluoropolymers using Focused Ion Beam (poster), *N. Fukutake, T. Urakawa, Y. Takasawa, T. Gowa, T. Takahashi, T. Hirano, M. Washio, A. Oshima, K. Okamoto, and S. Tagawa: Fluoropolymer 2008, Charleston, South Carolina, USA.

Dynamics of Radical Cations of Resist Model Compounds (poster), *K. Okamoto, M. Tanaka, T. Kozawa, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Microfabrication of Nano-scale Pattern on Crosslinked PTFE using Focused Ion Beam (poster), *N. Fukutake, T. Urakawa, Y. Takasawa, A. Oshima, M. Washio, A. Oshima, K. Okamoto, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Plasmonic Waveguides with Wavelength Selective Function (poster), *M. Haraguchi, Y. Matsuzaki, T. Tsuzura, T. Okamoto, M. Fukui, K. Okamoto, S. Seki, and S. Tagawa: Proceedings of SPIE-The International Society for Optical Engineering.

Dynamics of Guanine Radical Cations in Duplex DNA Studied by Pulse Radiolysis (poster), *K. Kobayashi, R. Yamagami, and S. Tagawa: 10th International Workshop Radiation Damage to DNA, Urabandai Japan.

Dynamics of Excess Electron in Duplex DNA Studied by Pulse Radiolysis (poster), R. Yamagami, K. Kobayashi, and S. Tagawa: 10th International Workshop Radiation Damage to DNA, Urabandai Japan.

Effect of Base Sequence and Deprtonation of Guanine Cation Radical in DNA (poster), K. Kobayashi, R. Yamagami, and S. Tagawa: Gordon Conference, Waterville, USA.

Dynamics of Excess Electron in Duplex DNA Studied by Pulse Radiolysis (poster), K. Kobayashi, R. Yamagami, and S. Tagawa: Gordon Conference, Waterville, USA.

Dynamics of Excess Electron in Duplex DNA Studied by Pulse Radiolysis (poster), K. Kobayashi, R. Yamagami, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Multispur effects in chemically amplified resists (poster), T. Kozawa, K. Okamoto, A. Saeki, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Feasibility Study on High-Sensitivity Chemically Amplified Resists by Polymer Absorption Enhancement in Extreme Ultraviolet Lithography (poster), T. Kozawa, K. Okamoto, J. Nakamura, and S. Tagawa: International Symposium on Extreme Ultraviolet Lithography, Lake Tahoe, California, USA.

Sensitization mechanisms of chemically amplified resists and resist design for 22 nm node (poster), T. Kozawa and S. Tagawa: 2009 International Workshop on EUV Lithography, Oahu, Hawaii, USA.

Electrode-less measurement of conductivity transients in poly(n-alkylthiophene)s induced by 193nm photoexcitation (poster), A. Saeki, S. Ohsaki, Y. Koizumi, S. Seki, and S. Tagawa: Conference of Photopolymer Science and Technology 2008.

Dynamics of Intermediates in Chemically Amplified EB Resist (poster), A. Saeki, T. Kozawa, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Charge dynamics in organic crystals, supermolecules, and dendrimers (poster), A. Saeki, S. Seki, and S. Tagawa: PULS'2008 (8th International Conference on Pulse Investigations in Chemistry, Biology and Physics).

Impact of Side-Chain Length on Alternating Current Mobility of Charge Carrier in Regioregular Poly(3-alkylthiophene) Films (poster), A. Saeki, S. Ohsaki, Y. Koizumi, S. Seki, and S. Tagawa: 18th Iketani Conference (International Conference on Control of Super-Hierarchical Structures and Innovative Functions of Next-Generation Conjugated Polymers).

Electrodeless Determination of Charge Carrier Mobility in Poly(3-hexylthiophene) Films Incorporating Perylene-3,4,9,10-tetracarboxylic diimide as Photoconductivity Sensitizer and Spectroscopic Probe (poster), A. Saeki, S. Ohsaki, S. Seki, S. Tagawa: Japan-Korea Polymer Young Scientist Symposium.

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	10 papers
Atomic Energy Society of Japan	2 papers
The Japan Society of Applied Physics:	12 papers
The Japan Society of Polymer Science	2 papers
The Japan Society of Biochemistry	3 papers

Academic Degrees**Doctor Degree for Engineering**

Ryuhei YAMAGAMI Sequence Dependent Dynamics of Hole and Electron in DNA

Master Degree for Engineering

Masafumi TANAKA	Formation dynamics of dimer radical cation of polystyrene derivatives
Hayato HIJIKATA	Development of bottom EUV-sensitive coating film for the evaluation of the absorption coefficient of extreme ultraviolet resist
Takahiro FUKUYAMA	Study of Acid Generator Distribution in Chemically Amplified Resist Films using Synchrotron Radiation

Sponsorships**Grant-in-Aid for Scientific Research (S)**

S. Tagawa	Femtosecond Pulse Radiolysis Study on Time Profile of Radiation-Induced Processes in Nanoscopic Region	¥20,900,000
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Grant-in-Aid for Scientific Research(C)

K. Kobayashi	Mechanism in Regulation of Transcription Factor containing Fe-S Clusters Sensing Oxidative Stress	¥1,200,000
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Grant-in-Aid for Young Scientists (A)

A. Saeki	Nanometer-scale dynamics of charge carriers in organic semiconductors by using radiations and microwave	¥9,100,000
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Grant-in-Aid for JSPS Fellows

R. Yamagami	Contact-less evaluation of intrinsic conductive property of single DNA molecule	¥1,000,000
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S. Tagawa	ASET	Research on reaction mechanism of chemically amplified resist	¥1,000,000
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Other Research Fund

S. Tagawa	JST CREST	Research on resist for ultrafine fabrication and development of process simulator	¥166,270,000
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S. Tagawa	ASET	Research on reaction mechanism of chemically amplified resist	¥1,000,000
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Other Research Fund

S. Tagawa	Nissankagaku company	Development of bottom EUV-sensitive coating film for the evaluation of the absorption coefficient of extreme ultraviolet resist	¥1,000,000
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S. Tagawa	SELETE	Research on EUV resists	¥5,000,000
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S. Tagawa	Matsushita company	Dissolution characteristics of extreme ultraviolet resist EUV resists	¥1,000,000
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Division of Next Industry Generation

Outline

Three new research departments have been established. The goal of each department is to provide advances in science and technology via close relationships with industry, which will lead to create a novel industry in the 21st century.

The departments are:

-Department of New Industrial Projection

Perform research on new projects that can lead to industrial-structure innovations in the next generation.

-Department of New Industry Generation System(s)

Investigate and develop novel business systems that enable transfer of academic research outcomes to a new industry effectively and promptly, and that intend to improve productivity through responding to social demands.

-Department of Intellectual Property Research

Perform the strategic world-leading study of intellectual property linked with potential needs of the society, where the academia is required to create intellectual properties efficiently from the wide-ranging knowledge accumulated from academic research of the new interdisciplinary fields of material, information, and biology.

Achievement

- The growth dynamics of Japanese firms classified by capital
- Development of a new intellectual property map
- Analysis and evaluation of intellectual property of Japanese universities
- Surveillance study on intellectual property exploitation in European universities

Department of New Industrial Projection

Professor: Hiroshi KATAYAMA-YOSHIDA
Designated Research Assoc.: Makoto NAKAZAWA
Supporting Staff: Mika ASADA, Ryoko ITO

Outline

Now in the 21st century, Japanese industrial structure is being transformed from a traditional industrial society to a knowledge-based society. In the knowledge-based society, instead of process innovation ("how to make"), product innovation ("what to make") is required. Thus new strategy for the change of the industrial structure is needed. We aim for the establishment of a framework to project new industries in future society (including the projection of the basic research required in the society) based on the analysis of the existing industries.

Current Research Projects

Analysis on growth dynamics of Japanese Manufacturing Industries

An analytical investigation has been made on statistical numerical indices of Japanese manufacturing companies in the process of new industrial projection based on the analysis of existing industries. We have investigated the capital size distribution and growth rates of Japanese manufacturing companies. It is found that the growth rates of profits are related to the capital sizes of the Japanese manufacturing companies. This result indicates that the capital size is an important reference index to discuss the growth potential of the industrial companies.

Development of Intellectual Property Map

The method for visualizing technology and market can be a very powerful tool to project new industries. To this end, we have developed an intellectual property map created by mapping both patent descriptions of interest and the keywords selected from the patent descriptions at the calculated position in the same plane. A new mapping method is developed by incorporating the clustering technique of closely related keywords in the descriptions of the patents in interest. This method will be developed to visualize the existing technologies, newly developed technologies and technologies demanded by market to project new industries based on new science and technology.

Department of Intellectual Property Research

Specially Appointed Professor: Hirokazu SHIMIZU

Specially Appointed Researcher: Seiichiro TAMAI(10.1.2008-)

Outline

The object of this department is to perform the strategic world-leading study of intellectual property linked with potential needs of the society, where the academia is required to create intellectual properties efficiently from the wide-ranging knowledge accumulated from academic researches of the new interdisciplinary fields of material, information, and biology.

Current Research Project

Analysis and evaluation of Intellectual Property of Japanese Universities

Analytical research has been made in the applied patents of Osaka University by using existing patent analysis and evaluation tools to clarify the problems and to investigate their measures for promoting utilization of the patents. It is found that the quality of the patents of Osaka University is low compared with Japanese major companies. It is also found that the patent descriptions of Osaka University are deficient in practicable statements. These tools are considered to be useful as a feedback action before filing the patents.

Survey Research on Intellectual Property Exploitation of European universities

We have investigated the policies and measures for industrialization of new technologies through academia-industry cooperation by visiting European universities and research organizations in France, Germany and England. The investigation has been made especially on industrialization of nanotechnologies. The R&D project of academia-industry cooperation on the assumption of production in strategic region of Germany and the industrialization system through networking in the incubation facilities for venture companies in England serve as useful references different from Japanese systems. It is noteworthy that each country is improving academia-industry cooperation systems for promoting next generation industries.

Publications

“How major companies establish and use intellectual property rights created in basic research?”, Seiichiro Tamai, Intellectual Property Seminar of Osaka University, Feb.5, 2009.

Division of Special Projects

Laboratory of Microbiology and Infectious Diseases

Associate Professor: Kunihiro NISHINO(2009.1.16-)
Graduate Students: Eiji NIKAI, Hiroki SAKATA, Tomoyuki NAKANO,
Tamami UEDA, Ikue SHIROSAKA, Manami TANAKA
Supporting Staff: Aiko FUKUSHIMA

Outlines

Multidrug-resistant bacteria are now encountered frequently and the rates of multidrug resistance have increased considerably in recent years. Genome annotation produces a considerable number of drug efflux pumps in bacteria. We previously identified efflux pumps related with bacterial multidrug resistance and virulence. Our discoveries support the notion that drug efflux pumps have specific physiological substrates because these pumps have been shown to have roles in bacterial virulence. We are trying to identify natural substrates of drug efflux pumps in order to understand physiological functions of pumps. This knowledge should promote the development of novel inhibitors or strategies that could counteract the contribution of efflux pumps to drug resistance and virulence.

Current Research Project

H-NS modulates multidrug resistance of *Salmonella enterica* serovar Typhimurium by repressing *acrEF* multidrug efflux genes.

Bacterial multidrug efflux pumps confer resistance to a wide range of antibiotics, dyes, and biocides. In Gram-negative bacteria, pumps belonging to the resistance-nodulation-cell division (RND) family are especially effective in conferring resistance. Our recent studies have shown that *S. enterica* has nine functional drug efflux pumps. Because many of these multidrug transporters have overlapping substrate spectra, it is intriguing that bacteria, with their economically organized genomes, harbor such large sets of multidrug efflux genes. The key to understanding how bacteria utilize these multiple efflux pumps lies in the regulation of pump expression. Currently available data show that multidrug efflux pumps are often expressed under precise and elaborate transcriptional control.

However, few data are available on the regulation of *S. enterica* multidrug efflux genes. We therefore screened for *S. enterica* mutations that increased multidrug resistance levels in this organism. During the study, we performed a genome-wide search for a regulator of multidrug resistance in *S. enterica* by random insertion and found that H-NS downregulates the expression of *acrEF*. We initially found by random insertion that the mutation in *hns* conferred oxacillin resistance on *Salmonella*. Then, we investigated the susceptibility of the strain lacking *hns* to various drugs, including common substrates of multidrug efflux pumps, and found that H-NS modulates *S. enterica* resistance to oxacillin, cloxacillin, nafcillin, cefamandole, methylene blue, and rhodamine 6G. DNA-binding protein H-NS is a global transcriptional regulator that

specifically silences horizontally acquired virulence genes in *Salmonella*. This process is achieved through interactions between H-NS and AT-rich DNA regions with low specificity. For the intergenic region located upstream of *acrE* in which H-NS was found to repress expression to 1/35 of the original level, the average GC content is 31.7%, whereas the average GC content of the entire *Salmonella* LT2 genome is 52.2%. It should be noted that this intergenic region harbors a 100 bp AT-rich DNA region located at 295 to 196 bp upstream of the start codon of *acrE*, which has a GC content of 16.0%. The AcrF efflux pump is highly homologous to AcrB in *S. enterica* with an 81.4% amino acid identity and similar substrate specificities. We found that *acrEF* is repressed by H-NS whereas *acrAB* is not and is constitutively expressed. Because overexpression of *acrEF* confers a similar effect as *acrAB*, H-NS represses *acrEF* and might confer a fitness advantage in this organism.

Role of the AraC-XylS family regulator YdeO in multi-drug resistance of *Escherichia coli*.

Multi-drug efflux pumps contribute to the resistance of *Escherichia coli* to many antibiotics and biocides. We discovered that the AraC-XylS family regulator YdeO increases the multi-drug resistance of *E. coli* through activation of the MdtEF efflux pump. Screening of random fragments of genomic DNA for their ability to increase beta-lactam resistance led to the isolation of a plasmid containing *ydeO*, which codes for the regulator of acid resistance. When overexpressed, *ydeO* significantly increased the resistance of the *E. coli* strain to oxacillin, cloxacillin, nafcillin, erythromycin, rhodamine 6G and sodium dodecyl sulfate. The increase in drug resistance caused by *ydeO* overexpression was completely suppressed by deleting the multifunctional outer membrane channel gene *tolC*. TolC interacts with different drug efflux pumps. Quantitative real-time PCR showed that YdeO activated only *mdtEF* expression and none of the other drug efflux pumps in *E. coli*. Deletion of *mdtEF* completely suppressed the YdeO-mediated multi-drug resistance. YdeO enhances the MdtEF-dependent drug efflux activity in *E. coli*. Our results indicate that the YdeO regulator, in addition to its role in acid resistance, increases the multi-drug resistance of *E. coli* by activating the MdtEF multi-drug efflux pump (*J. Antibiot.*[Nature Publishing Group] in press, 2009).

Publications

Original Papers

Regulation of the AcrAB multidrug efflux pump in *Salmonella enterica* serovar Typhimurium, E. Nikaido, I. Shirosaka, A. Yamaguchi, K. Nishino: Recent Advances in Clinical Pharmacology, (2009) in press.

Regulation and physiological function of multidrug efflux pumps in *Escherichia coli* and *Salmonella*, K. Nishino, E. Nikaido, A. Yamaguchi: BBA-Proteins & Proteomics, (2009) in press.

Role of the AraC/XylS family regulator YdeO in multidrug resistance of *Escherichia coli*, K. Nishino, Y. Senda, M. Hayashi-Nishino, A. Yamaguchi: J. Antibiot., (2009) in press.

H-NS modulates multidrug resistance of *Salmonella enterica* serovar Typhimurium by repressing *acrEF* multidrug efflux genes, K. Nishino, Y. Senda, M. Hayashi-Nishino, A. Yamaguchi: *Antimicrob. Agents Chemother.*, (2009) in press.

International Conferences

Physiological functions of multi-drug efflux systems in *S. enterica* (invited), *K. Nishino: Gordon Research Conference on Multi-Drug Efflux Systems (22-27 Mar. 2009, Texas, USA).

Roles of drug efflux pumps in bacterial multidrug resistance and virulence (invited), *K. Nishino: 3rd Annual Japanese-French Frontiers of Science Symposium (24-26 Jan. 2009, Kanagawa, Japan).

Publications in Domestic Meetings

82 th Japanese Society for Bacteriology	5 papers
The Japan <i>Pseudomonas aeruginosa</i> Infection Society	1 paper

Academic Degrees

Master Degree for Pharmaceutical Sciences

H. Sakata	Physiological functions of xenobiotic transporters in bacterial virulence
T. Nakano	Roles of xenobiotic transporters in polymyxin B resistance

Sponsorship

Grant-in-Aid for Young Scientists (S)

K. Nishino	Roles of orphan transporters in multidrug-resistant bacteria and development of therapeutic strategies to control infectious diseases	¥12,740,000
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Grant-in-Aid for Scientific Research on the Priority Area

K. Nishino	Resistome analysis of bacterial genome	¥4,700,000
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Grant-in-Aid for JSPS Fellows

E. Nikaido	Regulatory network of multidrug transporters reveals their physiological role in <i>Salmonella</i> virulence	¥600,000
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Entrusted Research

K. Nishino	Japan Science and Technology Agency • PRESTO	Roles of xenobiotic transporters in cellular physiology	¥15,600,000
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Other Research Fund

K. Nishino	Inamori foundation	Regulatory mechanisms of gene expression of drug efflux systems	¥1,000,000
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K. Nishino	Kanae foundation for the promotion of medical science	Structure, function and physiological roles of drug efflux systems	¥1,000,000
K. Nishino	Mochida memorial foundation for medical and pharmaceutical research	Roles of xenobiotic transporters in multidrug-resistant bacteria and development of therapeutic strategies to control infectious diseases	¥2,000,000
K. Nishino	Astellas foundation for research on metabolic disorders	Protection principles of pathogenic bacteria and host cell on bacterial infection	¥1,000,000
K. Nishino	The Uehara memorial foundation	Roles of efflux transporters and development of therapeutic strategies to control infectious diseases	¥3,000,000

Activities of Centers

Nanoscience and Nanotechnology Center

Director Professor: Katsuaki SUGANUMA
Support Staff: Mayo HAYASHI

Outline

Nanoscience and Nanotechnology Center was founded in April 2002 for developing Bottom-up Nanotechnology, Top-down Nanotechnology, and their Industrial Application. This center consists of four divisions; (1) Nanomaterial and Nanodevices, (2) Beam Science for Nanotechnology, (3) Nanoscience and Nanotechnology for Industrial Applications and (4) Nanocharacterization together with five laboratories (Radiation Laboratory, Electron Microscope Laboratory, Electronic Processing Laboratory, Nanofabrication Shop and Open Laboratory) and Nanotechnology Process Foundry.

Division of Nanomaterials and Nanodevices

Outline

The main purpose of this division is to construct function harmonized nano-materials which can mimic flexible data processing like human body. By using typical “Bottom-up Nanotechnology” of artificial lattice technique, we combine metal, inorganic and (bio)organic materials at an atomic/molecular level to new nano-materials. The object of this division is also to research molecular-scale devices based on the function of single molecule. We are developing new techniques for the measurement of physical and chemical properties of single or several molecules. Furthermore, design and syntheses of supramolecules such as artificial DNA, photosynthetic molecules, and a novel branched polythiophenes having more efficient and selective functions than those of single molecules are being investigated towards constructions of organized supramolecular systems such as artificial living cells and nano-devices and organic electronics materials exhibiting multifunction, complex properties, and conjugated functions. Proteins and their complexes with other biomolecules are regarded as nano bio devices. The research of our group is focused on structural and functional studies on such devices. We are also interested in developing highly sensitive biosensors and nano machines.

Achievement

- Construction of functional nano-materials, which can mimic flexible data processing like human body.
- Investigation of relationship with structure and material properties at nano-scale.
- Development of bottom-up nanotechnology and control of nano-scale interface.
- Fusion of Bottom-up and Top-down Nanotechnologies
- Creation of super-five senses sensor and brain type memory.
- Programmed self-assembly and self-organization for molecular device.
- Control of electrode-molecule interface for molecular devices.
- Construction of Gating Nanopore
- Construction of Nanowell biochip
- Charge separation in DNA.
- Mechanism of photosensitized one-electron oxidation of DNA.
- Development of a novel branched polythiophene as an organic electronics material.
- Structural analysis of reaction intermediates formed on the catalytic cycle of copper amine oxidase.
- Purification and crystallization of MFS-type bacterial drug exporter.

Department of Artificial Nanomaterials for Bio-Information

Systems

Professor: Hidekazu TANAKA
Assistant Professor: Teruo KANKI
Specially Appointed Assistant Professor: Nam Goo CHA
Under Graduate Students: Hidefumi TAKAMI
Supporting Staff: Megumi IKEDA

Outline

This research group focuses on functional oxide materials, which show huge response to external fields such as temperature, light, electric and magnetic fields, and establishes techniques and processes for controlling dimensionality and position in nano-scale space concerning optimal oxide materials by fusing two processes of “Bottom-up nanotechnology”, which is fabrication techniques of ultra-thin films, heterojunctions and artificial lattice using a pulsed laser deposition method, and “Top-down nanotechnology” for nanoimprint and /or atomic force microscopy (AFM) lithography methods. Our fruition in the near future will lead creation of novel multi-function-harmonized nano-materials/devices with sensing, information processing and memories. The main subjects in this year are (1) Nano-patterning of magnetic oxide nano-structures with large area by using nanoimprint lithography and evaluation of their physical properties, (2) fabrication of spinel ferrite nano-wire structures by using AFM lithography and evaluation of their physical properties, and (3) fabrication of vanadium oxide films with huge non-linear response against temperature and an electrical field.

Current Research Projects

Nano-patterning of magnetic oxide nano-structures with large area by using nanoimprint lithography and evaluation of their physical properties

The advance of nano-patterning techniques for functional oxide materials is an important subject toward not only construction of nano-integrated devices but also interest in nano-physics such as quantum effects. In the present situation, nano-fabrication techniques for oxide materials are not enough and the typical size of oxide devices are about several to hundreds micrometer orders by using photolithography. As one of promising methods for oxide nano-patterning, we note a nanoimprint technique in order to produce nano-patterned structures with a large area.

Device makers in the field of Si processing expect this technique as a future manufacturing method with a low cost. If we can apply this technique to the oxide nanofabrication process, it would be an effective tool to fabricate oxide nanopatterns with a large area. However, typical organic resist masks are not feasible because high temperature process over several hundreds degree Celsius include to form epitaxial oxide films. Here in our group, the Mo masks were used as the heat-enduring resist, having stable performance even at high temperature, instead of polymer resists. We show a nanoimprint process performed for spinel ferrite (Fe,Zn)₃O₄ (FZO) thin films as a example; (i) The Mo resist was sputtered on the PMMA layer patterned by

nanoimprint on a n-type Nb(0.2wt%)-SrTiO₃(100) substrate. (ii) The PMMA resist was removed by dissolving in acetone solvent and only the Mo nano-mask patterned remains. (iii) The FZO film was epitaxially deposited on this mask by a PLD technique under the condition of 360 degree for substrate-temperature and 10⁻⁴ Pa for oxygen-pressure. At that time the Mo nano-patterned resist endured against such a high temperature-fabrication-process. (iv) The Mo layer was removed by ultrasonication in H₂O₂ solvent. Finally, the FZO nano-pattern was formed.

Thus we successfully obtained nano-dot array of 300 nm to 1μm size of epitaxial FZO with a large area. Physical property of these nano-dot array structures showed a Schottky diode type character. We found that nano-dot FZO structure have high spin-polarized carriers from detail investigation. In addition, we made 3D gold nano-boxes by combining a nanoimprint and sputtering methods. This result has big step of creation of complicated 3D nano-structures.

Fabrication of spinel ferrite nano-wire structures by using AFM lithography and evaluation of their physical properties

Transition metal oxides have spatially inhomogeneous electrical and/or magnetic domains. That is why physical properties of the nano-structures would be quite different from that of bulk materials. In this research project, we made (Fe,Mn)₃O₄ nano-wire structures or nano-constricted structures. As results, one dimensional alignment of magnetic domains was observed in the nano-wire with 120nm-width. The 50nm-constricted nano-structure showed non-linear current-voltage property (I-V). This result experimentally made it clear that a nano-constricted part traps magnetic domains and work as a potential barrier in spin-polarized carriers, showing big magnetic resistance effect at room temperature. This achievement suggests possible to control a few magnetic domains in nano-space and to apply to other functional oxide materials.

Fabrication of vanadium oxide films with huge non-linear response to temperature and an electrical field

Vanadium oxide (VO₂) show drastic change of electronic and structural properties around 70°C. In order to apply this huge non-linear response to novel electronic functions, we fabricated VO₂ thin films in this year. The comparator property was observed in the films, showing non-linear response when input signal amplitude was beyond a threshold voltage. Another function of this film is for noise generator, using the phase-instability between monoclinic with high resistivity and triclinic with low resistivity. In addition, we succeeded in adjustment of the metal-insulator transition temperature in W-doped VO₂ thin films by control of doping level of W, and found the possibility of room temperature devices.

Publications

Original Papers

Crucial role of interdiffusion on magnetic properties of in situ formed MgO/Fe₃-delta O₄ heterostructured nanowires, A.Marcu, T.Yanagida, K.Nagashima, K.Oka, H.Tanaka, T.Kawai: Appl. Phys. Lett., 92 (2008) 173119.

Effect of Heterointerface on Transport Properties of In-situ Formed MgO/titanate

Heterostructured Nanowires, K. Nagashima, T. Yanagida, H. Tanaka, S. Seki, A. Saeki, S. Tagawa, T. Kawai: J. Am. Chem. Soc., 130 (2008) 5378-5382.

Hard X-ray Photoemission Spectroscopy Combined with Magnetic Circular Dichroism: Application to $\text{Fe}_{3-x}\text{Zn}_x\text{O}_4$ Spinel Oxide Thin Films, S. Ueda, H. Tanaka, J. Takaobushi, E. Ikenaga, J.-J. Kim, M. Kobata, T. Kawai, H. Osawa, N. Kawamura, M. Suzuki, and K. Kobayashi: Appl. Phys. Express, 1 (2008) 077003.

Growth atmosphere dependence of transport properties of NiO epitaxial thin films, K. Oka, T. Yanagida, K. Nagashima, H. Tanaka, T. Kawai: J. Appl. Phys., 104 (2008) 13711.

Mechanism of critical catalyst size effect on MgO nanowire growth by pulsed laser deposition, T. Yanagida, K. Nagashima, H. Tanaka, T. Kawai: J. Appl. Phys., 104 (2008) 16101.

Mechanochemical preparation of magnetite nanoparticles by coprecipitation, T. Iwasaki, K. Kosaka, N. Mizutani, S. Watano, T. Yanagida, H. Tanaka, T. Kawai: Materials Lett., 62 (2008) 4155-4157.

Ferromagnetic oxide Schottky diode of $(\text{Fe}, \text{Mn})_3\text{O}_4/\text{Nb}:\text{SrTiO}_3$ heterostructure with strongly correlated electrons, I. Satoh, J. Takaobushi, H. Tanaka, T. Kawai: Solid State Commun., 147 (2008) 397-400.

Epitaxial Nanodot Arrays of Transition-Metal Oxides Fabricated by Dry Deposition in Combined with a Nanoimprint-Lithography-Based Molybdenum Lift-Off Technique, N. Suzuki, H. Tanaka, S. Yamanaka, M. Kanai, B. K. Lee, H. Y. Lee, T. Kawai: Small, 4 (2008) 1661-1665.

Effect of ferrous/ferric ions molar ratio on reaction mechanism for hydrothermal synthesis of magnetite nanoparticles, N. Mizutani, T. Iwasaki, S. Watano, T. Yanagida, H. Tanaka, T. Kawai: Bulletin of Materials Sci., 31 (2008) 713-717.

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Implications of phase-segregation on structure, terahertz emission and magnetization of $\text{Bi}(\text{Fe}_{1-x}\text{Mn}_x)\text{O}_3$ ($0 \leq x \leq 0.5$) thin films, D. S. Rana, I. Kawayama, K. Takahashi, K. R. Mavani, H. Murakami, M. Tonouchi, T. Yanagida, H. Tanaka, T. Kawai: European Phys. Lett., 84 (2008) 67016.

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Non-volatile Bipolar Resistive Memory Switching in Single Crystalline NiO Heterostructured Nanowires, K. Oka, T. Yanagida, K. Nagashima, H. Tanaka, T. Kawai: J. Am. Chem. Soc., 131 (2009) 3434-3435.

Fabrication of $(\text{Fe,Mn})_3\text{O}_4$ ferromagnetic oxide nanostructure using Molybdenum nano-mask atomic force microscope lithography, K. Gotoh, H. Tanaka, T. Kawai: J. Appl. Phys., 105 (2009) 064301.

Patents

Comparator, noise generator and stochastic resonance devices, T. Kanki, Y. Hotta, N. Asakawa, T. Kawai, H. Tanaka, Tokugan2008-259480

Tunneling Magnetoresistive Element, Semiconductor Junction Element, Magnetic Memory and Semiconductor Light Emitting Element, H. Tanaka, T. Kawai, Patent No. US7, 468,282 B2

International Conferences

Ferroelectric Control of Carrier mediated Ferromagnetism in Spinel Ferrite with High Curie Temperature (poster), *H. Tanaka, J. Takaobuishi, T. Kanki and T. Kawai: The IEEE Nanotechnology Materials and Devices Conference 2008, Kyoto, Japan, Oct. 20-22, 2008.

Epitaxial $(\text{Fe,Mn})_3\text{O}_4$ Artificial Nano-Wire Structures Fabricated by a Combination of AFM Lithography and Molybdenum Lift-off with High Controllability in Their Shape and Positioning, K. Gotoh, *H. Tanaka and T. Kawai: MRS Fall Meeting 2008, Boston, USA, Dec. 1-5, 2008.

High Throughput Fabrication of Epitaxial Oxide Nano-dot and Nano-heterojunction Arrays Composed of Ferromagnetic Spinel Fe Oxide by Nanoimprint Lithography with Mo Lift-off Technique, H. Tanaka, *S. Yamanaka and T. Kawai: MRS Fall Meeting 2008, Boston, USA, Dec. 1-5, 2008.

Magnetic and electric properties of photo-induced magnet $(\text{Al,Ru,Fe})_3\text{O}_4$ spinel ferrite thin films (poster), *T. Kanki, Y. Hotta, N. Asakawa, M. Seki, E. Ikenaga, H. Tabata, H. Tanaka, K. Kobayashi, and T. Kawai: The IEEE Nanotechnology Materials and Devices Conference 2008, Kyoto, Japan, Oct. 20-22, 2008.

Magnetic and Electronic Characters of Photo-induced Magnet $(\text{Al,Ru,Fe})_3\text{O}_4$ Spinel Ferrite Thin Films, *T. Kanki, Y. Hotta, N. Asakawa, M. Seki, H. Tabata, H. Tanaka and T. Kawai: MRS Fall Meeting 2008, Boston, USA, Dec. 1-5, 2008.

Electronic Application of Stochastic Resonance by Utilizing Nonlinear Property of Vanadium Oxide: Toward Creation of Bio-Mimetic Devices (poster), *T. Kanki, Y.

Hotta, N. Asakawa, H. Tanaka and T. Kawai: MRS Fall Meeting 2008, Boston, USA, Dec. 1-5, 2008.

Contributions to International Conferences and Journals

H. Tanaka	The IEEE Nanotechnology Materials and Device Conference (NMDC 2008) (Sub-Committee Member)	
H. Tanaka	4th Handai Nano Science and Nanotechnology International Symposium (Organizing Committee Chair)	

Publications in Domestic Meetings

The Japan Society of Applied Physics	6 papers
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Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

T. Kanki	Creation of novel photoinduced-magnetic oxide materials and application to spintronic devices	¥23,000,000
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Entrusted Research

H. Tanaka	National Institute for Materials Science	Development of Hard X-ray Photoemission Microscope for 3 Dimensional Chemical State Analysis	¥1,050,000
H. Tanaka	Japan Society for the Promotion of Science	Fabrication of Nano-scale Oxide Heterostructures by Combination of Top-down and Bottom-up Nanotechnologies	¥1,200,000

Other Research Fund

H. Tanaka	The Mazda Foundation	¥2,000,000
H. Tanaka	Mitutoyo Association for Science and Technology	¥2,000,000
H. Tanaka	Suzuki Foundation	¥1,000,000
H. Tanaka	Research Foundation for the Electrotechnology of Chubu	¥5,000,000
H. Tanaka	Research Foundation for the Electrotechnology of Chubu	¥260,000
H. Tanaka	Kansai Research Foundation for Technology Promotion	¥300,000
T. Kanki	The Murata Science Foundation	¥2,000,000

Department of Single-Molecular Integrated Devices

Professor:	Tomoji KAWAI
Associate Professor:	Takuya MATSUMOTO
Specially Appointed Research Associate:	Bong-Kuk LEE
Support Staff:	Yumiko NOGI

Outlines

Notwithstanding the great anticipation of the potential of molecular-scale electronics, it is very difficult to fabricate molecular-devices, owing to the lack of effective technologies for wiring molecules and connecting molecules to electrode. Self-organization is a promising route to fabricating complicated nanostructure by “bottom-up” process with highly selective chemical-reactions.

The object of this department is to research molecular-scale devices based on the function of single molecule. We are developing new techniques for the measurement of electrical properties for molecular nanostructures. We are also developing an interconnect method to program three kinds of component molecules with their own functions, and to create a molecular device between nano-scale electrodes in a self-organized manner.

On the other hand, the multifunctional, electrochemical nanobiosensor system based on the self-assembly is developing for the analysis and detection of various biomolecules. For this, it is necessary to establish the elemental technologies, such as a nanopatterning of substrate using a top-down technique, the self-assembled nanoarray of probe biomolecule into the nanostructured substrate using a bottom-up technique, the integration of nanobiosensor system and the detection of the target biomolecules using an electrochemical technique. Then, the establishment of an each elemental technology necessary to develop the multifunctional electrochemical nanobiosensor system was researched aiming at current year.

Current Research Project

Imaging DNA and protein polarizations by Electrostatic force microscopy

Electrostatic force microscopy images of double-stranded DNA and transcription complex on an insulating mica substrate were obtained with molecular resolution using a frequency-mode noncontact atomic force microscope. The electrostatic potential images show that both DNA and transcription complexes are polarized with upward dipole moment. By analyzing potential differences of these molecules from the mica substrate, we determined that the values of dipole moments in zero external fields are 0.027 D/base and 0.16 D/molecule for isolated DNA and transcription complex, respectively. In contrast, we demonstrated that scanning capacitance microscopy gives characteristic contrast inversion between DNA and transcription complex images reflecting the difference of electric polarizability of these molecules. These findings indicate that the electrostatic properties of individual biological molecules can be imaged on an insulator substrate while retaining complex formation.

Electrical Resistivity of Molecular-Assembly Nanowire of Amphiphilic Charge Transfer Complex Characterized by PCI-AFM

Point-contact current-imaging atomic force microscope (PCI-AFM), which was developed in our laboratory, was applied to characterize electrical resistivity measurements of individual molecular-assembly nanowire of a CT complex between amphiphilic bis-TTF macrocycle (1) and 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-*p*-quinodimethane (F₄-TCNQ).^{3a} By applying Langmuir-Blodgett (LB) method to (1²⁺)(F₄-TCNQ)₂, oriented nanowire structure was constructed on mica substrate. Typical dimensions of nanowires were 2.5 nm in height, 10-100 nm in width and 1000 nm in length. Electrical resistivity of the nanowire was 10³-10⁵ Ωcm at room temperature measured on multi-layer LB films with electrode gap of 0.5 mm. Since electrode gap was much larger than the length of each nanowire, the conduction should be governed by hopping between nanowires. Therefore, characterization of electrical conduction within each nanowire was desired.

Nanopatterning of Inert Materials and Nanoarray of Lipid Bilayer

The best plan to construct a biomolecular nanoarray is to make the biomolecule array by using a stepwise self-assembly after the nanostructure is fabricated by the inert material that prevents nonspecific adsorption of biomolecules. Then, we established the elemental technologies to fabricate the nanostructures with the inert materials such as UV-curable polyvinyl alcohol and polyethylene glycol by using the UV- nanoimprint lithography (UV-NIL) as well as succeeded in the construction of the nanoarray of various biomolecules such as liposome and tethered-bilayer lipid raft (tBLR) on the pre-patterned substrate using the stepwise self-assembly.

Fabrication of Highly Durable Replica Mold

Recently, the nanoimprint lithography (NIL) attracts increasing attention as the next generation nanopatterning method. However, this technique has the problems such as the deformation and contamination of the expensive master mold by the mechanical contact with the resin and the master mold. One method of overcoming this problem is to reproduce the master mold without damage in a short time by an appropriate material with good mechanical strength, and to use it as mold for NIL. Then, we succeeded in the reproduction of the replica mold with good mechanical property (Young's modulus = 1.76 GPa) from master mold by using UV-curable organic-inorganic hybrid resin. This replica mold has high durability even if the imprinting is done repeatedly under UV-NIL and thermal-NIL conditions.

Publications

Original Papers

High-density DNA Alignment on an Au(111) Surface Starting from Folded DNA, H. Matsuura, A. Hirai, F. Yamada, T. Matsumoto, T. Kawai: J. Am. Chem. Soc., 130 (15) (2008) 5002-5003.

Self-Organized Functional Lipid Vesicle Array for Sensitive Immunoassay Chip, H.- Y. Lee, B.- K. Lee, J.- W. Park, H.- S. Jung, T. Kawai: Ultramicroscopy, 108 (10) (2008)

1325-1327.

Electrical Resistivity of Molecular-Assembly Nanowires of Amphiphilic Bis-TTF Macrocycle/2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-p-quinodimethane Charge Transfer Complex Characterized by PCI-AFM, R. Tsunashima¹, Y. Noda, Y. Tatewaki, S.- I. Noro, T. Akutagawa, T. Nakamura, T. Matsumoto, T. Kawai: Appl. Phys. Lett., 93 (29) (2008) 173102-1-3.

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Nanoarray of Tethered Lipid Bilayer Rafts on Poly(vinyl alcohol) Hydrogel, B.- K. Lee, H.- Y. Lee, P. Kim, K.- Y. Suh, T. Kawai: Lab on a Chip, 9 (1) (2009) 132-139.

Review Papers

Electrostatic force microscopy of nano-scale adsorbates on a insulating solid surface –application to biological molecules (in Japanese).

T.Matsumoto,F.Yamada,E.Satho-Mikamo,A.Takagi,T.Kawai

Journal of The Surface Science Society of Japan, 29, (2008) 246-252.

Nanoscale imaging of surface charges by scanning probe microscopy (in Japanese).

T.Matsumoto,T.Kawai

Journal of the Clay Science Society of Japan ,47 [1], (2008) 1-8.

Development of time-resolved electrostatic force detection using scanning probe microscopy (in Japanese)

T.Matsumoto,T.Kawai

MICROSCOPY, 43 [2], (2008) 149-151.

Nano Fabrication of Functional Transition Metal Oxide Thin Films (in Japanese)

N.Suzuki, Hide.Tanaka,Y.Yanagisawa,S.Yamanaka,L.Pellegrino,

B.-K.Lee,H.-Y.Lee,T.Kawai

Journal of the Vacuum Society of Japan, 51[1], (2008) 37-43.

Books

BioNanoProcess Introduction to Wet-Nanotechnology: *in aqua* Organization of Nano-Structures. Chapter 23: Creation of Nano-Material and Device by Programed self-assembly. (in Japanese)

N.Suzuki, K.Adachi, B.-K.Lee, T.Kawai

CMC, (2008) ISBN978-4-88231-995-5.

Patents

“Probe apparatus for measuring an electron state on a sample surface”

Takuya Matsumoto, Tomoji Kawai

(Feb. 10, 2009), US 7,486,667 B2

“Highly durable replica-molds for nanoimprint lithography and a method of manufacturing the same”

Tomoji Kawai , Hea Yeon Lee, Bong Kuk Lee , Lan-Young Hong, Dong-Pyo Kim,
(Sep.18.2008), Tokugan 2008-239827

Highly Durable Replica Mold for Nanoimprint Lithography and Fabrication Method,
Tomoji Kawai, Hea Yeon Lee, Bong Kuk Lee, Dong-Pyo Kim, Lan-Young Hong,
Korean (Jan. 29, 2009), 10-2009-0006902

International Conferences

Time-resolved Electrostatic Force Detection by Frequency Shift Mode (poster), T. Matsumoto, T. Kawai: 11th International Conference on Non-Contact Atomic Force Microscopy Madrid 2008, September 16-19, (2008), Madrid, Spain.

Electric Dipoles of Surface Nano-Structures on Insulating Substrates (poster), F. Yamada, A. Takagi, E. Mikamo-Satoh, T. Matsumoto, T. Kawai: 11th International Conference on Non-Contact Atomic Force Microscopy Madrid 2008, September 16-19, (2008), Madrid, Spain.

Integrated NanoBiochip through Soft NanoLithography (invited), B.- K. Lee, H.- Y. Lee, T. Kawai: The 4th Handai Nanoscience and Nanotechnology International Symposium, September 29–October 1, (2008) , Osaka, Japan.

Time-resolved Electrostatic Force Detection by Frequency Shift Mode, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology, November 9-13, (2008), Tokyo, Japan.

Molecule Recognition Imaging by Frequency Shift Detection on Liquid (poster), T. Matsumoto, T. Kawahara, H. Hokonohara, M. Kawano, T. Kawai: International Symposium on Surface Science and Nanotechnology, November 9-13, (2008), Tokyo, Japan.

Electric Dipoles of Surface Nano-Structures on Insulating Substrates (poster), F. Yamada, A. Takagi, E. Mikamo-Satoh, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology, November 9-13, (2008), Tokyo, Japan.

Force Measurement between Protein, IL-6 and IL-6 Receptor, Immobilized at N-terminal (poster), H. Hokonohara, A. Takagi, T. Matsuura, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology, November 9-13, (2008), Tokyo, Japan.

Arrays Mn12 Complex with DNA Template, Y. Segawa, F. Yamada, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology, November 9-13, (2008), Tokyo, Japan.

Conduction through Biomolecular Arrays, T. Matsumoto, T. Kawai: 4th International Meeting on Molecular Electronics elecml'08, December 8-12, (2008) Grenoble, France.

Transverse Conduction DNA Probed by Simultaneous Measurements of STM and Non-contact AFM (poster), T. Matsumoto, Y. Maeda, T. Kawai: 4th International Meeting on Molecular Electronics elecml'08, December 8-12, (2008) Grenoble, France.

Conduction through Biomolecular Arrays (poster), Takuya Matsumoto: Fifth International Conference on Molecular Electronics and Bioelectronics (M&BE5), March 15-18, (2009) Miyazaki, Japan.

Contributions to International Conferences and Journals

T. Matsumoto	Program Committee
	International Symposium on Surface Science and Nanotechnology (ISSS-5)

Publications in Domestic Meetings

The Japan Society of Applied Physics	4 papers
The Surface Science Society of Japan	2 papers
The Biophysical of Japan	2 papers
Others	1 paper

Sponsorship

Grant-in-Aid for Scientific Research on Innovative Areas

T. Matsumoto	Emergence of self-organized molecular system with top-down nanoelectdes	¥9,500,000
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Grant-in-Aid for Scientific Research (B)

T. Matsumoto	Analysis of molecular recognition in liquid by pulse-modulated attractive force microscopy	¥5,300,000
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Grant-in-Aid for Exploratory Research

T. Matsumoto	Nanoscale hopping conduction through self-organized molecular array with DNA templates	¥2,100,000
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Department of Supramolecular Chemistry

Professor: Tetsuro MAJIMA
Associate Professor: Kiyohiko KAWAI
Research Associate: Makoto KARAKAWA

Outlines

Towards the construction of organized supramolecular systems with multifunctionality, the design and syntheses of supramolecules such as spherical nanoparticles, artificial DNA, proteins, photosynthetic molecules, and metal-bridged polymers having more efficient and selective functions than those of single molecules have been investigated.

Development of a novel branched polythiophene as a organic electronics material are also studied.

Current Research Project

Sequence-Independent Rapid Charge Transfer through DNA

DNA forms self-assembled nano-structures like cubes as well as two-dimensional molecular sheets that we can control by programming the base sequence of the adenine-thymine (A–T) and guanine-cytosine (G–C) base-pairs, thus has the potential as a bottom-up material for nano-templates and nano-machines. Especially, the finding that DNA can conduct an electrical current has made it an interesting molecule for the design of nano-electronic circuits. However, because a hole migrates along DNA through the HOMO of the G bases, its conductivity decreases as the A–T base pair content increases. This means that there are limitations on what sequences can be used to construct functional nano-electronic circuits, particularly those rich in A–T pairs. Here we show that the charge transfer efficiency can be drastically increased in a G independent manner by adjusting the HOMO level of the A–T base-pair to be closer to that of the G–C pair. This is achieved by substituting the N7 nitrogen atom of A with a C–H group - to give deaza-adenine (Z) - which does not disturb the complementary base-pairing observed in DNA. The charge transfer efficiency through DNA was investigated for a DNA with a G–C and A–T mixed random sequence longer than 100 Å.

The charge transfer occurred as fast as $\tau = 0.45 \mu\text{s}$ over 100 Å by replacing the A–T base-pair with the Z–T base-pair. The charge transfer rate significantly decreased by more than three order of magnitude by converting one Z–T base-pair to a A–T base-pair showing that a rapid charge transfer through a mixed DNA sequence can be only achieved by replacing the A–T base-pair with the Z–T base-pair.

Development of a novel branched polythiophene as a organic electronics material.

π -Conjugated polymers based on thiophene molecules have been intensively investigated as an active material for organic field-effect transistors (OFETs) and photovoltaic cells. These π -conjugated polymers have several advantage, such as solution processability, higher hole mobility, structural flexibility and compatibility

with plastic substrates.

Our group has recently reported on an amorphous dendritic oligothiophene semiconductor for OFETs. The dendritic oligothiophene exhibited strong intermolecular interactions in a solution, constructing molecular self-aggregation which was detected by means of ^1H NMR and MALDI-TOF mass analyses. The aggregation property contributed to higher field-effect hole mobility. On the basis of these findings, we designed new polymer semiconductors containing branched units. The branched units of polymer material would exhibit a molecular aggregation property, leading to an effective hole hopping transportation in a film on an OFET.

We will investigate the syntheses of branched polythiophene derivatives, as new polymeric semiconductors, constructed from quater thiophenes and phenyl branching units, and also investigate the OFET characteristics based on the compounds. OFET devices using the branched polythiophene derivatives were prepared by spin-coating from a chloroform solution on a silicon-dioxide surface with pre-deposited source and drain gold electrodes. These devices exhibited typical p-type transistor behaviors. The FET performances were affected by the length of the branched units.

Publications

Original Papers

Intramolecular Excimer Formation and Photoinduced Electron Transfer Process in bis-1,8-Naphthalimide Dyads Depending on the Linker Length, D. W. Cho, M. Fujitsuka, A. Sugimoto, and T. Majima: *J. Phys. Chem. A*, 112 (31) (2008) 7208-7213.

Excitation Energy Dependence of Photoinduced Processes in Pentathiophene-Perylenediimide Dyads with a Flexible Linker, M. Fujitsuka, K. Harada, A. Sugimoto, and T. Majima: *J. Phys. Chem. A*, 112 (41) (2008) 10193-10199.

Photodecomposition Profiles of β -Bond Cleavage of Phenylphenacyl Derivatives in the Higher Triplet Excited States during Stepwise Two-Color Two-Laser Flash Photolysis, M. Yamaji, X. Cai, M. Sakamoto, M. Fujitsuka, and T. Majima: *J. Phys. Chem. A*, 112 (45) (2008) 11306-11311.

Properties of Excited Radical Cations of Substituted Oligothiophenes, S. Samori, M. Fujitsuka, and T. Majima: *J. Phys. Chem. A*, 112 (45) (2008) 11312-11318.

Photoinduced Charge Transfer Processes on MOF-5 Nanoparticles: Elucidating Differences between Metal-Organic Frameworks and Semiconductor Metal Oxides, T. Tachikawa, J. R. Choi, M. Fujitsuka, and T. Majima: *J. Phys. Chem. C*, 112 (36) (2008) 14090-14101.

Iodine-Doped TiO_2 Photocatalysts. Correlation between Band Structure and Mechanism, S. Tojo, T. Tachikawa, M. Fujitsuka, and T. Majima: *J. Phys. Chem. C*, 112 (38) (2008) 14948-14954.

Interfacial Electron Transfer Dynamics in a Single CdTe Quantum Dot-Pyromellitimide Conjugate, S.-C. Cui, T. Tachikawa, M. Fujitsuka, and T. Majima: *J. Phys. Chem. C*,

112 (49) (2008) 19625-19634.

Spatial Control of Protein Binding onto Lipid Bimembrane Using Photoeliminative Linker, K. Nakayama, T. Tachikawa, and T. Majima: *Langmuir (Letter)*, 24 (13) (2008) 6425-6428.

Fine-Tuning of Radiolysis Induced Emission by Variable Substitution of Donor-/Acceptor-Substituted Tetrakis(arylethynyl)benzenes, S. Samori, S. Tojo, M. Fujitsuka, E. L. Spitler, M. M. Haley, and T. Majima: *J. Org. Chem.*, 73 (9) (2008) 3551-3558.

Defect-Mediated Photoluminescence Dynamics of Eu^{3+} -Doped TiO_2 Nanocrystals Revealed at the Single-Particle or Single-Aggregate Level, T. Tachikawa, T. Ishigaki, J.-G. Li, M. Fujitsuka, and T. Majima: *Angew. Chem. Int. Ed.*, 47 (29) (2008) 5348-5352.

Two-laser-guided Three-dimensional Microfabrication and Processing in Flexible Polymer Matrix, M. Sakamoto, T. Tachikawa, M. Fujitsuka, and T. Majima: *Adv. Mater.*, 20 (18) (2008) 3427-3432.

Charge transfer in DNA assembly: effects of sticky end, Y. Osakada, K. Kawai, M. Fujitsuka, and T. Majima: *Chem. Commun.*, (2008) 2656-2658.

Two Different Mechanisms Operating in Photoinduced Electron Transfer of 1,8-Naphthalimide-linker-phenothiazine Dyads, D. W. Cho, M. Fujitsuka, U. C. Yoon, and T. Majima: *Phys. Chem. Chem. Phys.*, 10 (30) (2008) 4393-4399.

Kinetic of charge transfer in DNA containing a mismatch, Y. Osakada, K. Kawai, M. Fujitsuka, and T. Majima: *Nucl. Acids Res.*, 36 (17) (2008) 5562-5570.

Triplet Level Dependent Photoluminescence and Photoconduction Properties of π -Conjugated Polymer Thin Films Doped by Iridium Complexes, J. An, J. Chang, J. Han, C. Im, Y.-J. Yu, D. H. Choi, J.-I. Jin, and T. Majima: *J. Photochem. Photobiol. A*, 200 (2-3) (2008) 371-376.

Photoreactivity of As-Fabricated Au Clusters at the Single-Cluster Level, M. Sakamoto, T. Tachikawa, M. Fujitsuka, and T. Majima: *J. Am. Chem. Soc. (Commun.)*, 131 (1) (2009) 6-7.

Single-Molecule Observation of Photocatalytic Reaction in TiO_2 Nanotube: Importance of Molecular Transport through Porous Structures, K. Naito, T. Tachikawa, M. Fujitsuka, and T. Majima: *J. Am. Chem. Soc. (Commun.)*, 131 (3) (2009) 934-936.

α -Bond Dissociation of *p*-Phenylbenzoyl Derivatives in the Higher Triplet Excited State during Two-color Two-laser Flash Photolysis, M. Yamaji, X. Cai, M. Sakamoto, M. Fujitsuka, and T. Majima: *J. Phys. Chem. A*, 113 (9) (2009) 1696-1703.

Electron Transfer in Supramolecular Donor-Acceptor Dyad of Zinc Porphycene, M. Fujitsuka, H. Shimakoshi, S. Tojo, L. Cheng, D. Maeda, Y. Hisaeda, and T. Majima: *J. Phys. Chem. A*, 133 (14) (2009) 3330-3335.

Intramolecular Dimer Radical Anion of $[3_n]$ Cyclophanes: Transannular Distance Dependent Stabilization Energy, M. Fujitsuka, S. Tojo, T. Shinmyozu, and T. Majima: *Chem. Commun.*, (2009) 1553-1555.

High-Performance Poly(3-hexylthiophene) Field-Effect Transistors Fabricated by Slide-Coating Method, M. Karakawa, M. Chikamatsu, Y. Yoshida, M. Oishi, R. Azumi, K. Yase: *Appl. Phys. Express*, 1 (6) (2008) 061802.

Review Papers

Charge Transfer in DNA, Tetsuro Majima, *Chemistry and Biology* (in Japanese), 46[8] (2008) 520-522.

Development of New Photocatalysts of Titanium Oxide Nanoparticles, Takashi Tachikawa, Tetsuro Majima, *Chemical Engineering* (in Japanese), 53[8] (2008) 17-23.

Emissive Titanium Oxide Nanoparticles Doped by Eu Ions—Emission Measurement by Single-particle Spectroscopy, Takashi Tachikawa, Tetsuro Majima, *Ceramics* (in Japanese), 43[11] (2008) 958-960.

Fabrication of Metal Nanoparticles Arrays in Polymer Matrix by Two-color Two-laser Irradiation, Masanori Sakamoto and Tetsuro Majima, *Polyfile* (in Japanese), 45[538] (2008).

Chemistry Based on Single-molecule Observation—Application to Titanium Oxide Photocatalytic Reaction—, Takashi Tachikawa, Tetsuro Majima, *Chemistry* (in Japanese), 64[1] (2009) 55-60.

Two-color Two-Laser 3D Fabrication, Masanori Sakamoto and Tetsuro Majima, *Manufacturing and Technology* (Seisan-to-Gijutsu, in Japanese), 61[1] (2009) 55-61.

Light as a Construction Tool of Metal Nanoparticles: Synthesis and Mechanism, M. Sakamoto, M. Fujitsuka, and T. Majima, *J. Photochem. Photobiol. C*, 10[1] (2009) 33-56.

Physical Chemistry of DNA, Tetsuro Majima, Japan Chemical Society, Division Report of Physical Chemistry, 6. Biophysical chemistry, in Japanese, (2009) ①-83.

Photoinduced Electron Transfer in DNA, Tetsuro Majima, Japan Chemical Society, Division Report of Organic Chemistry, 12. Photochemistry, in Japanese, (2009) ⑥-54.

Photochemistry of DNA, Tetsuro Majima, Japan Chemical Society, Division Report of

Photochemistry, 12. Photochemistry, in Japanese, (2009) ②-16.

Quantum Yield and Photochemistry, Tetsuro Majima, Photochemistry (Kokagaku in Japanese), 40[1] (2009) 1.

Books

“Consecutive adenine sequences serve as potential targets in photosensitized oxidative DNA damage”, K. Kawai and T. Majima, Nova, USA, (2008).

Patents

Polymers, a thin-film and organic electronics device using the polymer, M. Karakawa, Y. Aso, M. Ueda, PCT/JP2009/052156

International Conferences

Development of New TiO₂ Photocatalyst: Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 213th Electrochemical Society meeting, Phoenix, USA, May 20, 2008.

Intramolecular Electron Transfer from Axial Ligands to S₂-Excited Tetraphenyl Porphyrins (invited), T. Tachikawa, M. Fujitsuka, and *T. Majima: 213th Electrochemical Society meeting, Phoenix, USA, May 20, 2008.

Charge Transfer in DNA (invited), T. Majima: 10th International Workshop on Radiation Damage to DNA, Fukushima, Japan, Jun. 8-12, 2008.

Real-Time Single Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species with Fluorescent Probes: Applications to TiO₂ Photocatalysts (poster), *K. Naito, T. Tachikawa, M. Fujitsuka, T. Majima: 21st IUPAC Symposium on Photochemistry, Gothenburg, SW, Jul. 28, 2008.

Single-Molecule Detection of Hole Transfer Through DNA (poster), *T. Tadao, M. Fujitsuka, and T. Majima: 21st IUPAC Symposium on Photochemistry, Gothenburg, SW, Jul. 28, 2008.

Charge Transfer in DNA (invited), *T. Majima, K. Kawai, and M. Fujitsuka: 236th ACS National Meeting, Philadelphia, PA, Aug. 17-21, 2008.

3-D Writing of metal nanoparticles in a polymer matrix with two-color laser beams (poster), *M. Sakamoto, T. Tachikawa, M. Fujitsuka, and T. Majima: 236th ACS National Meeting, Philadelphia, PA, Aug. 17-21, 2008.

Charge Transfer in DNA, K. Kawai, M. Fujitsuka, and *T. Majima: 2nd Asia-Pacific Symposium on Radiation Chemistry (APSRC-2008), Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Charge Transfer in DNA (invited), T. Majima: 2008 KOREA-JAPAN Symposium on

Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

Intermolecular Photoinduced Electron-Transfer of 1,8-Naphthalimides in Protic Polar Solvents (poster), *D. W. Cho, M. Fujitsuka, U. C. Yoon and T. Majima: 2008 KOREA-JAPAN Symposium on Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

Intramolecular Excimer Formation and Photoinduced Electron Transfer Process in *bis*-1,8-Naphthalimide Dyads Depending on the Linker Length (poster), *D. W. Cho, M. Fujitsuka, U. C. Yoon and T. Majima: 2008 KOREA-JAPAN Symposium on Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

Reversible Intramolecular Triplet-Triplet Energy Transfer in Benzophenone-*N*-methylphthalimide Dyad (poster), *S. S. Kim, M. Sakamoto, M. Fujitsuka, and T. Majima: 2008 KOREA-JAPAN Symposium on Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

Three-dimensional Fabrication of Metal Nanoparticles in Polymer Matrix (invited), T. Majima: Langmuir Symposium in Beijing, Beijing, China, Oct. 31, 2008.

Photochemical Fabrication of 3D Metal Nanoparticles in Polymer Matrix (invited), T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Solvent Effects on Photoinduced Electron Transfer in 1,8-Naphthalimide Dyads (poster), *D. W. Cho, U. C. Yoon, M. Fujitsuka, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Inter- and/or Intramolecular Excimer and Exciplex Emission in 1,8-Naphthalimide Derivatives (poster), *D. W. Cho, M. Fujitsuka, U. C. Yoon, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Emission Mechanism of Doubly Orth-Linked Quinoxaline/Diphenylfluorene or *cis*-Stilbene/Fluorene Hybrid Compounds Based on the Transient Absorption and Emission Measurements during the Pulse Radiolysis (poster), Y. Wei, S. Samori, S. Tojo, M. Fujitsuka, J.-S. Lin, *C.-T. Chen, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 9th Int Symp Ceramic Materials and Components for Energy and Environmental Application, Shanghai, China, Nov. 11, 2008.

Single-Molecule Observation of Photocatalytic Reaction in TiO₂ Nanotube: Importance of Molecular Transport through Porous Structures (poster), *K. Naito, T. Tachikawa, M. Fujitsuka, and T. Majima: Osaka University Forum in San Francisco: Global COE Program, Bio-Environmental Chemistry, San Francisco, USA, Dec.8-11, 2008.

Bilateral Cooperation between Korea and Japan: To the Future (invited), T. Majima: International Symposium on Core University Program between Japan and Korea -New

Processing and Nanostructure/Property Relationship for Multi-functional Materials - (The 21st JSPS-KOSEF CUP Seminar between Japan and Korea), Awajishima, Japan, Dec. 15, 2008.

Design of Cyclic Reaction Driven by the Two-color Two-photon Excitation (poster), M. Sakamoto, *S. S. Kim, M. Fujitsuka, T. Majima: International Symposium on Core University Program between Japan and Korea -New Processing and Nanostructure/Property Relationship for Multi-functional Materials - (The 21st JSPS-KOSEF CUP Seminar between Japan and Korea), Awajishima, Japan, Dec. 15, 2008.

Interfacial Electron Transfer Dynamics in a Single CdTe Quantum Dot-Pyromellitimide Conjugate (poster), *S.-C. Cui, T. Tachikawa, M. Fujitsuka, and T. Majima: International Symposium on Core University Program between Japan and Korea -New Processing and Nanostructure/Property Relationship for Multi-functional Materials - (The 21st JSPS-KOSEF CUP Seminar between Japan and Korea), Awajishima, Japan, Dec. 15, 2008.

Development of TiO₂ Photocatalyst: Real-Time Single Molecule Imaging of TiO₂ Photocatalytic Reactions (invited), T. Majima: The 10th International Symposium on Eco-materials Processing and Design, Xi'an, China, Jan. 13-16, 2009.

Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 2009 Korea-Japan Workshop on Photocatalysis and Solar Conversion, Pohang, Korea, Jan. 20, 2009.

Interfacial Electron Transfer Process in a Single CdTe Quantum Dot-Pyromellitimide Conjugate (poster), S.-C. Cui, *T. Tachikawa, M. Fujitsuka, and T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Defect-Mediated Photoluminescence Dynamics of Eu³⁺-Doped TiO₂ Nanocrystals Revealed at the Single-Particle Level (poster), *T. Tachikawa, T. Ishigaki, J.-G. Li, M. Fujitsuka, and T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Real-Time Single-Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species Generated on TiO₂ Photocatalysts (poster), K. Naito, T. Tachikawa, M. Fujitsuka, and *T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Single-Molecule Observation of Photocatalytic Reactions in Mesoporous TiO₂ Nanotube (poster), K. Naito, T. Tachikawa, M. Fujitsuka, and *T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Development of New TiO₂ Photocatalyst (invited), T. Majima: The 1st Hanyang-Osaka Symposium on Fusion-Tech based Materials, Seoul, Korea, Feb. 27, 2009.

Approach Toward Efficient Photo-electronic Devices by Supramolecular Chemistry (invited), *M. Fujitsuka, A. Sugimoto, and T. Majima: The 1st Hanyang-Osaka Symposium on Fusion-Tech based Materials, Seoul, Korea, Feb. 27, 2009.

Real-Time Single-Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species Generated on TiO₂ Photocatalysts (invited), T. Majima: Asian Academic Seminar 2008 on "Frontiers in the Photocatalysis and Photochemistry of Advanced Materials" Kawasaki, Japan, Mar. 2-6, 2009.

Charge Transfer in DNA (invited), T. Majima: Kyudai International Symposium on Photo and Supramolecular Chemistry, Fukuoka, Japan, Mar. 7, 2009.

Poly(3-hexylthiophene) Field-Effect Transistors Fabricated by Slide-Coating Method (poster), *M. Karakawa, M. Chikamatsu, Y. Yoshida, M. Oishi, R. Azumi, K. Yase: 5th International Conference on Moleculelectronics and Bioelectronics (M and Be5), Miyazaki, Japan, March 15-18, 2009.

Contributions to International Conferences and Journals

T. Majima	2007 Korea-Japan Symposium on Frontier Photoscience (Conference Chair)
T. Majima	2 nd Asia-Pacific Symposium on Radiation Chemistry (APSRC-2008) (Organizing Committee)
T. Majima	10 th International Symposium on Eco-materials Processing and Design (Organizing Committee)
T. Majima	Langmuir Symposium in Beijing 2008 (Organizing Committee)
T. Majima	2009 Korea-Japan Workshop on Photocatalysis and Solar Conversion (Organizing Committee)
T. Majima	1 st Hanyang-Osaka Symposium on Fusion-Tech based Materials' (Organizing Committee)
T. Majima	Langmuir, American Chemical Society (Senior Editor)

Publications in Domestic Meetings

The 30th Japan Photobiology and Photomedicine Meeting	1 paper
Photochemistry Meeting 2008	8 papers
The 23rd symposium on Biofunctional Chemistry	1 paper
The 51th Radiation Chemistry Meeting	2 papers
The 89th Japan Chemical Society Meeting	7 papers
The Japan Society of Applied Physics and Related Societies	1 paper

Sponsorship

Grand-in-Aid for Scientific Research (S)

T. Majima	Nanoscience of Photofunctionalized DNA	¥8,840,000
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Grand-in-Aid for Basic Scientific Research

T. Majima	Construction of devices for photoelectronic conversion using photochemical control of Tobacco Mosaic Virus supramolecules	¥800,000
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Other Research Fund

T. Majima	Sekisui Chemicals Co.	Super hydrophilicity by TiO ₂ photocatalytic reaction	¥400,000
T. Majima	Matsushita Electric Industrial Co.	Study on highly reactive nanostructured TiO ₂ photocatalysts	¥1,732,500
T. Majima	TOYOTA Co.	Hydrogen absorbing alloys with high surface area produced by photoreduction	¥5,000,000

Department of Nanobiology

Professor: Katsuyuki TANIZAWA
Associate Professor: Toshihide OKAJIMA
Research Associate: Ryousuke NAKASHIMA

Outlines

Proteins and those complexed with other biomolecules are regarded as nano bio devices. The research of our group is focused on structural and functional studies of the nano bio devices, as well as their applications in the interdisciplinary field. We are also interested in the development of highly sensitive biosensors and construction of nano machines.

Current Research Project

Biosynthesis of quinohemoprotein amine dehydrogenase containing novel intra-peptidyl crosslinks and peptide-derived quinone cofactor

Quinohemoprotein amine dehydrogenase (QHNDH), occurring in the periplasmic space of certain Gram-negative bacteria such as *Paracoccus denitrificans*, has a heterotrimeric structure, each subunit possessing distinct structural features. The largest α -subunit has a 4-domain structure with two hemes in the N-terminal domain. The middle-sized β -subunit has a 7-braded β -propeller structure frequently observed in quinoproteins. The smallest γ -subunit contains a peptidyl quinone cofactor, cysteine tryptophylquinone (CTQ), and intra-peptidyl thioether crosslinks formed between Cys and Asp/Glu residues. The cytoplasmic nascent γ -subunit possesses an N-terminal pre-sequence that must be cleaved off in the mature enzyme complex. Thus, the γ -subunit undergoes multiple post-translational modifications by itself or in a state associated with other subunits before translocation into the periplasm. We have previously shown that a putative [Fe-S]-cluster binding protein encoded in the second open reading frame (ORF) of the QHNDH operon is essential for modification of γ -subunit, presumably participating in the formation of intra-peptidyl thioether crosslinks. In the study reported here, we have focused on a subtilisin-like protein encoded in the fifth ORF of the same QHNDH operon and explored its role in the biogenesis of QHNDH.

First we have constructed an ORF5 gene-disrupted *P. denitrificans* strain by homologous recombination. While the wild-type strain produced an active, mature enzyme upon induction with *n*-butylamine, the mutant strain neither grew in the *n*-butylamine medium nor showed QHNDH activity. Both the *n*-butylamine-dependent growth and QHNDH activity of the Δ ORF5 strain were restored by expression of the plasmid-encoded ORF5 protein but not by that of its site-specific mutants at the putative catalytic-triad. In the Δ ORF5 strain grown independent of *n*-butylamine, α - and β -subunits were both detected in the periplasm, whereas γ -subunit was mostly present in the cytoplasm and stained negatively for redox-cycling quinone assay, showing the absence of CTQ. Western blotting and MALDI-TOF mass spectrometric analysis of the isolated γ -subunit revealed that the pre-sequence had not been removed, although the thioether crosslinks had been formed. These results unequivocally show that the ORF5

protein cleaves the pre-sequence of γ -subunit by acting as a specific processing protease in the cytoplasm. It is likely that the pre-sequence of γ -subunit is needed for guiding the [Fe-S]-containing ORF2 protein in the initial formation of the thioether crosslinks and its subsequent removal facilitates association with α -subunit to be translocated together into the final destination (periplasm), where two hemes are inserted into α -subunit, CTQ is generated within γ -subunit, and the active QHNDH complex is formed.

Crystallographic analysis of xenobiotic exporters.

Xenobiotic extruding pumps have recently been known to be widely distributed in living organisms from mammalian to bacteria as a host-defence mechanism in cellular level. These pumps not only confer multidrug resistance of cancer cells and pathogenic bacteria but also cause hereditary diseases through the mutation. We first determined the crystal structure of bacterial major xenobiotic exporter AcrB in 2002 and elucidated the molecular mechanism of xenobiotic export and the structural basis of multidrug recognition by determining the crystal structure of the drug-binding form of AcrB in 2006. In 2007, we continued to solve the substrate-binding form of AcrB with different substrates. In addition, we tried to crystallize the other type of exporters such as TetA.

Publications

Original Papers

Efficient bacterial production of functional antibody fragments using a phagemid vector, H. Kuba, A. Furukawa, T. Okajima and K. Furukawa: *Protein Expr. Purif.*, 58 (2) (2008) 292-300.

Identification of ubiquitin ligase activity of RBCK1 and its inhibition by splice variant RBCK2 and protein kinase C β , K. Tatematsu, N. Yoshimoto, T. Okajima, K. Tanizawa and S. Kuroda: *J. Biol. Chem.*, 283 (17) (2008) 11575-11585.

Yeast-based fluorescence reporter assay of G protein-coupled receptor signaling for flow cytometric screening: FAR1-disruption recovers loss of episomal plasmid caused by signaling in yeast, J. Ishii, T. Tanaka, S. Matsumura, K. Tatematsu, S. Kuroda, C. Ogino, H. Fukuda and A. Kondo: *J. Biochem.*, 143 (5) (2008) 667-674.

Enigma homolog 1 scaffolds protein kinase D1 to regulate the activity of the cardiac L-type voltage-gated calcium channel, A.D. Maturana, S. Wälchli, M. Iwata, S. Ryser, J. Van Lint, M. Hoshijima, W. Schlegel, Y. Ikeda, K. Tanizawa and S. Kuroda: *Cardiovascular Res.*, 78 (3) (2008) 458-465.

Crystal structures of *Lymnaea stagnalis* AChBP in complex with neonicotinoid insecticides imidacloprid and clothianidin, T. Okajima, M. Ihara, A. Yamashita, T. Oda, K. Hirata, H. Nishiwaki, T. Morimoto, M. Akamatsu, Y. Ashikawa, S. Kuroda, R. Mega, S. Kuramitsu, D.B. Sattelle and K. Matsuda: *Invert. Neurosci.*, 8 (2) (2008) 71-81.

Further insight into the mechanism of stereoselective proton abstraction by bacterial copper amine oxidase, M. Taki, T. Murakawa, T. Nakamoto, M. Uchida, H. Hayashi, K. Tanizawa, Y. Yamamoto and T. Okajima: *Biochemistry*, 47 (29) (2008) 7726-7733.

In vivo protein delivery to human liver-derived cells using hepatitis B virus envelope pre-S region, T. Kasuya, T. Yamada, A. Uyeda, T. Matsuzaki, T. Okajima, K. Tatematsu, K. Tanizawa and S. Kuroda: *J. Biosci. Bioeng.*, 106 (1) (2008) 99-102.

In vivo delivery of bio-nanocapsules displaying L4-PHA isolectin to malignant tumors overexpressing N-acetylglucosaminyltransferase V, T. Kasuya, J. Jung, H. Kadoya, T. Matsuzaki, K. Tatematsu, T. Okajima, E. Miyoshi, K. Tanizawa and S. Kuroda: *Hum. Gene Ther.*, 19 (9) (2008) 887-895.

Response regulator YycF essential for bacterial growth: X-ray crystal structure of the DNA-binding domain and its PhoB-like DNA recognition motif, T. Okajima, A. Doi, A. Okada, Y. Gotoh, K. Tanizawa and R. Utsumi: *FEBS Lett.*, 252 (23, 24) (2008) 3434-3438.

Expression of squamous cell carcinoma antigen-1 in liver enhances the uptake of HBV envelope-derived bio-nanocapsules in transgenic rats, T. Kasuya, S. Nomura, T. Matsuzaki, J. Jung, T. Yamada, K. Tatematsu, T. Okajima, K. Tanizawa and S. Kuroda: *FEBS J.*, 275 (22) (2008) 5714-572.

Review Papers

Structural basis of multidrug recognition by bacterial transporter, A. Yamaguchi, R. Nakashima, *Gene & Medicine MOOK*, 12 (2009) 61-66.

Books

“Copper Amine Oxidases: Structure, Catalytic Mechanism and Role in Physiopathology” (G. Floris and B. Mondovi, Eds.), Chapter 3: Cofactors of Amine Oxidases: Copper Ion and Its Substitution and the 2,4,5-Trihydroxyphenylalanine Quinone, S. Suzuki, T. Okajima, K. Tanizawa, and M. Mure, CRC Press, New York (2009) 19-37.

“Copper Amine Oxidases: Structure, Catalytic Mechanism and Role in Physiopathology” (G. Floris and B. Mondovi, Eds.), Chapter 8: Mechanism of TPQ Biogenesis in Prokaryotic Copper Amine Oxidase, T. Okajima and K. Tanizawa, CRC Press, New York (2009) 103-118.

International Conferences

In vivo delivery of bio-nanocapsules displaying L4-PHA isolectin to malignant tumors overexpressing N-acetylglucosaminyl-transferase V (poster), *T. Kasuya, J. Jung, H. Kadoya, T. Matsuzaki, K. Tatematsu, T. Okajima, E. Miyoshi, K. Tanizawa and S. Kuroda: 35th Annual Meeting & Exposition of the Controlled Release Society, New York, USA, July 12-16, 2008.

Direct observation of cell entry of hepatitis B virus envelope L-derived bio-nanocapsules (poster), *M. Yamada, T. Kasuya, T. Matsuzaki, K. Tanizawa and S. Kuroda: The Molecular Biology of Hepatitis B Viruses, San Diego, USA, August 17-21, 2008.

Enhancement of cellular uptake of HBV envelope L-derived bio-nanocapsules by liver-specific expression of SCCA1 in transgenic rat model (poster), *T. Kasuya, T. Matsuzaki, M. Yamada, K. Tanizawa and S. Kuroda: The Molecular Biology of Hepatitis B Viruses, San Diego, USA, August 17-21, 2008.

Analysis of the fusogenic activity of the HBV L protein utilizing bio-nanocapsule (poster), *T. Matsuzaki, Y. Sasaki, T. Kasuya, K. Tanizawa and S. Kuroda: The Molecular Biology of Hepatitis B Viruses, San Diego, USA, August 17-21, 2008.

Involvement of an iron sulfur protein and a subtilisin-like protease in the biogenesis of quinoxinoprotein amine dehydrogenase (invited), T. Okajima, K. Ono and *K. Tanizawa: Japan-Holland Joint Seminar on New Aspects in Enzyme Science and Biotechnology, Fukuoka, Japan, September 28-30, 2008.

X-ray crystal structure of Streptococcus mutans response regulator involved in biofilm formation (poster), *A. Tada, S. Nomura, Y. Eguchi, R. Utsumi, S. Kuroda, K. Tanizawa and T. Okajima: 4th Handai Nanoscience and Nanotechnology International Symposium, Suita, Osaka, Japan, Sept. 29-Oct. 1, 2008.

Conformational flexibility of the TPQ cofactor in bacterial copper amine oxidase (poster), *T. Okajima, S. Nakanishi, T. Murakawa, H. Hayashi and K. Tanizawa: The Second International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Athens, Georgia, USA, October 26-31, 2008.

Involvement of an iron sulfur protein and a subtilisin-like protease in the posttranslational modification of quinoxinoprotein amine dehydrogenase (invited), *K. Tanizawa, K. Ono and T. Okajima: The Second International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Athens, Georgia, USA, October 26-31, 2008.

Conformational Flexibility of the TPQ Cofactor in Bacterial Copper Amine Oxidase (poster), *T. Okajima, S. Nakanishi, and K. Tanizawa: 12th SANKEN International Symposium /Joint Meeting of The 7th SANKEN Nanotechnology Center Symposium/The 2nd SANKEN MSTeC Symposium/The 1st SANKEN Alliance Symposium, January 22, 2009, Suita, Osaka, JAPAN.

Contributions to International Conferences and Journals

K. Tanizawa	Federation of Asian and Oceanian Biochemists and Molecular Biologists (Delegate of Japan)
K. Tanizawa	The Journal of Biochemistry (Associate Editor)
K. Tanizawa	Journal of Nutritional Science and Vitaminology (Associate Editor)

Publications in Domestic Meetings

J Joint Annual Meeting of the Molecular Biology Society of Japan and the Japanese Biochemical Society (BMB2008) 6 papers
Annual Meeting of Japan Society for Bioscience, Biotechnology, and Agrochemistry 4 papers

12th Spring-8 Symposium

1 paper

Sponsorships

Grant-in-Aid for Scientific Research (B)

K. Tanizawa	Mechanisms of Biosynthesis and Catalysis of Built-in Type Quinone Cofactor	¥2,600,000
T. Okajima	Mechanism of Proton and Electron Transfer in Enzyme Containing Built-in Type Quinone Cofactor	¥3,900,000

Grant-in-Aid for Young Scientists (B)

R. Nakashima	Crystallization of tetracycline efflux protein	¥1,560,000
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Entrusted Research

T. Okajima	Bio-oriented Technology Research Advancement Institution (BRAIN)	Development of Drugs Inhibiting Bacterial Signal Transduction Based on X-ray Crystal Structures	¥5,200,000
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Other Research Fund

K. Tanizawa	Vitamin B Committee	¥250,000
K. Tanizawa	Japan Foundation for Applied Enzymology	¥1,000,000

Department of Nanosystem Design

Guest Professor: Masafumi ATA (2008.4.1-6.30)

Outlines

Main target of research in the period was to propose a new methodology of responsible R&D of emerging nanotechnology, in which research on societal implication of nanotechnology is concurrently carried out and reflected into the development of core technology. Effective creation of socio-economic value by the responsible R&D was discussed, a novel relationship between Science&Technology and Society to enable the sustainable future society, as well. In practice, scientific approach to EHS and ELSI issues of nanotechnology were integrated in the research as key issues in societal implication of nanotechnology. Finally, trend of domestic and international effort to achieve the management of nano materials and nanotechnology standardization was analyzed from a view point of public engagement of nanotechnology.

Achievement

Nanotechnology R&D and Effective Engagement of Public

Mizuki Sekiya, SoonHwa An, Saori Ishizu, Tadashi Tanabe and Masafumi Ata

4th International Nanotechnology Conference on Communication and Cooperation

April 15, 2008. Tokyo

Public Acceptance and Economic Effects on Nanotechnology-EHS Related Issue:
Japanese Experience

SoonHwa An, Mizuki Sekiya, Saori Ishizu, Tadashi Tanabe and Masafumi Ata

APO Study Meeting on Strategic Industries: Nanotechnology

July 11, 2008. Taipei

Nanotechnology in Society

Mizuki Sekiya, SoonHwa An, Saori Ishizu, Tadashi Tanabe and Masafumi Ata

SEMI Forum Japan 2008, July 19, 2008

Strategic Issue in Public Engagement of Nanotechnology; Responsible R&D to
Innovation

SoonHwa An, Mizuki Sekiya, Saori Ishizu, Tadashi Tanabe and Masafumi Ata

Lecture at Nanotechnology Center, The Institute of Scientific and Industrial Research,
Osaka University, June 20, 2008

Comprehensive Approach to Standardization of Nanotechnology and Public Acceptance
of Nanotechnology; What's going on in Nanotechnology Standardization

Masafumi Ata

Lecture at Organization for the Promotion of Research on Nanoscience and
Nanotechnology, Osaka University, June 27, 2008

Department of Nano System Design

Guest Associate Professor: Yasushi KANAZAWA (2008.4.1-6.30)

Outlines

Camera calibration is a quite important preprocess for accurate geometrical analysis including range measurement and 3D reconstruction in computer vision. In previous calibration methods for perspective cameras, the intrinsic and extrinsic parameters are simultaneously estimated during calibration. However, in some situations, only estimation of the intrinsic parameters is necessary as the extrinsic parameters are not used. In these cases, each intrinsic parameter, is not sufficiently robust to combat the image processing noise, which is absorbed by both parameter types, during calibration. The proposed method observes parallel light pairs which are projected on different points to calibrate the intrinsic parameters.

Achievement

Multiple feature points are extracted as approximately infinite scene points and they are used as parallel light observations. Because feature point correspondence under various camera position and orientation is needed, we discuss a method of local feature-based image correspondence. After a pair of the feature points (parallel lights) are chosen, the intrinsic parameter estimation is accomplished by applying the constraint that the relative angle of two parallel rays is constant even if they are projected on any points. This method focuses only on the intrinsic parameters and the calibrations are robust as demonstrated in this study. Moreover, our method can visualize the error of the calibrated result and the degeneracy of the input data.

Department of Nanosystem Design

Guest Professor: Toshiaki Kaneko (2008.7.1-2008.9.30)

Outlines

An attosecond/femtosecond electron beam is a powerful tool to study the ultrafast reactions or phenomena in nanospace in materials. It is suggested that a specific phenomenon is induced such as the collective ionization of the material by the attosecond pulse. This specific phenomenon was formulated and studied theoretically for an interaction between the electron bunch and materials.

Achievement

Formulation and Theoretical study for stopping power and range of femtosecond/attosecond electron beam pulse in materials

The interactions of an attosecond electron beam with materials become to be dominant coherently, not a single electron. The interactions are suggested that a specific phenomenon is induced such as the collective ionization of the material by the attosecond pulse. This specific phenomenon was formulated and studied theoretically for an interaction between the electron bunch and materials. New effect of quantum beam irradiation for the material is expected for physics, chemistry, and material science.

Publications

T. Kaneko and S. Ikegami, "Average charge of MeV/atom carbon cluster ions impacted on foils", Nucl. Instr. Meth. in Phys. Res. B, 258, 57-60, (2007)

Department of Nanosystem Design

Guest Professor: Hiroyuki AKINAGA (2008.10.1-12.31)

Outlines

Oxide nanostructures are expected to show various interesting phenomena, which cannot be realized by Si-based materials and devices. In this study, fabrication of functional-oxide exotic nanostructures, such as the functional-oxide interface and nano-structured materials, and the nanoelectronic application are investigated. More concretely, non-volatile memory effects, such as resistive switch and tunnel magnetoresistance effects, are studied. The goal of this study is making them to the high performance, as well as the promotion of the integration to Si technology.

Advent of nanotechnology and the progress the nanotechnology network project, MEXT, such as The Handai Multi-Functional Nanofoundry and AIST Nano processing partnership platform, are also discussed.

Achievement

Oxide nanostructures are expected to show various interesting phenomena, which cannot be realized by Si-based materials and devices. In this study, fabrication of functional-oxide exotic nanostructures, such as the functional-oxide interface and nano-structured materials, and the nanoelectronic application were investigated. Comprehensive understanding of electronic properties in functional-oxide nanostructures has been achieved.

Advent of nanotechnology and the progress the nanotechnology network project, MEXT, such as The Handai Multi-Functional Nanofoundry and AIST Nano processing partnership platform, have been discussed. The discussion formulated a common understanding regarding the prospect of nanotechnology.

Department of Nanosystem Design

Guest Associate Professor: Kenji MURAKAMI (2008.7.14-10.14)

Outlines

Dye-sensitized solar cell consists of the semiconductor-based photoelectrode, the dye for sunlight harvesting, the electrolyte for a redox reaction and the counter electrode. A catalytic activity is required for the counter electrode to enhance the redox reaction in electrolyte, and thus platinum is usually used as the counter electrode. It is, however, necessary to reduce an amount of platinum for the practical applications. In this study, a formation of nano-structured platinum electrode is aimed to improve the catalytic activity, and the surface morphologies are observed in detail by using the atomic force microscopy (AFM).

Achievement

Platinum layers with the different thicknesses were deposited successively on the chromium conductive layers on glass substrates by using the magnetron sputtering method. It is found from the AFM observations that the chromium conductive layer is porous and the sputtered platinum particles are seemed to fill in gaps between the chromium grains at the small amount of platinum. On the other hand, when the platinum layer is formed on the dense titanium layer/chromium/glass, the sputtered platinum layer is not observed. It is pointed out that a formation method for platinum layer should be also considered. Furthermore, a lecture entitled “Development of dye-sensitized solar cells and nanotechnology” was given to researchers and graduate students.

Department of Nanosystem Design

Guest Professor: Masami NAKAMOTO (2009.1.4 - 2009.3.31)

Outline

In order to develop metallic nanoparticles for ink-jet printing wiring, synthesis conditions and ink properties are directly connected. The design concept for the synthesis was discussed. This project focused on the design approach based on the wide range of chemistry/metallurgy/electronics system integration crossover fields.

Achievement

The synthesis process control is one of the key issues for the fabrication of metallic inks, especially easily oxidized elements such as copper. The atmosphere control design was discussed and future collaboration on this base was planned.

Division of Beam Science for Nanotechnology

Outlines

The division of beam science for nanotechnology is composed of five research departments: beam science for nanofabrication, quantum beams for nanotechnology, beam processing for nanotechnology, advanced nanofabrication, and ultra-fast spectroscopy of nanostructures. Quantum beam science is one of the most important fields for nanoscience and nanotechnology. The researches are performing by using ultra-short electron beam, slow positron beam, ion beam, electron lithography and so on. The studies such as time-space reaction analysis with ultra-short electron beam, nano-structure analysis with slow positron beam and nano-beam process, are expected for ultimate nanofabrication and a new nano-beam science.

Achievements

- Generation of femtosecond/attosecond electron source
- Femtosecond pulse radiolysis based on equivalent velocity spectroscopy
- Double-decker electron accelerator and attosecond pulse radiolysis
- Primary Process of Quantum Beam-Induced Nanofabrication
- Analysis of spur reactions for nanofabrication
- Radiation chemistry of ionic liquids
- Improvement of L-band linear accelerator for nanoscience
- Researches on FEL and THz
- Generation of intense slow-positron beam
- Study of annihilation process of positrons in polymeric materials using AMOC
- Study of primary radiation reactions in resists using positron annihilation technique
- Single-particle induced chemical reactions and nanotechnology
- Study of physical properties of single molecular by using quantum beam
- Study of nano-process with quantum beam
- Modeling of nano-process in resist

Department of Beam Science for Nanofabrication

Professor: Yoichi YOSHIDA
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Outline

A femtosecond/attosecond pulse radiolysis based on a photocathode electron beam accelerator is being developed for the study of such ultrafast reactions in nano-space. The study of ultrafast reactions in nano-space of the materials is very important for the development of ultimate fabrication process with quantum beam for the next nanotechnology (e.g. EUV lithography).

In 2008, a femtosecond pulse radiolysis system was developed and used successfully to study the dynamics of solvation and geminate ion recombination in materials on femtosecond time scales. In the femtosecond pulse radiolysis, a femtosecond electron bunch which was generated from a laser photocathode electron gun accelerator, while a time-synchronized femtosecond laser was used as a analyzing source. The femtosecond solvation dynamics of electrons produced by electron-beam-induced ionization in water was firstly observed by using the femtosecond pulse radiolysis. It found that the most of hydrated electrons are formed in water pulse radiolysis by passing through the pre-hydrated state (wet electron). The wet electron formation time and lifetime are 180 fs and 540 fs, respectively, which are in agreement with the case of photo-ionization.

Moreover, the generation of an attosecond electron bunch was studied theoretically. The equivalent velocity spectroscopy and the double-decker electron accelerator were continued to be studied for the next new pulse radiolysis in the attosecond time region.

Current Research Programs

1. Femtosecond pulse radiolysis and femtosecond reactions/phenomena

The pulse radiolysis is a powerful tool to reveal the hidden chemical kinetics and radiation primary processes or reactions by using ultrafast pulse radiolysis. In the pulse radiolysis, a short electron beam, which is almost produced by radio-frequency (rf) electron linear accelerator (linac) with energy from a few MeV to a few tens MeV, is used as a pump or irradiative source. The electron-induced reactions or phenomena in matter are analyzed by a short-pulse analyzing light (e.g. synchronized lasers or Cherenkov light emitted from the electron beam) with the time-resolved stroboscopic technique. The resolution limit in pulse radiolysis is determined by the pulse width of the electron beam and the analyzing light, and by the synchronized time jitter between the electron pulse the light pulse.

Our group has been successfully generated a 98-femtosecond electron beam by using the advanced photocathode rf electron accelerator. A femtosecond pulse radiolysis based on the femtosecond electron beam was constructed to study the chemical kinetics

and radiation primary processes in femtosecond time region. In pulse radiolysis, a time-synchronized precisely femtosecond laser light was used as the analyzing source. A double-pulse injection technique was developed to compensate the change of the signal due to the fluctuation of the laser power during the measurement. The stability of the signal was successfully reduced to be below 1%. The stabilization of the electron beam on the charge and position was carried out. Finally, a 0.1-mm-thick sample has been used successfully in the pulse radiolysis. The time resolution of 150 fs, which is a new world record in pulse radiolysis, was successfully achieved.

The femtosecond pulse radiolysis was opened the femtosecond dynamics of electrons produced by electron-beam-induced ionization in liquids; e.g. salvation and geminate ion recombination. In the water pulse radiolysis, it found that the most of hydrated electrons are formed in water pulse radiolysis by passing through the pre-hydrated state (wet electron). The wet electron formation time and lifetime are 180 fs and 540 fs, respectively, which are in agreement with the case of photo-ionization.

2. Attosecond electron beam generation and attosecond science

An attosecond pulse radiolysis was begun to study in our laboratory. The electron beam pulse duration and the time jitter between the electron pulse and the analyzing light pulse, however, are key elements to reach the attosecond time region. A new advanced generation method was developed and studied theoretically by exciting the photocathode with a femtosecond laser to generate a femtosecond electron beam directly, and then compressing the femtosecond electron bunch into attosecond with the magnetic compression technique. A 780-attosecond electron beam is generated and expected in the pulse radiolysis.

The laser technologies can, recently, synchronize the laser output with the external rf down to the sub-100 femtosecond time region. However, the time jitter problem is remained. To reduce the time jitter, a double-decker electron beam accelerator was developed for pulse radiolysis; one of the electron beam is used as an irradiation source while another is used to change a radiation light source as the analyzing source without the use of laser light, resulting in reducing the time jitter. The double-decker electron beams are generated with one or a few cycle of the rf packets. The resolution due to the synchronized time jitter will reach lower than 1 fs.

Besides the pulse duration and the time jitter, there is another temporal spread that imposes an often more severe limitation on the time resolution. When the light is propagated into the sample, the velocity of the light becomes to be slow (c/n) due to the refractive index (n), where c is the light speed in vacuum. For the electrons accelerated at a few tens MeV, the electron velocity is approximate to c , resulting in the difference in group velocities of the electrons and the light in the sample. This difference leads to a large degradation of time resolution during propagation in the sample, e.g. 11 ps for the 1-cm-thick water sample. In the previous reports, this problem was considered in ultrafast pulse radiolysis and conditions were established for minimizing the velocity mismatch by reducing the sample thickness, such as a 0.1-mm-thick sample was used for improving the time resolution into the femtosecond region. However, no solution was offered to reduce it beyond 1 fs.

To solve this problem, we have proposed an equivalent velocity spectroscopy (EVS) method to overcome the effect of group velocity mismatch between the electrons and

the light in sample by rotating the electron pulse such that both the electron and the light pulses are precisely coincidence at every point and throughout the propagation time. In 2008, the method how to rotate the electron pulse with a deflecting cavity and how to measure the electron pulse rotation was developed. The beam simulation was carried out.

Publications

Original Papers

Dynamic Optical Modulation of an Electron Beam on a Photocathode RF Gun: Toward Intensity-Modulated Radiation Therapy (IMRT), T. Kondoh, H. Kashima, J. Yang, Y. Yoshida, S. Tagawa: *Radiat. Phys. Chem.*, 77 (2008) 1142– 1147.

Effects of emittance and space-charge in femtosecond bunch compression, K. Kan, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: *Nucl. Instrum. Methods A*, 597 (2008) 126–131.

Reactions of Solvated Electrons with Imidazolium Cations in Ionic Liquids, K. Takahashi, T. Sato, Y. Katsumura, J. Yang, T. Kondoh, Y. Yoshida, R. Katoh: *Radiat. Phys. Chem.*, 77 (2008) 1239– 1243.

Molar Absorption Coefficient and Radiolytic Yield of Solvated Electrons in Diethylmethyl(2-methoxy)ammonium bis (trifluoromethanesulfonyl)imide Ionic Liquid, A. Asano, J. Yang, T. Kondoh, K. Norizawa, R. Nagaishi, K. Takahashi, Y. Yoshida: *Radiat. Phys. Chem.*, 77 (2008) 1244– 1247.

Picosecond Pulse Radiolysis: Dynamics of Solvated Electrons in Ionic Liquid and Geminate Ion Recombination in Liquid Alkanes, J. Yang, T. Kondoh, K. Norizawa, R. Nagaishi, M. Taguchi, K. Takahashi, R. Katoh, S. V. Anishchik, Y. Yoshida, S. Tagawa: *Radiat. Phys. Chem.*, 77 (2008) 1233– 1238.

Study on the Reaction of Chlorophenols in Room Temperature Ionic Liquids with Ionizing Radiation, A. Kimura, M. Taguchi, T. Kondoh, J. Yang, Y. Yoshida, K. Hirota: *Radiat. Phys. Chem.*, 77 (2008) 1253– 1257.

xtension of the Heavy Ion Beam Pulse Radiolysis Using Scintillators, T. Kondoh, J. Yang, K. Kan, Y. Yoshida, H. Shibata, S. Kurashima, M. Taguchi and K. Hirota: *JAEA-Review*, 55 (2008) 158.

International Conferences

Spatial Resolution and Contrast of the Intensity Modulated Electron Beam by the Photocathode RF Gun for the Radiation Therapy (poster), T. Kondoh, J. Yang, Y. Yoshida, H. Kashima, K. Kan, K. Norizawa, A. Ogata, S. Tagawa: The 11th European Particle Accelerator Conference(EPAC'08), Genoa, Italy, June 23-27, 2008.

Femtosecond Photocathode Electron Source (poster), J. Yang, K. Kan, T. Kondoh, K. Tanimura, Y. Yoshida, J. Urakawa: The 11th European Particle Accelerator Conference(EPAC'08), Genoa, Italy, June 23-27, 2008.

Collective Ionization by Attosecond Electron Bunches (poster), A. Ogata, T. Kondoh, K. Norizawa, J. Yang, Y. Yoshida: The 11th European Particle Accelerator Conference(EPAC'08), Genoa, Italy, June 23-27, 2008.

Pulse Radiolysis Study of Ion-Species Effects on the Solvated Electrons in Alkyl Ammonium Ionic Liquids, T. Kondoh, A. Asano, J. Yang, K. Norizawa, K. Takahashi, M. Taguchi, R. Nagaishi, R. Katoh, Y. Yoshida: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Breaking Time-Resolution Limits in Pulse Radiolysis, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida, S. Tagawa: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Pulse Radiolysis Study of Trapped Electron in $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ Single Crystal (poster), K. Norizawa, T. Kondoh, J. Yang, A. Ogata, Y. Yoshida: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Observation of Optical Reflection Change due to Electron Pulse Irradiation in GaAs for Femtosecond Electron Pulse Measurement (poster), K. Kan, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Development of Heavy Ion Beam Pulse Radiolysis in a Single Ion Nano-track (poster), T. Kondoh, J. Yang, K. Kan, Y. Yoshida, K. Norizawa, H. Shibata, M. Taguchi, S. Kurashima, T. Kojima and K. Hirota: The 4th Handai Nanoscience and Nanotechnology International Symposium, Sep. 29-Oct. 1, 2008.

Study of Electron-induced Ultrafast Phenomena in GaAs for Femtosecond Electron Measurement (poster), K. Kan, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 4th Handai Nanoscience and Nanotechnology International Symposium, Sep. 29-Oct. 1, 2008.

Femtosecond Pulse Radiolysis for Study of Nanofabrication Process (poster), J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 4th Handai Nanoscience and Nanotechnology International Symposium, Sep. 29-Oct. 1, 2008.

Femtosecond reaction analysis based on a femtosecond electron beam and a femtosecond laser light (poster), J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 12th Sanken International Symposium, Jan. 22, 2009.

Optical Modulation of Electron Beam by Digital Micromirror Device for Radiation Therapy based on Photocathode RF Gun (poster), T. Kondoh, H. Kashima, J. Yang, K. Kan, K. Norizawa, A. Ogata, Y. Yoshida, S. Tagawa: The 12th Sanken International Symposium, Jan. 22, 2009.

Optical Absorption Spectrum of Hydrated Electron in MgSO_4 Aqueous Solution (poster), K. Norizawa, T. Kondoh, J. Yang, Y. Yoshida: The 12th Sanken International Symposium, Jan. 22, 2009.

Femtosecond electron source and its applications (invited), J. Yang: The 4th workshop on electron beam applications, Dwajeon, Korea, Mar. 13, 2009.

Publications in Domestic Meetings

The Japan Society of Physics	2 papers
The Japan Society of Radiation Chemistry	4 papers
The Particle Accelerator Society of Japan	4 papers
Atomic Energy Society of Japan	2 papers
Symposium on RF Electron Gun	4 papers
Symposium on TIARA	1 paper

Academic Degrees

Doctor Degree of Engineering

Koichi Kan Study on femtosecond and attosecond electron beam generation

Master Degree of Engineering

Haruki Tanaka Study of radiation primary processes by femtosecond pulse radiolysis

Hiroaki Kashima Electron beam modulation for IMRT

Sponsorship

Grant-in-Aid for Basic Research (A)

Y. Yoshida Research on Equivalent Velocity Spectroscopy for Subfemtosecond and Attosecond Pulse Radiolysis ¥10,790,000

Grant-in-Aid for Basic Research (C)

J. Yang High LET based on Heavy Ion Pulse Radiolysis ¥2,210,000

Collaborative Researches

J. Yang	KEK	Development of photocathode femtosecond electron source	¥1,200,000
Y. Yoshida	JAERI Tokai	High time resolution study on radiation-induced reaction in nanostructure	
	JAERI Tokai	Pulse radiolysis study of Ionic Liquid	
	JAERI Takasaki	Mechanism of micro sphere generation in phenol solution	
	JAERI Takasaki	Radical study by using ion pulse radiolysis	
	National Institute of Radiological Science	Beam control technique on the intensity modified radiation therapy	

Department of Quantum Beams for Nanotechnology

Professor: Goro ISOYAMA
Associate Professor: Yoshihide HONDA
Assistant Professor: Norio KIMURA

Outline

In this department, we conduct research on development of new measurement methods in the nanometer range using quantum beams, which are expected to form bases for nanotechnology, and on their applications as well as on development of quantum beams. To put it concretely, we are developing a highly intense and bright positron beam using an electron linac and its applications to materials science. Positrons have a nature to concentrate in holes and free volumes in materials and consequently measurements using positrons are widely received as an effective method to analyze sizes and distributions of free volumes. The positron beam is highly expected to play an important role in analyzing not only the sizes but also the distributions of nanometer size spaces and free volumes in porous materials such as polymers. We conduct research for better understanding interactions of positrons and positroniums, which are formed by an electron and a positron as a bound state, with materials, and for analyzing free volumes, surfaces and interfaces in thin polymer films, and finally for developing new materials. Since high-quality positron beams are necessary for conducting such researches, we also make studies on production of intense, bright, and short-pulsed slow positron beams using an electron linac, and on development of new measurement methods. We also take part in management and operation of the Radiation Laboratory, which has the experimental apparatuses for these studies.

Current Research Projects

1. Commissioning of the S-band Linac

The S-band linac, which has been used for production of a slow positron beam, has three acceleration tubes and the nominal energy of the accelerated electron beam is 150 MeV. This linac is under reconstruction.

2. Development of New AMOC System Based on Angular Correlation

In the measurements for polymer electrolyte membrane (PEM), Nafion-117, S-parameter, which is an index representing Doppler broadening of photopeak, has found to be a sensitive parameter to express the degradation of the membrane rather than lifetime of *o*-Ps. However, the S-parameter would be affected by both annihilation γ -rays originating free positron and *o*-Ps. To identify which effect is dominant in S-parameter, AMOC (age-momentum correlation) measurement was carried out. This system usually consists of one high purity Germanium detector (HPGe) to get S-parameter and two BaF₂ scintillators to get lifetime of positron. However, the resolution of HPGe for the analysis of the momentum of annihilated electron is not so good as that of angular correlation. Indeed the resolution of HPGe for 511 keV was estimated to be about 1.3 keV, corresponding to the E_e of 6.6 eV. This means the change in lower energy region would not be detected well. Thus we designed

a new measuring system based on AMOC with angular correlation, pursuing detailed analysis of annihilated electron. In such a system, intense positron source such as linac based slow positron beam is suitable to get proper counting rate.

The new system is aiming at both high momentum resolution of annihilated electron and high time resolution and consists of BaF₂ and BGO scintillators attaching to the position sensitive photomultipliers to get the information of incident position of annihilation γ -rays, and a conventional BaF₂ scintillator to get a start signal in lifetime spectroscopy. Additional photomultiplier is set on the side surface of BaF₂ to produce stop signal. In the present design, only the thickness of scintillators and the arrangement of experimental setup were taken into account for angular correlation measurement.

The resolution decided by ADC is about 100 eV/channel, and the equivalent angle spread for the new angular correlation system is about 0.4 mrad. In general, as the space resolution and quantum efficiency is in trade-off, the numerical calculations were carried out using EGS4 program and the thickness of BaF₂ scintillator was decided to be 1 inch and to set more than 1 m apart from the sample. Preliminary experiments to get lifetime spectrum were carried out using 1 inch thick BaF₂ scintillator with 2 inch diameter. Detection of luminescence with photomultiplier tube set on the side surface of the BaF₂ scintillator to produce stop signal was difficult due to the lack of the light reflected from the bottom side facing position sensitive photomultiplier tube. Though the lifetime spectrum could be measured by amplifying the stop signal, the obtained resolution function for lifetime spectrum was not satisfied. Further improvement would be made. The incident position of γ -ray on BGO scintillator could be deduced and the estimation of their spatial resolution is under investigation.

3. Investigation of Degradation Process of Polymer Electrolyte Membrane by Using Positron

Understanding degradation mechanism of polymer electrolyte membrane (PEM) for fuel cell is very important from the view of developing robust membranes with longer lifetime in actual fuel cell environment. The chemical and the structural changes of PEM have already been investigated elsewhere by using conventional techniques such as X-ray diffraction, infrared spectroscopy, electron spin resonance (ESR) techniques, etc.. A positron, which is sensitive to such changes, is thought to be suitable for the analysis of degradation process in PEM. The changes in the structure or the electronic state of the polymer may be reflected on the changes in the lifetime of *o*-Ps or line-shape parameter (S-parameter) of the photopeak of annihilation γ -ray.

To investigate the degradation process of PEM, Nafion[®]-117 was exposed to γ -ray with different dose to reveal intrinsic degradation process instead of usually used degradation methods such as Fenton test. As a result, we got a good linear correlation between proton conductivity and S-parameter, where the larger S-parameter corresponded to the lower proton conductivity.

To investigate whether this correlation holds for another degradation process, Nafion-117 was damaged in various ways and investigated in the similar methods. Several samples, such as as-purchased one, treated with hydrogen peroxide, exposed to Fenton reagents and kept for 8 months in air after purchase, were exposed to γ -ray with different dose. Another samples were heated with different temperature. For all samples, the linear correlations were obtained to some extent between proton conductivity and S-parameter. In case of γ -ray irradiated sample, the correlation showed almost linear up to 100 kGy, but the plot for 1000 kGy was apart from the correlation line. Also the

samples heated up to 120°C were plotted in linear, but the plot for the sample of 140 °C was apart from the line. These seem to be the evidences that the extreme condition damaged chemical bonding, especially hydrogen bond, leading to the destruction of cluster in PEM. In the middle rage, no more than 100 kGy or 120 °C, the slopes characterizing the correlation were different for different treatment. The aged samples showed the steepest slope and the sample treated with hydrogen peroxide, including Fenton tested one, showed mild slope. What define the slope is under investigation.

Publications

Original Papers

Interlaboratory comparison of positron annihilation lifetime measurements for synthetic fused silica and polycarbonate, K. Ito, T. Oka, Y. Kobayashi, Y.. Shirai, K. Wada, M. Matsumoto, M. Fujinami, T. Hirade, Y. Honda, H. Hosomi, Y. Nagai, K. Inoue, H. Saito, K. Sakaki, K. Sato, A. Shimazu, A. Uedono: J. Appl. Phys., 104 (2) (2008) 026102 1-3.

Radiation chemical yield for loss of carbonate ester bonds in PADC films exposed to gamma ray, Y. Mori, T. Ikeda, T. Yamauchi, A. Sakamoto, H. Chikada, Y. Honda, K. Oda: Radiation Measurements, 44 (2) (2009) 211-213.

International Conferences

Analysis of Radiation Induced Phenomena in a Polymer Electrolyte Membrane with Positron Annihilation Technique (poster), Y. Honda, N. Kimura, P. K. Pujari, G. Isoyama, S. Tagawa, H. Miyauchi, Y. Shibahara, H. S. Sodaye, Y. Akiyama, Y. Izumi, S. Nishijima: 9th International Workshop on Positron and Positronium Chemistry, May. 11-15, 2008, Wuhan, China.

Development of A New Detection System Using Positron (poster), Y. Honda, N. Kimura, G. Isoyama, S. Tagawa, H. S. Sodaye, Y. Shibahara, Y. Akiyama, S. Nishijima: 12th SANKEN International Symposium, Jan. 22, 2009, Osaka, Japan.

Application of coincidence Doppler broadening technique for polymer electrolyte membrane (poster), Y. Shibahara, H. S. Sodaye, Y. Miyauchi, Y. Akiyama, Y. Izumi, S. Nishijima, Y. Honda, N. Kimura, G. Isoyama, S. Tagawa: The 15th International Conference on Positron Annihilation, Jan. 18-23, 2009, Kolkata, India.

Aging Phenomenon in Nafion-117 Probed by Positron Annihilation Spectroscopy (poster), H. S. Sodaye, Y. Shibahara, H. Miyauchi, Y. Akiyama, Y. Izumi, S. Nishijima, Y. Honda, N. Kimura, P. K. Pujari, G. Isoyama, S. Tagawa: The 15th International Conference on Positron Annihilation, Jan. 18-23, 2009, Kolkata, India.

Publications in Domestic Meetings

Meeting of Atomic Energy Society of Japan

1 paper

Grant-in-Aid for Scientific Research (C)

Y. Honda	Evaluation of polymer electrolyte membrane with positron	¥910,000
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Department of Beam Science for Nanotechnology

Professor:	Seiichi TAGAWA
Associate Professor:	Takahiro KOZAWA
Specially Appointed	Kazumasa OKAMOTO
Assistant Professor:	

Outline

The targets of the present department are the establishment of initiatives of quantum beams for nanoscience and nanotechnology. Quantum beams mean both beams such as photons and beams inducing interactions with materials in the nanoscopic level of quantum mechanics. The beams potentially have applicability for imaging with ultra fine patterns, and the present department aims to use the fine patterns as the probes for nano-structured material sciences and devices.

Current Research Projects

Reaction Mechanisms in Polymeric Materials for Micro- and Nano-electronics

Chemically amplified resist system is one of the most practical candidates in the future technology in semiconductor fabrication. Reaction mechanisms in the system are analyzed upon exposure to electron beams, X-rays, and laser beams to design a new lithography technique in the present program. The correlation between C_{37} parameter and acid generation efficiency was clarified.

Radiation-Induced Reactions in Nanoscopic Region

Electron beam lithography has the highest resolution among top-down writing systems. The ultimate spatial resolution is closely related to the reaction mechanism of resist materials. The relation between line edge roughness and reaction mechanisms was investigated by a subpicosecond pulse radiolysis.

Nanosize distributions of Polymer Matrices and Acid Generators in Resist Films

The feature sizes in micro-fabrication have shrunk with the progresses in lithography technology. The decrease in deviation of resist pattern has been also needed to molecular size. Thus, distribution of photo-acid generator (PAG) and orientation of polymer matrix have been important issues. X-ray reflectivity measurements were carried out to understand PAG distribution and polymer orientation from the resist film density map in-depth.

Publications

Original Papers

Line edge roughness after development in a positive-tone chemically amplified resist of post-optical lithography investigated by Monte Carlo simulation and dissolution model, A. Saeki, T. Kozawa, S. Tagawa, H. B. Cao, H. Deng, and M. J. Leeson:

Nanotechnology, 19 (2008) 015705.

Point Spread Function for the Calculation of Acid Distribution in Chemically Amplified Resists for Extreme Ultraviolet Lithography, T. Kozawa, A. Saeki, and S. Tagawa: Appl. Phys. Express, 1 (2008) 027001.

Dependence of Acid Generation Efficiency on Molecular Structures of Acid Generators upon Exposure to Extreme Ultraviolet Radiation, R. Hirose, T. Kozawa, S. Tagawa, T. Kai, and T. Shimokawa: Appl. Phys. Express, 1 (2008) 027004.

Enhancement of Acid Production in Chemically Amplified Resist for Extreme Ultraviolet Lithography, H. Yamamoto, T. Kozawa, S. Tagawa, H. Yukawa, M. Sato, and J. Onodera: Jpn. J. Appl. Phys., 1 (2008) 047001.

Difference in Reaction Schemes in Photolysis of Triphenylsulfonium Salts between 248 nm and Dry/Wet 193 nm Resists, Y. Matsui, H. Sugawara, S. Seki, T. Kozawa, S. Tagawa, and T. Itani: Appl. Phys. Express, 1 (2008) 047001.

Resolution degradation caused by multispur effect in chemically amplified extreme ultraviolet resist, T. Kozawa, S. Tagawa, and M. Shell: J. Appl. Phys., 103 (2008) 084306.

Relationship between Sensitivities of Chemically Amplified Resist Based on Adamantane Derivatives upon Exposure to ArF Excimer Laser, K. Furukawa, T. Kozawa, S. Seki, and S. Tagawa: Appl. Phys. Express, 1 (2008) 067001.

X-ray reflectivity study on depth profile of acid generator distribution in chemically amplified resists, T. Fukuyama, T. Kozawa, S. Tagawa, R. Takasu, H. Yukawa, M. Sato, J. Onodera, I. Hirose, T. Koganesawa, and K. Horie: Appl. Phys. Express, 1 (2008) 065004.

Feasibility Study of Chemically Amplified Extreme Ultraviolet Resists for 22 nm Fabrication, T. Kozawa, K. Okamoto, J. Nakamura, and S. Tagawa: Appl. Phys. Express, 1 (2008) 067012.

Feasibility Study of Chemically Amplified Extreme Ultraviolet Resists for 22 nm Fabrication, T. Kozawa, S. Tagawa, J. J. Santillan, M. Toriumi, and T. Itani: Jpn. J. Appl. Phys., 47 (2008) 4465-4468.

Effects of Rate Constant for Deprotection on Latent Image Formation in Chemically Amplified Extreme Ultraviolet Resists, T. Kozawa, S. Tagawa, J. J. Santillan, M. Toriumi, and T. Itani: Jpn. J. Appl. Phys., 47 (2008) 4926-4931.

Study of the Reaction of Acid Generators with Epithermal and Thermalized Electrons, K. Natsuda, T. Kozawa, A. Saeki, S. Tagawa, T. Kai, and T. Shimokawa: Jpn. J. Appl. Phys., 47 (2008) 4932-4935.

Impact of nonconstant diffusion coefficient on latent image quality in 22 nm fabrication using extreme ultraviolet lithography, T. Kozawa, S. Tagawa, J. J. Santillan, and T. Itani: *J. Photopolym. Sci. Technol.*, 21 (2008) 421-427.

Quencher Effects at 22 nm Pattern Formation in Chemically Amplified Resists, T. Kozawa, S. Tagawa, J. J. Santillan, and T. Itani: *Jpn. J. Appl. Phys.*, 47 (2008) 5404-5408.

Simulation of amine concentration dependence on line edge roughness after development in electron beam lithography, A. Saeki, T. Kozawa, S. Tagawa, H. B. Cao, H. Deng, and M. J. Leeson: *J. Appl. Phys.*, 104 (2008) 024303.

Formation of Intramolecular Poly(4-hydroxystyrene) Dimer Radical Cation, K. Okamoto, T. Kozawa, K. Natsuda, S. Seki, and S. Tagawa: *J. Phys. Chem. B*, 112 (2008) 9275-9280.

Theoretically Study on the Dependence of Acid Distribution on Material Properties of Chemically Amplified Extreme Ultraviolet Resists, T. Kozawa, S. Tagawa, and M. Shell: *Jpn. J. Appl. Phys.*, 47 (2008) 6288-6292.

Difference between Acid Generation Mechanism in Poly(hydroxystyrene)-and Polyacrylate-Based Chemically Amplified Resists upon Exposure to Extreme Ultraviolet Radiation, R. Hirose, T. Kozawa, S. Tagawa, D. Shimizu, T. Kai, and T. Shimokawa: *Jpn. J. Appl. Phys.*, 47 (2008) 7125-7127.

Theoretically Study on Difference between Image Quality Formed in Low- and High-Activation-Energy Chemically Amplified Resists, T. Kozawa, and S. Tagawa: *Appl. Phys. Express*, 1 (2008) 107001.

Side Wall Degradation of Chemically Amplified Resists Based on Poly(4-hydroxystyrene) for Extreme Ultraviolet Lithography, T. Kozawa and S. Tagawa: *Jpn. J. Appl. Phys.*, 47 (2008) 7822-7826.

High-Absorption Resist Process for Extreme Ultraviolet Lithography, T. Kozawa and S. Tagawa: *Jpn. J. Appl. Phys.*, 47 (2008) 8354-8359.

Effects of Polymer Interference during Acid Generation on Latent Image Quality of Extreme Ultraviolet Resists, T. Kozawa and S. Tagawa: *Jpn. J. Appl. Phys.*, 47 (2008) 8328-8332.

Latent image formation in chemically amplified extreme ultraviolet resists with low activation energy for deprotection reaction, T. Kozawa, S. Tagawa, J. J. Santillan, and T. Itani: *J. Vac. Sci. Technol. B*, 26 (2008) 2257-2260.

Dissolution characteristics of chemically amplified extreme ultraviolet resist, T. Itani, K.

Kaneyama, T. Kozawa, and S. Tagawa: J. Vac. Sci. Technol. B, 26 (2008) 2261-2264.

International Conferences

Chemically Amplified Molecular Resist Based on Fullerene Derivative for Nanolithography (poster), *H. Yamamoto, T. Kozawa, S. Tagawa, T. Ando, K. Ohmori, M. Sato, and J. Onodera: SPIE Advanced Lithography San Jose, California, USA.

Dependence of Acid Generation Efficiency on Molecular Structure and Concentration of Acid Generator in Chemically Amplified EUV Resists (poster), *R. Hirose, T. Kozawa, S. Tagawa, T. Kai, and T. Shimokawa: SPIE Advanced Lithography San Jose, California, USA.

Acid-base equilibrium in chemically amplified resist (poster), *K. Natsuda, T. Kozawa, K. Okamoto, and S. Tagawa: SPIE Advanced Lithography San Jose, California, USA.

Base quencher effects in chemically amplified resist at sub-30-nm fabrication (poster), *T. Kozawa, S. Tagawa, J. J. Santillan, M. Toriumi, and T. Itani: SPIE Advanced Lithography San Jose, California, USA.

Evaluation of Admantane derivatives for chemically amplified resist-a comparison between ArF, EUV and EB exposures- (poster), K. Furukawa, S. Seki, T. Kozawa, and S. Tagawa: SPIE Advanced Lithography San Jose, California, USA.

Study on Reactivity of Halogenated Resist Polymer with Low-energy Electrons (poster), *H. Yamamoto, T. Kozawa, A. Saeki, S. Tagawa, T. Miura, H. Yukawa, and J. Onodera: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Effect of acid generator structure on its depth distribution in chemically amplified resist films
Fluorine Atom on Acid Generation in Chemically Amplified EUV Resists (poster), *T. Fukuyama, T. Kozawa, K. Okamoto, S. Tagawa, M. Irie, T. Mimura, T. Iwai, J. Onodera, I. Hirose, T. Koganesawa, and K. Horie: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Effect of molecular structures of acid generators on acid generation in chemically amplified resists upon exposure to 75 keV electron beam (poster), *K. Natsuda, T. Kozawa, K. Okamoto, and S. Tagawa: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Dynamics of Radical Cation of Poly(4-Hydroxystyrene) and its Complex (poster), *K. Okamoto, M. Tanaka, T. Kozawa, and S. Tagawa: 21st International Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Effects of Polymer Interference in Acid Generation on Latent Image Quality of Extreme Ultraviolet Resists (poster), *T. Kozawa, and S. Tagawa: 21st International

Microprocesses and Nanotechnology Conference, Fukuoka, Japan.

Latent image formation in chemically amplified extreme ultraviolet resists with low activation energy for deprotection reaction (poster), T. Kozawa, S. Tagawa, J. J. Santillan, and T. Itani: 52nd International Conf. Electron, Ion, and Photon Beam Technology & Nanofabrication, Portland, Oregon, USA.

Multispur in chemically amplified electron beam resists (poster), T. Kozawa, K. Okamoto, and S. Tagawa: 52nd International Conf. Electron, Ion, and Photon Beam Technology & Nanofabrication, Portland, Oregon, USA.

Study on acid generation of acid generators in chemically amplified resists for electron beam Reactivity of Halogenated Resist Polymer with Low-energy Electrons (poster), *K. Natuda, T. Kozawa, K. Okamoto, and S. Tagawa: International Workshop on Molecular Information and Dynamics 2008, Taipei, Taiwan.

Nano-fabrication of Fluoropolymers using Focused Ion Beam (poster), *N. Fukutake, T. Urakawa, Y. Takasawa, T. Gowa, T. Takahashi, T. Hirano, M. Washio, A. Oshima, K. Okamoto, and S. Tagawa: Fluoropolymer 2008, Charleston, South Carolina, USA.

Dynamics of Radical Cations of Resist Model Compounds (poster), *K. Okamoto, M. Tanaka, T. Kozawa, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Microfabrication of Nano-scale Pattern on Crosslinked PTFE using Focused Ion Beam (poster), *N. Fukutake, T. Urakawa, Y. Takasawa, A. Oshima, M. Washio, A. Oshima, K. Okamoto, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Plasmonic Waveguides with Wavelength Selective Function (poster), *M. Haraguchi, Y. Matsuzaki, T. Tsuzura, T. Okamoto, M. Fukui, K. Okamoto, S. Seki, and S. Tagawa: Proceedings of SPIE-The International Society for Optical Engineering.

Multispur effects in chemically amplified resists (poster), T. Kozawa, K. Okamoto, A. Saeki, and S. Tagawa: 2nd Asia-Pacific Symposium on Radiation Chemistry, Waseda University, Japan.

Feasibility Study on High-Sensitivity Chemically Amplified Resists by Polymer Absorption Enhancement in Extreme Ultraviolet Lithography (poster), T. Kozawa, K. Okamoto, J. Nakamura, and S. Tagawa: International Symposium on Extreme Ultraviolet Lithography, Lake Tahoe, California, USA.

Sensitization mechanisms of chemically amplified resists and resist design for 22 nm node (poster), T. Kozawa and S. Tagawa: 2009 International Workshop on EUV Lithography, Oahu, Hawaii, USA.

Contributions to International Conferences and Journals

T. Kozawa	21 st Microprocess and Nanolithograph Conference (Paper Committee Section Head)	
T. Kozawa	2008 International Workshop on EUV Lithography (Technical Steering Committee)	
T. Kozawa	2008 International Extreme Ultraviolet Lithography (EUVL) Symposium (Paper Committee)	
T. Kozawa	The 2nd Asia-Pacific Symposium on Radiation Chemistry (APSRC-2008) (Executive Committee)	

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	4 papers
Chemical Society of Japan	2 papers
The Japan Society of Applied Physics	3 papers
The Society of Polymer Science, Japan	1paper

Academic Degrees

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas (S)

S. Tagawa	Femtosecond Pulse Radiolysis Study on Nano Spatial-temporal Reactions	¥27,170,000
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Grant-in-Aid for Scientific Research on Priority Areas (B)

T. Kozawa	Nano-space Reaction for Establishment of Academic Basis toward Realization of Ultrafine Fabrication by Extreme Ultraviolet Light	¥5,980,000
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Grant-in-Aid for Scientific Research, Encouragement of Young Scientist (B)

K. Okamoto	Elucidation of Molecular Dynamics and Reaction Mechanism for Control of Nano-size Roughness in Resist Materials	¥1,200,000
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Entrusted Research

S. Tagawa	JST-CREST	Research on Resist for Ultra-fine Fabrication and Development of Process Simulator	¥99,450,000
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Other Research Fund

S. Tagawa	SELETE	Research on EUV Resist	¥5,000,000
S. Tagawa	Matsushita Electric Industrial Co.	Dissolution Property of EUV Lithography Resist	¥1,000,000

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: Hossain Akther Kashem Mohammad (2008.10.1-12.31)

Outlines

I intend to search for new nanocrystalline ferrite materials which exhibit high permeability and high resonance frequency. Both spinel ferrites and hexaferrites with high frequency are suitable for many applications. They have immense potential for applications in the areas of high density data storage, ferrofluids, magnetic resonance imaging and magnetic refrigeration. With the rapid development of mobile communication and information technology, the electronic component with small size, high efficiency and low cost are urgently demanded. Multilayer chip inductor (MLCI) is such a component which is widely used in electronic products, such as cellular phone, note book computer and video cameras. The Ni-Cu-Zn ferrites have been the dominant materials for MLCI due to its better magnetic properties at high frequency and low sintering temperature.

In solid-state reaction technique, there are some limitations of having homogeneous and smaller particle size. In this respect, combustion technique is suitable for the preparation of nano-sized powders. The advantages of combustion method are that the method is (i) simple, because all the reactions takes place only in a few minutes, not like the other methods that require tedious process, (ii) it involves simple equipment, i.e., complicated equipment are not needed in this method, and (iii) it includes low cost, because all the materials used in this method are cheap. Combustion technique is expected to produce nano-sized powder. Samples prepared from these powders may have different magnetic properties compared to the properties of the materials prepared by other techniques.

Various nano-sized $\text{Ni}_{0.50-x}\text{Cu}_x\text{Zn}_{0.50}\text{Fe}_2\text{O}_4$ powders will be prepared by combustion technique and hence to investigate the influence of copper in the surface morphology, structural, magnetic and electrical properties of the proposed ferrites.

Department of Ultrafast Spectroscopy of Nanostructures

Guest Researcher: Kyusik YUN (2008.7.10-8.15)

Outlines

Nanoparticles with carbohydrates as functional ligands are called glyconanoparticles (GNPs), which has a multifunctional role in nanobiotechnology. Here I report a facile fabrication of silver-glucosamine GNPs starting with metal nanoclusters obtained under hydrothermal condition using (LSS strategy) ethanol-linoleic acid (liquid), sodium linoleate-metal (solid) and ethanol-water (solution) [1].

Achievement

The resulted metal colloid was first physisorbed with the monolayer of Tween-20 prior to chemisorption of alkanethiols resulted in surface-modified colloidal metal, which is stable over a broader range of pH values [2]. The adsorbed layer of Tween-20 prevents irreversible aggregation of the nanoparticles by means of steric interactions due to the presence of oligo-(ethylene glycol) moieties on the headgroup of the surfactant. Further the physisorbed metal colloid was covalently immobilized by carboxyl-terminated alkanethiol and the terminal carboxyl group was bonded with side-chain amino group of glucosamine surface in phosphate buffered saline through EDC/NHS coupling reaction. The synthesized silver-GNPs can be exploited as a chemo-sensitizer with an active target for the treatment of malignant cancers via transglutaminase 2 inhibition [3]. Furthermore, there is vast array of intriguing applications for GNPs in carbohydrate interactions, biolabels, drug delivery, and as anti-adhesion agents in inhibition of metastasis or as anti-cancer vaccines.

References

- [1] X. Wang, J. Zhuang, Q. Peng, Y. Li, *Nature*, **437.**, 121 (2005).
- [2] K. Aslan, V.H. Prez-Luna, *Langmuir*, **18.**, 6059 (2002).
- [3] D.S. Kim, K.S. Park, K.C. Jeong, B.I. Lee, C. H. Lee, S.Y. Kim, *Cancer Letters*, **273.**, 243 (2009).

Department of Ultrafast Spectroscopy of Nanostructures

Visiting Research Scholar: Jan Ivanco (2009.2.2-2009.3.13)

Outlines

Semiconductors form the heart of electronic devices which are indispensable for the modern society. Properties of both ultrathin dielectric films and their interfaces to semiconductors strongly affect device characteristics and therefore investigations on electronic and chemical properties of interfaces are fundamental in both the basic and applied research. While the semiconductors have been historically associated with inorganic elements only, recent progress reveals a commercial competitiveness of 'plastic' semiconductors especially in low cost applications, e.g. flexible displays. Nevertheless, the understanding of processes in molecular films and their interfaces is in its infancy and fundamental research has to be done to exploit the full potential of organic electronics. During the stay, electronic phenomena in organic films like band bending were investigated.

Achievement

The band bending was analyzed by means of "the X-ray photoelectron spectroscopy under biases", the method invented and elaborated in our laboratory. The method bases on the detection of core level shifts - which would indicate the band bending - in the semiconducting film induced by external bias. The core levels are inspected through a biased ultrathin metallic film. The characterization is sensitive to the optimal sample design and preparation.

In our study, phthalocyanine and sexithiophene molecular films were evaporated in UHV on Au foils. An ultrathin (~2.5 nm) insulating film of SiO₂ was grown by electron beam induced evaporation followed by an ultrathin Pt film (~2.5 nm) evaporation through a mask. The Pt film was contacted by a gold wire so to apply voltage across the organic layer. As carbon is dominating element in organic materials, the C 1s core level was chosen for the determination of the shift induced by the external bias. The measurement and analysis of the measured data are in progress.

Division of Nanoscience and Nanotechnology for Industrial Applications

Outline

This division involves five laboratories, i.e., Department of Nanomaterials and Environmentally Conscious Technology, Department of Computational Nanomaterials Design, Department of Nano-Bio-Intelligent Systems Science, Department of Propatent Strategy for Nanotechnology (Domestic visiting researcher), Department of Nanotechnology Transfer (Foreign visiting researcher). All of these laboratories have the same direction to make contribution to society and industries through their own nanotechnology. Through the activity of these laboratories in the first year, establishments are listed as follows.

Achievements

Suganuma Lab.

- Basic design and science of high temperature lead-free soldering
- R&D of low temperature lead-free soldering and improvement of oxidation resistance
- Development of Printed Electronics technology with nano particles paste
- Basic design of high reliability conductive adhesives and evaluation methods

Mizoguchi Lab.

- Development of contents management system based on nanotechnology ontology
- Towards interoperable description of phenotypes based on ontological investigation of quality and quantity
- Advancement of ontology building tool Hozo for clinical ontology building
- Development of an e-textbook using clinical ontology
- Advancement of databases in life science domains using ontological engineering

Katayama-Yoshida Lab.

- Development of materials design engine and materials design for semiconductor spintronics
- Development of pseudopotential electronic-structure calculation codes “Osaka2002_nano”
- Material design for superconductivity of icosahedron-based boron
- Mechanism of fast diffusion of Cu impurity in Si
- Material design for Cu gettering in crystal Si
- Microscopic roles of hydrogen in crystal Si

Department of Nanomaterials and Environmentally Conscious Technology

Professor:	Katsuaki SUGANUMA
Assistant Professor:	Masahiro INOUE, Keun-Soo KIM
Post Doctoral Fellows:	Jinting JIU, Sun-Sik KIM
Graduate Students:	Seiji KUMAMOTO, Masafumi KURAMOTO, Daisuke WAKUDA, Seong-Jun KIM, ALONGHENG, Ki-Ju LEE, Min Kang, Chang-Jae KIM, Takahiro KUWANA, Natsuki KOMODA
Support Staff:	Mariko HATAMURA, Noriko KAGAMI, Kyoko HAMASAKI, Kozue IDE, Misa MATSUSHITA.

Outlines

Through nanotechnologies and knowledge for organic/inorganic materials, we are conducting the development of environmentally conscious fine technologies for electronics packaging area, i.e., lead-free soldering and conductive adhesives, and the composite materials based on metals and intermetallic compounds. We set our route towards contributions to our society in near future.

Current Research Project

Development of alternative technology for high-temperature soldering

Isotropic conductive adhesives have excellent attributes as heat-resistant lead-free high temperature interconnection materials as well as those enabling low temperature manufacturing of circuits. Ag metallic particles from nano-scale to micron-scale are combined with organic matrix to provide sound high-temperature lead-free interconnection. The purpose of the project is to understand the current characteristics of conductive adhesives as the alternative to leaded solders, and, especially focusing on their characteristics of high temperature resistance and of low temperature manufacturing process, new conductive adhesives are targeted to be developed by the improvement of the current drawbacks.

Development of new room temperature wiring method for Printed electronics

Room temperature wiring is one of the last goals for Printed Electronics. Room temperature fabrication enables to use the wide variety of functional materials into one circuit board without thermal stress or damage as well as environmental consciousness. Metallic nanoparticles can be sintered to form dense microstructure if both the surface of nanoparticles and the environment are clean without any oxidation or contamination. Ag nanoparticles are, however, usually protected by an organic layer. It is desirable to remove this organic layer by certain chemical processes with or without light heating or other kinds of energy processes, which do not have any serious damage on organic devices and substrate weak against heating. Recently, we developed a new process, by which the paste of Ag nanoparticles protected with them can be successfully

sintered at room temperature in air atmosphere.

Development of soft human/machine interfaces using super-flexible wiring technology

Recently, the super-flexible (bendy and stretchable) wiring technology using elastomer-based conductive adhesives was developed in our group. By using the super-flexible wiring, stretchable tactile sensor systems including piezoelectric sensor and novel electrostatic sensor systems for humanoid robots and related applications were successfully fabricated. In addition, these sensor systems were connected to a self-organized network of distributed processors in order to realize the fail-safe data processing system and shown to work successfully.

Publications

Original Papers

Physical Factors Determining Thermal Conductivities of Isotropic Conductive Adhesives, M. Inoue, H. Muta, T. Maekawa, S. Yamanaka, K. Suganuma: J. Electron. Mater., 38 (2009) 430-437.

Interfacial Reaction and Die Attach Properties of Zn-Sn High-Temperature Solders, S.J. Kim, K.S. Kim, S.S. Kim, K. Suganuma: J. Electron. Mater., 38 (2009) 266-272.

High-temperature lead-free solders: properties and possibilities, K. Suganuma, S.J. Kim, K.S. Kim: JOM, 61 (2009) 64-71.

Synthesis and nanostructure of boron nitride nanotubes grown from iron-evaporated boron, T. Oku, N. Koi, K. Suganuma: Diamond and Related Materials, 17 (2008) 1805-1807.

Room temperature sintering of Ag nanoparticles by drying solvent, D. Wakuda, K.S. Kim, K. Suganuma: Scripta Materialia, 59 (2008) 649-652.

Structures and purification of boron nitride nanotubes synthesized from boron-based powders with iron particles, N. Koi, T. Oku, M. Inoue, K. Suganuma: J. Materials Science, 43 (2008) 2955-2961.

Characteristics of Zn-Al-Cu Alloys for High Temperature Solder Application, S.J. Kim, K.S. Kim, S.S. Kim, C.Y. Kang, K. Suganuma: Materials Transactions, 49 (2008) 1531-1536.

Variations in polymeric structure of ferroelectric poly(vinylidene fluoride) films during annealing at various temperatures, M. Inoue, Y. Tada, K. Suganuma, H. Ishiguro: J. Applied Polymer Science, 111 (2008) 2837-2843.

Joint Strength and Microstructure for Sn-Ag-(Cu) Soldering on an Electroless Ni-Au Surface Finish by Using a Flux Containing a Cu Compound, S. Kumamoto, H. Sakurai,

Y. Kukimoto, K. Suganumai: J. Electron. Mater., 37 (2008) 806-814.

Electronic and optical properties of boron nitride nanotubes, T. Oku, N. Koi, K. Suganumai: J. Physics and Chemistry of Solids, 69 (2008) 1228-1231.

Temperature dependence of electrical and thermal conductivities of an epoxy-based isotropic conductive adhesive, M. Inoue, H. Muta, T. Maekawa, S. Yamanaka, K. Suganuma: J. Electron. Mater., 37 (2008) 462-468.

Review Papers

Trends of ink jet technology (In Japanese), K. Suganuma, Denshi Zairyo, 48-2 (2009) 67-73.

Trends of conductive adhesives in electronics (In Japanese), K. Suganuma, D. Shindo, K. Ohtsuka, Y. Kariya, J. Japan Institute of Electronics Packaging, 12-1 (2009) 79-85.

Trends of printed electronics technology (In Japanese), K. Suganuma, Converttech, 36-7 (2008) 29-32.

Production innovation by ink jet technology (In Japanese), K. Suganuma, D. Wakuda, K.S. Kim, Monthly Display, 14-6 (2008) 41-47.

Books

Metallic nano particle inks for printable electronics, 2009 Printable Electronics (In Japanese), K. Suganuma, D. Wakuda, K. S. Kim, Electronics Journal Co., (2008) 89-95.

Patents

Object detection sensor, K. Suganuma, Y. Tada, H. Ishigoro, M. Inoue, T. Kawasaki, Y. Kawahito, JP 2008-190902

Synthesis method of Ag paste containing metal silver obtained from β -keto-carboxylic acid silver, T. Yamaguchi, M. Hatamura, K. Suganuma, JP 2008-159535

International Conferences

Interfacial Reaction and Thermal Cycling Reliability of Zn-Sn High Temperature Lead-Free Solders, *S.J. Kim, K.S. Kim, G. Izuta, K. Suganuma: 138th TMS Annual Meeting & Exhibition, San Francisco, CA, USA, Feb.15-19, 2009.

Degradation Mechanism of Conductive Adhesive/Sn Interface under High Humidity, *S.S. Kim, K.S. Kim, S.J. Kim, K. Suganuma: 41st Annual International Symposium on Microelectronics (IMAPS 2008), Rhode Island Convention Center, Providence, Rhode Island USA, Nov. 2-6, 2008.

Reliability of die attached AlN-DBC module using Zn-Sn high temperature lead-free solders, *S.J. Kim, K.S. Kim, G. Izuta, K. Suganuma: 2nd Electronics System-Integration Technology Conference (ESTC 2008), Greenwich, London, UK, September 1-4, 2008.

Degradation Mechanism of Ag-Epoxy Conductive Adhesive Joints by Heat and Humidity Exposure, *S.S. Kim, K.S. Kim, K. Suganuma, H. Tanaka: 2nd Electronics System-Integration Technology Conference (ESTC 2008), Greenwich, London, UK, September 1-4, 2008.

Room Temperature Sintering Mechanism of Ag Nanoparticle Paste, *D. Wakuda, C.J. Kim, K.S. Kim, K. Suganuma: 2nd Electronics System-Integration Technology Conference (ESTC 2008), Greenwich, London, UK, September 1-4, 2008.

Room Temperature Sintering of Ag Nano-scale particles with drying of the solvent, *D. Wakuda, K.S. Kim, K. Suganuma: 7th IEEE Conference on Polymers & Adhesives in Microelectronics & Photonics, Germany, August 17-20, 2008.

Developing the Stencil Printing Process for 01005 Lead-Free Assemblies, *Y.W. Lee, K.S. Kim, K. Suganuma, J.H. Kim: 2008 International Conference on Electronic Packaging Technology & High Density Packaging (ICEPT-HDP 2008), Shanghai, China, July 28-31, 2008.

Large-scale synthesis of micrometer-scale single-crystal gold nanosheets by polyol process, *J. Jiu, K. Suganuma, K.S. Kim, T. Nemoto, T. Ogawa, S. Isoda: 2008 International Materials Research Conference, Chongqing, China, June 9-12, 2008.

Electrical and thermal properties of electrically conductive adhesives using a heat-resistant epoxy binder, *M. Inoue, J. Liu: 2nd Electronics System-Integration Technology Conference (ESTC 2008), Greenwich, London, UK, September 1-4, 2008.

Recent progress of thermal interface materials, *J. Liu, T. Wang, B. Carlberg, M. Inoue: 2nd Electronics System-Integration Technology Conference (ESTC 2008), Greenwich, London, UK, September 1-4, 2008.

Contributions to International Conferences and Journals

K. Suganuma	TMS Annual Meeting Committee of Phase Stability, Phase Transformation, and Reactive Phase Formation in Electronic Materials
K. Suganuma	Electronic Components and Technology Conference (ECTC), Materials Processing Committee

Publications in Domestic Meetings

Japan Institute of Electronics Packaging	5 papers
Japan Institute of Metals	1 paper
Japan Society of Thermophysical Properties	1 paper

Academic Degrees

Master Degree for Engineering

Min Kang	Improvement of impact test method for micro joining system, and impact property evaluation of lead-free high-temperature interconnection materials
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Doctor Degree for Engineering

Seongjun Kim	Joining properties and joint reliability of Si die-attached joint with Zn-Sn based high temperature lead-free solders
Seiji Kumamoto	Joining mechanism of lead-free soldering on an electroless Ni-Au surface finish by using a flux containing a Cu compound

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

Grant-in-Aid for Scientific Research (A)

K. Suganuma	Establishment of bases for synthesis of metal nano-particles and for wiring technology using nano-pastes	¥4,940,000
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Entrusted Research

K. Suganuma	JEITA	Standardization of conductive adhesive testing methods	¥2,298,000
K. Suganuma	NEDO	R&D of flexible thermoelectric module for curved drainpipes of hot waste water	¥5,937,000
	NEC Co. Ltd.	Development of interconnecting technology using conductive Adhesives	¥1,050,000

Other Research Fund

K. Suganuma	Mitsubishi Chemical Co.	¥10,143,000
K. Suganuma	Mitsubishi Electric Co.	¥4,000,000
K. Suganuma	Teijin Ltd.	¥850,000
K. Suganuma	Denso Co.	¥450,000
K. Suganuma	Nippon Avionics Co. Ltd.	¥1,500,000
K. Suganuma	Senju Metal Industry Co. Ltd.	¥4,000,000
K. Suganuma	Toppan Forms Co. Ltd	¥2,000,000
K. Suganuma	Showa Denko K. K.	¥2,000,000
K. Suganuma	Toray Engineering Co. Ltd.	¥1,000,000
K. Suganuma	C. Uyemura & Co., Ltd.	¥1,000,000

K. Suganuma	NOF Co.	¥900,000
K. Suganuma	Bando Chemical Industries, Ltd.	¥500,000
K. Suganuma	ROHM Co. Ltd.	¥500,000
K.S. Kim	Japan Copper and Brass Association	¥300,000

Department of Computational Nanomaterials Design

Professor: Hiroshi KATAYAMA-YOSHIDA
Associate Professor: Koun SHIRAI
Research Associate: Kazunori SATO
Post Doctoral Fellows: Van An DINH, Ikutaro HAMADA, Susumu YANAGISAWA
Graduate Students: Hiddetoshi KIZAKI, Masayuki TOYODA,
Tetsuya FUKUSHIMA, Hideki HAYASHIDA,
Kenji TOYODA, Haruhiko DEKURA, Kunihiro HARADA,
Motohiko ETO, Yousuke NAKANO,
Hironobu YAMAGUCHI, Akihumi UOZUMI,
Hideyuki JIPPOU
Under Graduate Students: Yuki TERATANI, Ryusuke TOMINAGA
Supporting Staff: Mika ASADA, Ryoko ITO

Outlines

The primary activities of this department are theoretical study of electronic properties of nanomaterials, which are different from those of bulk crystals. The first-principles calculations based on the density-functional theory are used, in order to exclude any empirical parameters. More importantly, we wish to predict unknown features of new nanostructure and design novel nanomaterials. Lead of the area of material research from the theoretical viewpoint is one of our goals.

At the same time, efforts are continued to keep development in the methodologies in order to solve difficult problems encountered in this field, because nanoscience is different from study of bulk materials with many respects.

Current Research Project

Development of Pseudopotential Electronic-structure Calculation Codes “Osaka2002_nano”

Improvement and extension of our developed first-principles calculation code ‘Osaka2002_nano’ have been in progress. In particular, in this year, improvements have been made on extension of phonon calculation. Usual calculation by frozen-phonon method allow to calculate only for zone-center modes. For study of crystal dynamics, full information over the full zone is necessary. For this end, a method of constructing force constants has been developed. For superconductivity research, an improvement has been made in calculating Fermi surfaces.

Material Design for Superconductivity of Icosahedron-based Boron

Growing interests are addressed to solid boron and its compounds because of its superconducting transition at high pressures. Among the variety of polymorphs of boron, α -boron is particularly interesting, because of its high potentiality of superconductivity. A problem of α -boron is difficulty in obtaining good-quality crystals. We have theoretically created the phase diagram for boron, which was previously not available in experiment. Based on this phase diagram, we find a promising path for synthesizing

α -boron with good quality. In addition, an efficient method for doping has been devised: Li or H can be efficiently doped at high pressures, which could lead to high T_c superconductivity to boron.

Material design for superconducting semiconductors by heavy doping

Usually, semiconductors do not exhibit superconductivity. However, it has been demonstrated that heavily doping leads the matrix semiconductor exhibit superconductivity. This was for the first time demonstrated on B-doped diamond by Ekimov. He realized this by high-temperature high-pressure method. However, no one has analyzed this process theoretically. We have made theoretical study on the crystal growth of his method. Not only our study succeeded to clarify his method, but also leads to further possibility of heavily doping, resulting in further high T_c materials.

Material design for light-emitting devices using Cu complex in Si

In addition to its high diffusivity, Cu impurities have distinct properties among TM impurities in Si. Some fraction of Cu impurities can form a complex, which exhibit photo-luminescence with high efficiency. Its structure has been for a long time believed in a wrong way, i.e., Cu pair. Recent studies of isotope shift of photo-luminescence clearly shows that the complex must be Cu_4 . We have theoretically shown that the most stable complex is Cu_4 , and its microscopic structure which is compatible with experiment. Moreover, we are able to explain the complicated isotope shifts of photo-luminescence.

Physics of vacancy in crystalline Si and use for process design for crystal growth

It is well known that a vacancy in Si exhibits a Jahn-Teller distortion. Recently, ultrasonic measurement has demonstrated that another effect of vacancy is softening at low temperature. This could lead to a new and efficient method for measurement of vacancy, which is very important for controlling crystal growth of Si crystals. We have studied the dynamical aspect of vacancy. This dynamical aspect can solve some important contradictions which were recognized among different measurements. This dynamics leads to dynamic Jahn-Teller effect in fundamental physics.

Design of co-doping method in DMS

We have proposed co-doping method for increasing solubility of magnetic impurities in dilute magnetic semiconductors (DMS). The concentration dependences of the mixing energy of DMS, such as (Ga, Mn)N, (Ga, Cr)N, (Ga, Mn)As and (Zn, Cr)Te, show large convexity and these systems have a tendency toward spinodal decomposition. By introducing compensating impurities, e.g. O or Si, into these DMS, it is found that the mixing energy shows gradual transition from convex to concave concentration dependence resulting in negative mixing energy of magnetic impurities. This result suggests that the co-doping method dramatically increases the solubility of magnetic impurities in DMS, thus high concentration doping of magnetic impurities into DMS becomes possible.

However, the co-doped impurities kill the ferromagnetism of DMS. In order to remove the co-doped impurities after crystal growth, we propose interstitial impurities such as Li, Be, B, Na, Mg, K, Ca, Cu and Ag for co-dopants in (Ga, Mn)As. With these interstitials, the mixing energy of (Ga, Mn)As are strongly reduced and for low

concentration of Mn it becomes negative. Next, to simulate low temperature annealing of Li-co-doped (Ga, Mn)As, we calculate binding energy between substitutional Mn and interstitial Li in GaAs by using STATE-SENRI package. The calculated binding energy is smaller than the binding energy between substitutional Mn and interstitial Mn. By performing kinetic Monte Carlo simulations with ab-initio binding energies, we have calculated effective diffusion constant of Li in (Ga, Mn)As. Due to the small binding energy, Li diffuse rather easily in (Ga, Mn)As and Li interstitials can be removed by the low temperature (lower than 580 degree C) annealing treatment. Thus, we have shown that by using the Li interstitials the solubility limit is enhanced and high concentration Mn doping becomes possible. Moreover, by low temperature annealing after the crystal growth Li can be diffuse out from the sample to recover the ferromagnetism.

Materials design of oxide based magnetic materials for spintronics

We have proposed a materials design of MgO based magnetic materials as a spin polarizer in semiconductor spintronics devices. By using the KKR-CPA method (MACHIKANNEYAMA2002 package) we calculate the electronic structure of Ni-, Co-doped MgO and N-doped MgO, CaO, SrO and BaO. By performing monte Carlo simulations with ab-initio exchange interactions we estimate Curie temperature of these compounds. It is found that N-doped MgO, CaO, SrO and BaO are ferromagnetic inspite of the absence of magnetic impurities. In these compounds, N carries large part of the magnetization. Moreover, these compounds show half-metallic density of states, and this means that they are promising candidates for a spin polarizer. It is pointed out that to realize high-T_c the control of spinodal decomposition in these compounds is of significant importance.

Materials design for dilute magnetic semiconductors with IV-group elements

We have proposed a materials design of Si- and Ge-based dilute magnetic semiconductors. They are very much coherent with the present semiconductor electronics. In this sense, the fabrication of ferromagnetic DMS based on Si and Ge is very important. In order to design environmentally safe and cheap materials, we consider Fe and Mn as a magnetic impurity. By using the KKR-CPA method (MACHIKANNEYAMA 2002 package) we calculate the electronic structure of Mn- and Fe-doped Si and Ge. It is found that Mn atoms avoids nearest-neighbor configuration in Ge and in this configuration the Mn atoms couple ferromagnetically. Moreover calculated pair interactions between Mn are attractive and this result well explains the observed nano-column formation in Mn-doped Ge systems.

Publications

Original Papers

Calculation of Fermi surface and its applicaion to Li-doped α -boron, H. Dekura, K. Shirai, A. Yanase: J. Comput. And Theor. Nanoscience, (2008) (in press).

The stable site and diffusion of impurity Cu in Si, H. Yamaguchi, K. Shirai, H. Katayama-Yoshida: J. Comput. And Theor. Nanoscience, (2008) (in press).

A new structure of Cu complex in Si, K. Shirai, H. Yamaguchi, A. Yanase, H.

Katayama-Yoshida: J. Phys.: Condens. Matter, 21 (2009) 064249(7pages).

Utilization of high pressure for synthesizing superconducting semiconductors: -analysis of Ekimov's method-, K. Shirai, H. Dekura: Phys. Status Solidi B, 246 (2009) 673-678.

Computational nano-materials design for the wide band-gap and high-Tc semiconductor spintronics, H. Katayama-Yoshida, K. Sato, T. Fukushima, M. Toyoda, H. Kizaki and V. A. Dinh: Semiconductors and Semimetals, 82 (2008) 433-454.

Materials Design of CuAlO₂-based Dilute magnetic semiconductors by First-principles calculations and Monte Carlo Simulations, H. Kizaki, K. Sato and H. Katayama-Yoshida: Jpn. J. Appl. Phys., 47 (2008) 6488-6495.

Computational nano-materials design for II-VI compound semiconductor-based spintronicss, H. Katayama-Yoshida, K. Sato, T. Fukushima, M. Toyoda, H. Kizaki, V. A. Dinh and P. H. Dederichs: J. Korean Phys. Soc., 53 (2008) 1-12.

New high-Tc half-Heusler ferromagnets NiMnZ (Z = Si, P, Ge, As), V. A. Dinh, K. Sato and H. Katayama-Yoshida: J. Phys. Soc. Jpn., 77 (2008) 014705(6pages).

Review Papers

“Control of impurity diffusion in semiconductors by IR excitation”, K. Shirai, Hikari-Gigyutu contact, 46 (2008) 22-29.

Books

“Fundamentals and applications of boron and its compounds”(Organizing committee of 16th Int. Conf. Boron, Borides, and Related Materials), K. Shirai, CMC Pub. 2008, 34-48.

International Conferences

A new structure of Cu complex in Si (poster), *H. Yamaguchi, K. Shirai, A. Yanase, H. Katayama-Yoshida: International Conference on Quantum Simulation and Design 2008, May 31-June 3, 2008, Tokyo, Japan.

Effect of vacancy on the elastic properties of Si (poster), *J. Ishisada, K. Shirai, A. Yanase: International Conference on Quantum Simulation and Design 2008, May 31-June 3, 2008, Tokyo, Japan.

Utilization of high pressure for synthesizing superconductivity in semiconductors: -analysis of Ekimov's method- (poster), *K. Shirai, H. Dekura: International Workshop on Superconductivity in Diamond and Related Materials (IWSDM2008), July 7-9, 2008, Tsukuba, Japan.

Cu complex in silicon and its photoluminescence, *K. Shirai, H. Yamaguchi, K. Matsukawa, A. Yanase, S. Emura: 29th International Conference on the Physics of Semiconductors, July 27-Aug 1, 2008, Rio de Janeiro, Brazil.

An investigation of material design for gettering (poster), K. Matsukawa, *K. Shirai, H. Katayama-Yoshida: 29th International Conference on the Physics of Semiconductors, July 27-Aug 1, 2008, Rio de Janeiro, Brazil.

Utilization of high pressure for synthesizing superconducting semiconductors (invited), *K. Shirai, H. Dekura, A. Yanase: 13th High Pressure Semiconductor Physics -HPSP13, July 22-25, 2008, Fortaleza, Ceara, Brazil.

A new doping method to semiconducting boron for superconductivity application, *K. Shirai, H. Dekura, A. Masago: 16th International Symposium on Boron, Borides and Related Materials, Sept. 7-12 2008, Matsue, Japan.

Metalization of α -boron for superconductive material (poster), *H. Dekura, K. Shirai, A. Yanase: 16th International Symposium on Boron, Borides and Related Materials, Sept. 7-12 2008, Matsue, Japan.

Possibility of defect in α -boron (poster), *H. Dekura, K. Shirai, A. Yanase: 16th International Symposium on Boron, Borides and Related Materials, Sept. 7-12 2008, Matsue, Japan.

An investigation of material design for gettering (poster), *K. Matsukawa, K. Shirai, H. Katayama-Yoshida: Pacific Rim Meeting on Electrochemical and Solid-State Science (PRIME); The Joint International Meeting of 214th Meeting of the Electrochemical Society and 2008 Fall Meeting of the Electrochemical of Japan, Oct12-17, 2008, Hawaii.

Metallization of electron-phonon coupling in icosahedral α -B₁₂ and Li-doped B₁₂ (poster), *H. Dekura, N. Vast, E. Bettrandy, K. Shirai, V. Trinité: 14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, 8-10 Jan 2009, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

MD simulation of phonon decay processes (poster), *K. Shirai, H. Dekura, J. Ishisada: 1st International Conference of the Grand Challenge to Next-Generation Integrated Nanoscience, June 3-7, 2008, Tokyo.

Improvement of the gettering efficiency of Cu by BO Complexes (poster), *K. Shirai, K. Matsukawa, N. Yamaguchi, H. Katayama-Yoshida: 11th Sanken, 6th Nanotechnology Center and 1st MSTEC International Symposium, Feb. 4-5 2008, Awaji Yumebutai International Conference Center.

The theoretical study of elemental solid boron under high pressure (poster), *H. Dekura, K. Shirai, H. Katayama-Yoshida: 11th Sanken, 6th Nanotechnology Center and 1st MSTEC International Symposium, Feb. 4-5 2008, Awaji Yumebutai International Conference Center.

The stable site and electronic states of Copper in Silicon (poster), *H. Yamaguchi, K.

Shirai, H. Katayama-Yoshida: 11th Sanken, 6th Nanotechnology Center and 1st MSTEC International Symposium, Feb. 4-5 2008, Awaji Yumebutai International Conference Center.

The effects of monovacancy on the elastic properties of Si (poster), *J.Ishisada, K. Shirai, H. Katayama-Yoshida: 11th Sanken, 6th Nanotechnology Center and 1st MSTEC International Symposium, Feb. 4-5 2008, Awaji Yumebutai International Conference Center.

Electronic structure and pressure-induced transformation of graphite (poster), *N. Nakae, K. Shirai: 4th Handai Nanoscience and Nanotechnology International Symposium Sep.29-Oct.1 2008, Icho Kaikan, Osaka Univ.

Imperfection of α -B (poster), *H. Dekura, K. Shirai, A. Yanase: 4th Handai Nanoscience and Nanotechnology International Symposium Sep.29-Oct.1 2008, Icho Kaikan, Osaka Univ.

Molecular Dynamic Study of Single Lattice Vacancy in Si (poster), *J. Ishida, K. Shirai, A. Yanase: 4th Handai Nanoscience and Nanotechnology International Symposium Sep.29-Oct.1 2008, Icho Kaikan, Osaka Univ.

Electronic study of B-C system for superconductivity application (poster), *N. Nakae, K. Shirai, A. Yanase: The 12th SANKEN International Symposium (Joint Meeting of the 7th SANKEN Nanotechnology Center Symposium, The 2nd SANKEN MSTeC Symposium, The 1st SANKEN Alliance Symposium), Jan.22 2009, Convention Center, Osaka Univ.

Superconductivity Research on Boron Solids (poster), *K. Shirai, H. Dekura, A. Yanase: The 12th SANKEN International Symposium (Joint Meeting of the 7th SANKEN Nanotechnology Center Symposium, The 2nd SANKEN MSTeC Symposium, The 1st SANKEN Alliance Symposium) Jan. 22 2009, Convention Center, Osaka Univ.

Molecular Dynamic Study of Single Lattice Vacancy in Si (poster), J. Ishisada, K. Shirai: The 12th SANKEN International Symposium (Joint Meeting of the 7th SANKEN Nanotechnology Center Symposium, The 2nd SANKEN MSTeC Symposium, The 1st SANKEN Alliance Symposium) Jan. 22 2009, Convention Center, Osaka Univ.

First-Principles study on Electronic Structure of Co-doped TiO₂ (rutile) within Self-Interaction-Corrected LDA (poster), *H. Kizaki, M. Toyoda, K. Sato, and H. Katayama-Yoshida: International Conference on Quantum Simulation and Design 2008, June 1, 2008, Tokyo, Japan.

A theoretical study of codoping with Li interstitials in Mn-doped GaAs (poster), *Lars Bergqvist, Kazunori Sato, Peter Heinz Dederichs and Hiroshi Katayama-Yoshida: International Conference on Quantum Simulation and Design 2008, June 1, 2008, Tokyo, Japan.

Design of Colossal Solubility of Magnetic Impurities for Semiconductor Spintronics by Co-doping method (poster), *T. Fukushima, K. Sato and H. Katayama-Yoshida: International Conference on Quantum Simulation and Design 2008, June 1, 2008, Tokyo, Japan.

Design of dilute magnetic semiconductors with room temperature ferromagnetism by controlling spinodal decomposition (poster), *K. Sato, T. Fukushima and H. Katayama-Yoshida: International Conference on Quantum Simulation and Design 2008, June 1, 2008, Tokyo, Japan.

First principle study on the half-metallic ferromagnetism in half-heusler alloys XMnSi (poster), *Van An Dinh, Kazunori Sato, and Hiroshi Katayama-Yoshida: International Conference on Quantum Simulation and Design 2008, June 1, 2008, Tokyo, Japan.

Design of dilute magnetic semiconductors with room temperature ferromagnetism by controlling spinodal decomposition (poster), *K. Sato, T. Fukushima, H. Katayama-Yoshida: The 1st International Conference of the Grand Challenge to Next-Generation Integrated Nanoscience, June 4, 2008, Tokyo, Japan.

Design of Dilute Magnetic Semiconductors with room Temperature Ferromagnetism by Controlling Spinodal Decomposition (poster), *K. Sato, T. Fukushima, and H.K.-Yoshida: 29th International Conference on the Physics of Semiconductors, July 29, 2008, Rio de Janeiro, Brazil.

First Principle Prediction of Half-Metallicity and Ferromagnetism above room Temperature in Half-Heusler Alloys (poster), *V.A. Dinh, K.Sato, and H.K.-Yoshida: 29th International Conference on the Physics of Semiconductors, July 29, 2008, Rio de Janeiro, Brazil.

Design of Colossal Solubility of Magnetic Impurities for Semiconductor Spintronics by Co-Doping Method (poster), *T. Fukushima, K.Sato, and H.K.-Yoshida: 29th International Conference on the Physics of Semiconductors, July 29, 2008, Rio de Janeiro, Brazil.

Design of High Solubility of Magnetic Impurities for Semiconductor Spintronics by Codoping Method (poster), *T. Fukushima, K. Sato, and H. Katayama-Yoshida: Fifth International Conference on Physics and Applications of Spin-related Phenomena in Semiconductors, Aug 4, 2008, Iguacu, Brazil.

Design of Dilute Magnetic Semiconductors by Controlling Spinodal Decomposition (poster), *K. Sato, T. Fukushima, and H. Katayama-Yoshida: Fifth International Conference on Physics and Applications of Spin-related Phenomena in Semiconductors, Aug 4, 2008, Iguacu, Brazil.

First Principle Study of Spinodal Decomposition Thermodynamics in Half-heusler Alloys (poster), *V. A. Dinh, K. Sato, and H. Katayama-Yoshida: Fifth International Conference on Physics and Applications of Spin-related Phenomena in Semiconductors,

Aug 4, 2008, Iguacu, Brazil.

Ab-initio Electronic Structure Calculations of (Ti,Co)O₂ Within Self-interaction-corrected LDA (poster), *H. Kizaki, M. Toyoda, K. Sato, and H. Katayama-Yoshida: Fifth International Conference on Physics and Applications of Spin-related Phenomena in Semiconductors, Aug 4, 2008, Iguacu, Brazil.

Computational Nano-materials Design for Semiconductor Nano-Spintronics (invited), *H. Katayama-Yoshida: Joint European Magnetic Symposia, Sep 19, 2008, Trinity College Dublin, Ireland.

First-Principles Calculations of Electronic Structure on(Ti,Co)O₂ within Self-Interaction-Corrected LDA, *H. Kizaki, M. Toyoda, K. Sato, H. Katayama-Yoshida: 2nd International Symposium on Transparent Conductive Oxides, Oct 22, 2008, Crete.Greece.

Control of spinodal decomposition in dilute magnetic semiconductors and computational materials design for semiconductor spintronics (invited), *K. Sato: Computational Magnetism and Spintronics International Workshop, Nov 7, 2008, Dresden.Germany.

First-Principles Calculations of Electronic Structure on(Ti,Co)O₂ within Self-Interaction-Corrected LDA, *H. Kizaki, M. Toyoda, K. Sato, H. Katayama-Yoshida: 2nd International Symposium on Transparent Conductive Oxides, Oct 22, 2008, Crete.Greece.

Control of spinodal decomposition in dilute magnetic semiconductors and computational materials design for semiconductor spintronics (invited), *K. Sato: Computational Magnetism and Spintronics International Workshop, Nov 7, 2008, Dresden.Germany.

Contributions to International Conferences and Journals

K. Shirai 16th International Symposium on Boron, Borides and Related Compounds (Organizing Committee)

Publications in Domestic Meetings

The Physical Society of Japan	12 papers
The Japan Society of Applied Physics	4 papers
Publications in Domestic Meetings	4 papers

Academic Degrees

Master Degree for Engineering

J. Ishisada	Effect of single lattice vacancy in Si on its elastic properties
K. Harada	Ab initio materials design for environmentally sustainable

spintronics

Master Degree for Science

A. Fujii Ab initio design interstitial Li co-doping method for high-Tc magnetic semiconductors

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

K. Sato	Development and application of computational nano-materials design engine	¥10,800,000
K. Shirai	Superconductivity research on Icosahedron-Based Semiconducting Boron	¥1,300,000

Grant-in-Aid for Scientific Research for Young Researcher (B)

K. Sato	Ab initio calculation for electric transport properties by non-local CPA method	¥1,690,000
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Entrusted Research

K. Shirai	Japan Science and Technology Corporation Collaborative Development of Innovative Seeds	Prediction and Experimental Confirmation of New Gettering Method for Transition-Metal Impurities in Semiconductors	¥18,000,000
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Other Research Fund

H. Katayama-Yoshida	Japan Science and Technology Corporation	Case study on advanced measurements and analysis	¥1,960,000
H. Katayama-Yoshida	Japan Atomic Energy Agency	Analysis and Materials design simulation in Grid computing	
H. Dekura	Murata Science Foundation	Support for student to visit abroad	¥350,000

Department of Nano-Bio Intelligent Systems Science

Professor: Riichiro MIZOGUCHI

Assistant Professor: Kouji KOZAKI (Associate Professor, 2008.8.1-)

Outlines

The research on development of Nano-Bio intelligent help system, data mining from the nano-bio data, systematization of nano-bio knowledge, ontology engineering is conducted aiming at amalgamation of knowledge research and nano-biotechnology. Special emphasis is placed on systematization of nanotechnology.

It is highly expected that bridging the gap between several domains of nanotechnology to facilitate creative design by enabling reuse of knowledge across these domains. Ontology engineering is an advanced AI technology which has a great potential to achieve the goal. This is why we have been intensively involved in ontology engineering. The concrete objectives include development of nanotechnology ontology, development of function achievement ways for nanomaterials and development of a system for supporting creative design of nanomaterials at the functional level together with an ontology engineering environment.

The current research projects include: development of an intelligent help system based on nanotechnology ontology, ontology construction for clinical medicine and supporting systems for ontology development.

Current Research Project

Development of Nano-Bio Intelligent Help System based on Ontology Engineering

In the domains including chemical engineering, we develop a common ontology in the light of nanotechnology knowledge systematization. A preliminary ontology has been developed by analyzing textbooks, papers and patents under the consultation of the domain experts. And we developed a prototype of content management system based on the ontology. In 2007, we refined nanotechnology index ontology based on an ontological consideration of function and quality and evaluated the ontology through development of a search system using it.

Development of Clinical Ontology and its Applications

Ontology is one of the most promising techniques for enabling semantic interoperability of medical information among various data across domains/tasks. This is why there have been developed some ontologies such as SNOMED-CT, ICD-10, Galen, etc. In this situation, there has been strong need of a sophisticated medical ontology in Japanese which is highly expected to compatible with those existing ontologies.

In this background, we considered fundamental issues of medical ontology based on ontological theory. We focus on "anatomical structure of organs" and "abnormal states in the human body". On the basis of the investigation, we distinguish organ-specific types from those independent of any organ to maximize the explicitness of ontology.

The next feature of our ontology is to allow on-demand reorganization of is-a hierarchy of diseases instead of one fixed hierarchy to cope with various viewpoints which physician might have. In 2008, we developed upper level ontology of clinical medicine focusing on diseases and human body. We also developed a prototype of navigation system for medical knowledge based on the ontology.

An Environment for Ontology Development and its Use

We developed **Hozo**, an ontology engineering environment, which enables a user to build and use an ontology and instance models. It consists of Ontology editor, Concept factory and ontology server.

Ontology editor

It provides a friendly user interface as well as powerful functions necessary for ontology building and editing.

Concept factory

A guidance system based on AFM(Activity-First Method) has been implemented to guide ontology developers who build an ontology from technical documents.

Ontology server

A server for ontologies and models has been developed. It is based on the client-server architecture and enables human/computer agents to access them through internet.

We published the Ontology editor at the web site (<http://www.hozo.jp>), and we improved the Graphical User Interface of the system based on feedbacks from its users. And we developed API for ontology-based system and applied it to our content management system and creative design support system.

In 2008, we developed a reasoning system for Hozo and several new functions using it. The new functions include a function to validate ontologies, supporting functions for ontology modification, advanced search and so on. We have started theoretical considerations about several fundamental issues of ontology development for improvement of Hozo. The topics include identity of instances, view point management of ontologies and the notorious issue related to conflict of *is-a* and *part-of* relations.

Publications

Original Papers

Toward Knowledge Structuring of Sustainability Science Based on Ontology Engineering, Terukazu Kumazawa, Osamu Saito, Kouji Kozaki, Takanori Matsui and Riichiro Mizoguchi: Sustainability Science, 4 (1) (2009) 99-116.

International Conferences

Semantics of the Integrated BioMedical Database Project -A Japanese National Project-, Jun Nakaya, Saburo Sakota, Riichiro Mizoguchi, Kouji Kozaki, Kaei Hiroi, Keisuke Ido, Michio Kimura, Hiroshi Tanaka: 9th International HL7 Interoperability Conference (IHIC2008), Crete, Greece, Oct.8-11, (2008).

Toward Integration of Mouse Phenotype Information, Hiroshi Masuya and Riichiro Mizoguchi: Second Interdisciplinary Ontology Meeting, Tokyo, Japan, February 28 - March 1, (2009) 35-44.

Understanding Semantic Web Applications, Kouji Kozaki, Yusuke Hayashi, Munehiko Sasajima, Shinya Tarumi and Riichiro Mizoguchi: 3rd Asian Semantic Web Conference (ASWC 2008), LNCS 5367, February 2-5, Bangkok, Thailand, (2008) 524-539.

Instance Management Problems in the Role Model of Hozo, Kouji Kozaki, Satoshi Endo and Riichiro Mizoguchi: 10th Pacific Rim International Conference on Artificial Intelligence (PRICAI-08), LNAI 5351, December 15-19, Hanoi, Vietnam, (2008) 614-625.

Knowledge Structuring Process of Sustainability Science based on Ontology Engineering, Terukazu Kumazawa, Takanori Matsui, Keishiro Hara, Michinori Uwasu, Yohei Yamaguchi, Yugo Yamamoto, Kouji Kozaki, Osamu Saito and Riichiro Mizoguchi: 8th International Conference on Eco Balance, December 10-12, Tokyo, Japan, (2008).

Knowledge Structuring Tool for Sustainability Science Based on Ontology Engineering, Terukazu Kumazawa, Osamu Saito, Kouji Kozaki, Takanori Matsui and Riichiro Mizoguchi: 1st International Workshop on Intelligent Systems for Environmental (Knowledge) Engineering and EcoInformatics (i-SEEK' 09), Fukuoka, Japan, March 16-19, (2009) 1138-1143.

Knowledge Structuring and an Exploration System for Global Sustainability and its Application to the Biofuel Issue, Osamu Saito, Kouji Kozaki, Takeru Hirota, Riichiro Mizoguchi: Climate Change: Global Risks, Challenges and Decisions, Copenhagen, Denmark, March 10-12, (2009).

HOZO: An ontology building environment (poster), Riichiro Mizoguchi and Kouji Kozaki: Demonstrations Program of 9th International Conference of Intelligent Tutoring Systems (ITS'08), Motreal, Canada, June 23-27, (2008) 35-36.

Development of a Conceptual Map Generation Tool for Exploring Ontologies (poster), Kouji Kozaki, Takeru Hirota and Riichiro Mizoguchi: Poster Noets of the 5th European Semantic Web Conference (ESWC 2008), Tenerife, Spain, Jun. 1-5th, (2008).

Divergent Exploration of an Ontology (poster), Takeru Hirota, Kouji Kozaki and Riichiro Mizoguchi: Poster & Demo Notes of the 7th International Semantic Web Conference (ISWC 2008), October 26-30, Karlsruhe, Germany, (2008).

Contributions to International Conferences and Journals

R. Mizoguchi Semantic Web Science Association (Vice-president)

R. Mizoguchi International Journal of Web Semantics(Editors-in-Chief)

R. Mizoguchi	International Artificial Intelligence in Education Society (Executive Committee)
R. Mizoguchi	Asia-Pacific Society for Computers in Education (APSCE) (Board member)
R. Mizoguchi	The 16 th International Conference on Computers in Education (ICCE2008) Conf. on AIED/ITS & Adaptive Learning (Program Co-Chair)
R. Mizoguchi	The Tenth Pacific Rim International Conference on Artificial Intelligence (PRICAI-08) (PC Vice-Chair)
R. Mizoguchi	The 3 rd European Conference on Technology Enhanced Learning (EC-TEL 2008) (PC member)
R. Mizoguchi	The 9 th International Conference on Intelligent Tutoring System (ITS2008) (PC member)
R. Mizoguchi	The 9 th International Conference on Intelligent Tutoring System (ITS2008) (Panel Chair)
R. Mizoguchi	The 5 th European Semantic Web Conference (ESWC2008) (PC member)
R. Mizoguchi	The 2008 IEEE International Conference on Information Reuse and Integration (IEEE IRI-08) (PC member)
R. Mizoguchi	The 17 th International World Wide Web Conference Semantic Web Track (PC Chair)
R. Mizoguchi	ODBASE 08 : Intl. Conf. on Ontologies, DataBases, and Applications of Semantics (PC member)
R. Mizoguchi	The 3 rd Asian Semantic Web Conference (ASWC2008) (PC member)
R. Mizoguchi	The 7 th international semantic web conference (ISWC2008) (Vice Chair)
R. Mizoguchi	EKAU 2008 - 16th International Conference on Knowledge Engineering and Knowledge Management Knowledge Patterns (PC member)
R. Mizoguchi	Formal Ontologies Meet Industry: FOMI 2008 (PC member)
R. Mizoguchi	IIP2008 - 5th International Conference on Intelligent Information Processing (PC member)
R. Mizoguchi	14th Collaboration Researchers' International Workshop on Groupware (PC member)
R. Mizoguchi	The 6 th International Workshop on Applications of Semantic Web Technologies for E-Learning (SWEL'08) (Workshop Organizers)
R. Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
R. Mizoguchi	International Journal of Applied Ontology (Editorial board)
R. Mizoguchi	Research and Practice in Technology Enhanced Learning (Editorial board)
R. Mizoguchi	International Journal of Artificial Intelligence in Education (Editorial board)

R. Mizoguchi	Frontiers in AI and Application (Editorial board)
R. Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)
R. Mizoguchi	Asian Semantic Web Conference (Steering committee chair)
K.Kozaki	The 3 rd Asian Semantic Web Conference (ASWC2007) (PC member)
K.Kozaki	The 1 st International Workshop on Intelligent Systems for Environmental (Knowledge) Engineering and EcoInformatics (i-SEEK'09) (PC member)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	7 papers
Japanese Association for Medical Informatics	1 paper

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

R. Mizoguchi	Technical documents integration based on an artifact ontology	¥5,000,000
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Grant-in-Aid for Young Scientists (A)

K. Kozaki	Application Platform for Multi-Dimension Knowledge Structuring based on Ontological Engineering	¥3,510,000
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Entrusted Research

R. Mizoguchi	The University of Tokyo	Research on development of a medical knowledge database for medical information systems; Design of a semantic relational model	¥15,000,000
R. Mizoguchi	The University of Tokyo	Biofuel Use Strategies for Sustainable Development; Restructuring problems of biofuel use by using Ontology and developing policy-making supporting tools.	¥2,401,000

Cooperative Research

R. Mizoguchi	Idemitsu Kosan Co., Ltd.	Development of knowledge base systems for nano-materials	¥3,300,000
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Department of Nanotechnology Transfer

Guest Associate Professor: Mohamed Almokhtar ABDEL-MOLA (2008.6.30-9.21)

Outlines

Double-quantum-well (DQW) superlattice structure consisting of ferromagnetic and non-ferromagnetic layers is one of the most important structures for spintronics devices. GaGdN/AlGaN DQW superlattice with room temperature ferromagnetic layer GaGdN and non-ferromagnetic barrier layer AlGaN was grown by molecular beam epitaxy method. In this work, we study the structural, optical and magnetic properties of this DQW superlattice structure. Especially, we focus on the interlayer exchange coupling in the GaGdN/AlGaN DQW superlattice between ferromagnetic layers of GaGdN.

Achievement

The surface morphology of GaGdN/AlGaN QDW superlattice structure was investigated by atomic force microscopy (AFM), and samples show very well crystalline quality because atomic steps were observed. Satellite peaks in the X-ray diffraction rocking curves were observed, which show smooth hetero-interface of GaGdN and AlGaN in the superlattice. Room temperature ferromagnetic behavior was found by using SQUID measurement. Strong photoluminescence from quantum well of GaGdN was observed on the lower energy side of GaN template. With decreasing the thickness of GaGdN layer, the peak from GaGdN quantum well showed blue shift.

Department of Nanotechnology Transfer

Guest Professor: Sung Sik KIM (2008.11.27-2009.2.27)

Outlines

Fabrication of the metal nanostructure has been studied using a new cyclic reaction based on the concept of two-color two-photon excitation.

Achievement

Fabrication of metal nanostructure using the two-color two-photon reduction cycle

We propose to fabricate the metal nanostructure using a new cyclic reaction based on the concept of two-color two-photon excitation. *N*-Methylphthalimide (MePI)-linked 4-methoxybenzophenone (MeOBP) (**1**) was synthesized. The excited benzophenone ketyl radical formed by the two-color two-photon excitation reduces the MePI moiety to form the diphenylmethanol cation and the MePI radical anion (MePI^{•-}). The cation quickly deprotonates to regenerate MeOBP. In the presence of an appropriate electron acceptor, MePI^{•-} reduces the acceptors to regenerate the initial MePI. As a result, the circular reaction is completed. The proposed cyclic reaction produces one reducing reagent (radical anion) and one proton from two photons (UV and vis light) and a hydrogen donor.

We tried to fabricate the metal nanostructure on the **1**-coordinated substrate using the above reduction cycle. The Ag nanostructures were successfully fabricated through the reduction of metal ions using the two-color two-photon cycle.

Publications

Original Papers

Reversible Intramolecular Triplet-Triplet Energy Transfer in Benzophenone-*N*-Methylphthalimide Dyad Aprotic Polar and Protic Polar Solvents, M. Sakamoto, S. S. Kim, M. Fujitsuka, A. Sugimoto, and T. Majima, *J. Phys. Chem. A*, 112[7] (2008) 1403-1407.

Division of Nanocharacterization

Outline

Division of Nanocharacterization has four departments: Department of Advanced Nanostructural Characterization, Department of Advanced Characterization for Nano-Processing, Department of Quantum Materials and Devices Characterization, and Department of Computational Nanocharacterization. This division aims at development and establishment of high-precision methods in evaluating nanoproceses, nanostructures and quantum-materials/devices specially suited for the unique features of nanotechnology, focusing on atomic-level surface layer formation, atomic arrangements and their relations to electron states, next-generation materials/devices properties.

Achievement

- Direct observations of the recording mark in phase change recording materials
- Elucidation of fundamental mechanism of electron beam lithography of semiconductor surfaces
- Finding of Plasmon-induced structural instability on Si surfaces
- Formation of sp^3 -bonded carbon nanostructures by femtosecond laser excitation of graphite
- Stochastic resonance effects of photoinduced bond rupture on Si(111)7x7
- Nano-characterization of GaGdN nanorod structures
- Nano-characterization of GaCrN/AlN multi-quantum disk nanorod structures

Department of Advanced Nanostructural Characterization

Assistant Professor: Muneyuki NAITO

Outlines

The purpose of this department is to develop new electron microscopy methods to characterize atomic structures, atomic bonding and electronic structures of functional nanomaterials in order to contribute to the development and realization of novel functional materials and devices.

Current Research Project

Electron irradiation-induced phase transformation in α -FeSi₂

Structural changes of α -FeSi₂ induced by electron beam irradiation have been investigated using transmission electron microscopy (TEM). Single crystals of Si(111) were implanted with 120 keV Fe ions at -150 °C to a fluence of 1.0×10^{17} /cm², followed by thermally annealing at 350-550 °C. Cross-sectional and plan-view TEM observations revealed the formation of the metastable α -FeSi₂ in the annealed samples. Under high-energy electron beam irradiation, the α -phase changed to a metastable crystalline phase whose structure is close to the CsCl structure. The phase transformation was caused mainly by displacement damage processes and suggest a low displacement energy for Fe atoms (< 9eV). To explain these observations, it was considered that vacancies in α -FeSi₂ are responsible for the electron irradiation-induced phase transformation.

Publications

Original Papers

Low temperature thermal annealing-induced α -FeSi₂ derived phase in an amorphous Si matrix, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez, K. E. Sickafus: Appl. Phys. A, 91 (2008) 353-356.

Direct observations of thermally induced structural changes in amorphous silicon carbide, M. Ishimaru, A. Hirata, M. Naito, I.-T. Bae, Y. Zhang, W. J. Weber: J. Appl. Phys., 104 (2008) 033503(1)-033503(3).

Electron irradiation-induced phase transformation in α -FeSi₂, M. Naito, M. Ishimaru, J. A. Valdez, K. E. Sickafus: J. Appl. Phys., 104 (2008) 073524(1)-073524(6).

Structural characterization of metastable iron silicides formed in the Fe ion implanted Si, M. Naito, M. Ishimaru: Proc. 9th Asia-Pacific Microscopy Conf., (2008) 822-823.

Review Papers

Recrystallization Processes of High-Dose Fe Implanted Si, M. Naito and M. Ishimaru, Materia Japan 47 (2008) 640 (in Japanese).

International Conferences

Formation of metastable iron silicides in the Fe implanted Si, *M. Naito, M. Ishimaru: 16th International Conference on Ion Beam Modification of Materials, Dresden, Germany (August 31 - September 5, 2008).

Local structure analysis of metastable iron silicides formed in the Fe ion implanted Si, *M. Naito, M. Ishimaru: 7th Polish-Japan Joint Seminar on Micro and Nano Analysis, Warsaw, Poland (September 7-10, 2008).

Structural relaxation in amorphous SiC studied by in situ transmission electron microscopy, *M. Ishimaru, A. Hirata, M. Naito, I.-T. Bae, Y. Zhang, W. J. Weber: 9th Asia-Pacific Microscopy Conference, Jeju, Korea (November 2-7, 2008).

Structural characterization of metastable iron silicides formed in the Fe ion implanted Si, *M. Naito, M. Ishimaru: 9th Asia-Pacific Microscopy Conference, Jeju, Korea (November 2-7, 2008).

Transmission electron microscopy study on electron beam irradiation induced phase transformation of niobium nitride (poster), *J. H. Won, J. A. Valdez, K. E. Sickafus, M. Ishimaru, M. Naito: Materials Research Society 2008 Fall Meeting, Boston, USA (December 1-5, 2008).

Structural changes of amorphous SiC during post-implantation thermal annealing (invited), *M. Ishimaru, A. Hirata, M. Naito, I.-T. Bae, Y. Zhang, W. J. Weber: 16th International Conference on Ion Beam Modification of Materials, Dresden, Germany (August 31 - September 5, 2008).

Publications in Domestic Meetings

Japanese Society of Microscopy	1 paper
The Japan Institute of Metals	1 paper

Sponsorship

Grant-in-Aid for Encouragement of Young Scientists (B)

M. Naito	Direct observations of recording marks in the phase-change disk	¥2,700,000
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Entrusted Research

M. Naito	Nissan Arc, Ltd.	Structure analysis of amorphous Si layers in the lithium-ion secondary battery	¥1,000,000
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Other Research Fund

M. Naito	Kazato Research Foundation	Travel Grants for International Conference	¥100,000
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Department of Advanced Characterization for Nano-Processing

Professor: Katsumi TANIMURA
Associate Professor: Jun'ichi KANASAKI

Outlines

For fabricating highly functional nano-structured devices in future technology, it is important to establish the ways to control structures and compositions of materials in atomic levels. Electronic excitations, which induce and promote atomic processes with strongly site-sensitive rates, can be a promising method for creating nano-scaled structures possessing new properties and functions, that are not achieved by conventional thermal process. Our targets are to understand completely the fundamentals of underlying physics concerning the excitation-induced atomic processes, and finally to establish advanced surface nano-processing technologies fully exploiting unique features of electronic-excitation effects. For this purpose, we have studied laser or low-energy electron induced structural changes of semiconductor and graphite surfaces by means of the direct imaging of the surface structures using scanning tunneling microscopy (STM).

Current Research Project

• Excitation-induced Instability of Semiconductor Surfaces

Systematic studies of structural instabilities of semiconductor surfaces induced by laser beams, low-energy electron beams, and carriers injected from STM tips have revealed that the excitations cause bond rupture at intrinsic surface sites, resulting in formation of vacancies selectively on the outermost atomic layer. We have successfully established the unified theoretical mechanism of the excitation-induced bond rupture based on the two-hole localization of valence holes at intrinsic surface sites.

In order to deepen our understanding of the excitation-induced instabilities, we have studied further two topics as follows:

1. Mechanism of bond rupture on Si(111)7x7 induced by low-energy electron beam excitation

The quantum nature of low-energy (several eV - 10eV) electrons (LEEs) is obvious in most processes, and the Born approximation cannot be used for describing the scattering of LEEs. Therefore, the primary mechanisms of the LEE interaction with solids have not yet been completely understood. We have studied the structural responses of Si(111)7x7 surface induced by LEE beams by means of STM, and found that the excitation removes Si atoms on the surface with a strongly site-dependent efficiency. The bond rupture efficiency (or the cross section) has been measured as a function of the maximum energy E_{av} available for inelastic excitation. The rate shows a clear threshold energy at $E_{av}=8 \pm 2$ eV, and then forms the maximum around $E_{av}=14$ eV. The available energy giving the maximum efficiency coincides with the plasma excitation

energy of Si crystal. Therefore, the result provides the first evidence for the bond rupture on semiconductor surfaces induced by plasmon excitation.

2. Stochastic resonance effects of photoinduced bond rupture on Si(111)7x7

We have studied the temperature dependent effects on the fs-laser induced bond rupture rate to reveal synergistic effects of thermal fluctuation of the lattice system and dynamical relaxation process of two-hole localization. STM studies of the excitation-induced structural changes of Si(111)7x7 at several different temperatures between 200 and 500 K have revealed a type of stochastic resonance of the dynamical process with the thermal fluctuation effects.

• Formation of A Novel sp^3 -Bonded Nanostructures by Femtosecond Laser Excitation of Graphite

Hexagonal graphite crystal is characterized by the stacking of strongly sp^2 -bonded planes (graphene sheets) by van der Waals interaction, and phenomena associated with its anisotropic bonding nature in graphite have attracted fundamental and technological interests. We have obtained the first direct atomic-scale evidence of the non-thermodynamic formation of a novel carbon phase about 5nm in diameter by fs-laser excitation of graphite. We have examined the nanostructures by means of STM, and found that the structures exhibit sp^3 -type interlayer bonds but differ from a diamond lattice: the structures have been termed '*diaphite*'. Also we have measured the local density of states (LDOS) at the nanostructures, and found the remarkable peaks of LDOS centered at $\pm 0.3\text{eV}$ relative to the Fermi level. Theoretical studies of total energy calculation with LDA method have confirmed that the diaphite is a metastable phase of graphite, separated by a barrier of 0.5 eV, which is enough to stabilize the diaphite phase during STM analysis. The structure and LDOS calculated for the diaphite structure agree with the experimental results derived from our STM/STS analyses. This study opens up the possibility of finding more new phases of carbon through simple optical methods.

Publications

Original Papers

Formation of sp^3 -bonded carbon nanostructures by femtosecond laser excitation of graphite, J. Kanasaki, E. Inami, K. Tanimura, H. Onishi, and K. Nasu: Physical Review Letters 102 [8] (2009) 087402-1-4.

Excitation-induced atomic desorption and structural instability of III-V semiconductor surfaces, K. Tanimura and J. Kanasaki: Surface Science 602 [20] (2008) 3162-3171.

International Conferences

Local bond rupture on Si surfaces induced by low-energy electron-beam excitation, J. Kanasaki, and K. Tanimura, Electron Induced Processes at Molecular Level, Low-Energy Electron Molecule Interaction, Electron Controlled Chemical Lithography,

Roscoff, France, May 7-11, 2008.

Interlayer bond formation of a graphite crystal induced by femtosecond laser excitation, J. Kanasaki, E. Inami, K. Tanimura, and K. Nasu, 25th European Conference on Surface Science, Liverpool, UK, July 26-August 1, 2008.

Local bond rupture on silicon surfaces induced by low-energy electron-beam excitation, J. Kanasaki and K. Tanimura, 12th SANKEN International Symposium, 7th Nanotechnology Center International Symposium, 2nd MSTEC International Symposium, 1st SANKEN Alliance Symposium, Osaka, January 22, 2009

Contributions to International Conferences and Journals

K.Tanimura	International Workshop on Desorption Induced by Electronic Transitions (International Steering Committee)
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Publications in Domestic Meetings

The Physical Society of Japan	4 papers
Others	5 papers

Sponsorship

Grant-in-Aid for Specially Promoted Science

K. Tanimura	Dynamical Studies of Photoinduced Phase Transitions	¥175,760,000
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Department of Quantum Materials and Devices Characterization

Professor: Hajime ASAH
Assistant Professor: Yi-Kai ZHOU

Outline

The department of quantum materials and devices characterization makes researches on new characterization methods and the characterization of structural and physical properties of quantum materials and quantum devices in order to contribute to the development and realization of novel functional quantum materials and devices.

- Development and application of nano-characterization methods for the physical properties of quantum materials.
- Development and application of nano-characterization methods for the structural and physical properties of quantum devices including next generation LSIs.
- Development and application of nano-characterization methods for the device properties of quantum devices.

Current Research Projects

1. Nano-Characterization of GaN-Based Magnetic Semiconductor Nanostructures

Quantum nanostructures are basic structures for devices. Nanostructures using diluted magnetic semiconductors perform very important roles for the fabrication of spin devices. GaCrN nanorods were formed by MBE. We have already clarified the relation between GaCrN nanorods and their growth conditions by STM. In 2008, GaGdN nanorods were grown on the Si substrates by MBE at relatively low temperature of 550°C to suppress second phase formation and to incorporate higher concentration of Gd. X-ray diffraction measurement revealed that GaGdN nanorods are oriented to c-axis and that the hexagonal GaGdN diffraction peak shows a shift to low diffraction angle side with increasing Gd concentration because of the larger lattice constant of GaGdN than GaN (radius of Gd ion is large than that of Ga). Magnetization measurement with alternating gradient magnetometer on GaGdN nanorod samples confirmed room temperature ferromagnetism. With increasing Gd concentration, the saturation magnetization becomes large. The GaGdN nanorod sample grown with Gd cell temperature of 1150 °C showed the saturation magnetization of 3.7×10^{-6} emu.

2. Nano-Characterization of Fe thin film on GaN

Spin injection behavior from magnetic metals into diluted magnetic semiconductors (DMSs) is very important to realize semiconductor spintronics devices in addition to operate spin polarized scanning tunneling microscopy (SP-STM) to DMSs. So far, we have evaluated crystal structures and magnetic properties of Fe nanodots on GaN. It was found that magnetic characteristics greatly depend on the amount of deposited Fe metals and their structures. In 2008, magnetic properties of Fe nanodots were studied using SP-STM. It was found that Fe nanodots with some ordered orientation show spin-dependent current-voltage characteristics.

3. XAFS and SX-MCD Characterization of Ferromagnetic semiconductor GaGdN

The element-selected magnetic circular dichroism (MCD) between Gd core states is observed in soft X-ray region (1150–1250 eV). The dichroism intensity for the transition from 3d to 4f orbital of Gd atomic state is very strong and reaches up to about 30% at 15K. The temperature dependence of the MCD intensity shows ferromagnetic phase around 50–80K in addition to room temperature ferromagnetic phase. X-ray absorption near edge structures (XANES) is different from other Gd compounds. It seems to relate to the strength of the ferromagnetic behaviors. It is found that the XANES, which also reflects the local structure around the selected element more sensitively, produces the weak hump on the high-energy side of the white peak. The hump is not observed in pure and high quality GdN, Gd₂O₃ and Gd metal. Therefore, the hump suggests that the local coordination around the Gd ions deforms. As it is clearly observed, the deformation is strong, and considering the ionic radius of Gd ion, it is highly possible that an N vacancy is made in vicinity of the Gd ion. This fact may support a model proposed by German groups and strongly relates to the ferromagnetism generation of GaGdN. Therefore, N vacancies neighboring Gd ions enhance or mediate the ferromagnetic behaviors of GaGdN.

Publications

Original Papers

Low temperature molecular-beam epitaxy growth of cubic GaCrN, S. Kimura, S. Emura, Y. Yamauchi, Y. K. Zhou, S. Hasegawa and H. Asahi: J. Cryst. Growth, 310 (2008) 40-46.

Large magnetization in high Gd concentration GaGdN and Si-doped GaGdN grown at low temperatures, Y.K. Zhou, S.W. Choi, S. Emura, S. Hasegawa and H. Asahi: Appl. Phys. Lett., 92(6) (2008) 6062505-1 - 6062505-3.

Growth and characterization of InCrN and (In,Ga,Cr)N, S. Kimura, S. Emura, K. Tokuda, Y. Hiromura, S. Hayakawa, Y.K. Zhou, S. Hasegawa and H. Asahi: Phys. Stat. Sol. (c), 5 (6) (2008) 1532-1535.

Molecular-beam epitaxy fabrication and analysis of GaN nanorods on patterned silicon-on-insulator substrate, J.U. Seo, S. Hasegawa, and H. Asahi: Phys. Stat. Sol. (c), 5(9) (2008) 3004-3007.

Selective growth of InP on localized areas of silicon (100) substrate by molecular beam epitaxy, K. Araki, S. Hasegawa and H. Asahi: Phys. Stat. Sol. (c), 5(9) (2008) 2766-2768.

Selective growth of InP on areas (1 μ m $\times$ 1 μ m) of silicon (100) substrate by molecular beam epitaxy, K. Araki, S. Hasegawa and H. Asahi: Proc. of the 20th Intern. Conf. on Indium Phosphide and Related Materials, (2008) WeP12-1 - WeP12-4.

Studies on TlInGaAsN Double Quantum Well Structures, D. Krishnamurthy, M. Ishimaru, M. Ozasa, Y. Tanaka, S. Hasegawa, Y. Hirotsu and H. Asahi: Proc. of the 20th Intern. Conf. on Indium Phosphide and Related Materials, (2008) WeP10-1 -

WeP10-4.

Electronic structure of Ga_{1-x}Cr_xN and Si-doping effects studied by photoemission and X-ray absorption spectroscopy, G. S. Song, M. Kobayashi, J. I. Hwang, T. Kataoka, M. Takizawa, A. Fujimori, T. Ohkouchi, Y. Takeda, T. Okane, Y. Saitoh, H. Yamagami, F.-H. Chang, L. Lee, H.-J. Lin, D. J. Huang, C. T. Chen, S. Kimura, M. Funakoshi, S. Hasegawa, and H. Asahi:, (2008) 033304-1 – 033304-4.

Local Structural Change in paramagnetic and Charge-Ordered Phase of Sn_{0.2}Pr_{0.3}Sr_{0.5}MnO₃: an EXAFS Study, K.R. Priolkar, V. Kulkarni, P.R. Sarode, and S. Emura: J. Phys.: Condensed matter, 20 (2008) 335227 – 335231.

Review Papers

Advances and future prospects of semiconductor hetero-epitaxy, H. Asahi, Oyobutsuri, 77(5) (2008) 489-499 (in Japanese).

Books

Vacuum and vacuum evaporation, H. Asahi: in *Handbook of Thin Films* (Ohm-sha, 2008) 10-14 (in Japanese).

International Conferences

TlInGaAsN Novel Semiconductors and Temperature-Stable Lasing Wavelength Laser Diodes (invited), H. Asahi, S. Hasegawa, A. Fujiwara and D. Krishnamurthy: 2008 SPIE Photonics West Conference.

Selective growth of InP on areas (1μm×1μm) of silicon (100) substrate by molecular beam epitaxy (poster), K. Araki, S. Hasegawa and H. Asahi: 20th International Conference on Indium Phosphide and Related Materials, Versailles, France,.

Studies on TlGaInNAs Double Quantum Well Structures (poster), D. Krishnamurthy, M. Ishimaru, M. Ozasa, Y. Tanaka, S. Hasegawa, Y. Hirotsu and H. Asahi,: 20th International Conference on Indium Phosphide and Related Materials, Versailles, France,.

Formation of aligned CrN nano-clusters in Cr-delta-doped GaN (poster), Y. K. Zhou, S. Kimura, S. Emura, S. Hasegawa and H. Asahi: International Conference on Quantum Simulators and Design 2008, Tokyo.

Crystal growth and characterization of GaCrN nanorods on Si substrate (poster), H. Tambo, S. Kimura, Y. Yamauchi, Y. Hiromura, S. Emura, S. Hasegawa and H. Asahi: The 2nd International Symposium on Growth of III-Nitrides, Izu, Japan.

Effects of morphologies on field emission characteristics of GaN nanorods grown on Si by MBE (poster), J. U. Seo, S. Hasegawa, and H. Asahi: The 2nd International Symposium on Growth of III-Nitrides, Izu, Japan.

Orbital ordering on dilute Cr³⁺ ions doped in GaN (poster), S. Emura, S. Kimura, K. Tokuda, Yi-Kai Zhou, S. Hasegawa and H Asahi: 29th International Conference on Physics of Semiconductors, Brazil.

Third magnetic phase of GaGdN detected by SX-MCD (poster), M. Takahashi, Y. Hiromura, S. Emura, T. Nakamura Y.K. Zhou, S. Hasegawa and H. Asahi: 29th International Conference on Physics of Semiconductors, Brazil.

Structural properties of AlCrN, GaCrN and InCrN (poster), S. Kimura, K. Tokuda, Y. K. Zhou, S. Emura, S. Hasegawa and H. Asahi: 15th International Conference on Molecular Beam Epitaxy, Vancouver, Canada.

MBE growth and characterization of TlGaInNAs double quantum well structures (poster), D. Krishnamurthy, M. Ozasa, Y. Tanaka, S. Hasegawa and H. Asahi: 15th International Conference on Molecular Beam Epitaxy, Vancouver, Canada.

Annealing effect in GaDyN on optical and magnetic properties (poster), Y. K. Zhou, M. Takahashi, S. Emura, S. Hasegawa, H. Asahi: 5th International Conference on Physics and Applications of Spin-Related Phenomena in Semiconductors, Foz do Iguacu, PR, Brazil.

Magnetic properties of GaGdN studied by SQUID and SX-MCD (poster), M. Takahashi, Y.K. Zhou, S. Emura, T. Nakamura, S. Hasegawa, and H. Asahi: 5th International Conference on Physics and Applications of Spin-Related Phenomena in Semiconductors, Foz do Iguacu, PR, Brazil.

Structural properties of AlCrN, GaCrN and InCrN (poster), K. Tokuda, S. Kimura, Y. K. Zhou, S. Emura, S. Hasegawa and H. Asahi: XXI International Union of Crystallography, Osaka, Japan.

Crystal growth condition dependence of local structure around Gd in GaN nanorods (poster), S. Emura, H. Kameoka, H. Tambo, Y.K. Zhou, S. Hasegawa and H. Asahi: XXI International Union of Crystallography, Osaka, Japan.

Growth and characterization of GaN nanorods towards the application to field emitters (invited), S. Hasegawa, J.U. Seo and H. Asahi: 14th Seoul International Symposium on the Physics of Semiconductors and Applications, Jeju Island, Korea.

SX-MCD and XAFS Analysis on GaGdN (poster), M. Takahashi, Y. Hiromura, S. Emura, T. Nakamura, Y.K. Zhou, S. Hasegawa, and H. Asahi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Gd concentration dependence of local structures around Gd atoms in GaGdN nanorod (poster), H. Kameoka, S. Emura, H. Tambo, Y.K. Zhou, S. Hasegawa and H. Asahi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Growth and characterization of Fe nanostructures on GaN (poster), Y. Honda, M. Sotani, S. Hasegawa and H. Asahi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Growth and characterization of transition-metal and rare-earth doped III-nitride based

magnetic semiconductors for nano-spintronics (invited), H. Asahi, S. Hasegawa, S. Emura and Y.K. Zhou: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka.

Influence of native silicon oxides on the growth of GaN nanorods on Si (001) (poster), S. Hasegawa, J. K. Seo, K. Uchida, H. Tambo, H. Kameoka, M. Ishimaru, and H. Asahi: International Workshop on Nitride Semiconductors (IWN-2008), Montreux, Switzerland.

Degradation mechanisms of GaAs PHEMTs under operation in high humidity conditions (poster), T. Hisaka, H. Sasaki, Y. Nogami, K. Hosogi, N. Yoshida, J.A. del Alamo, S. Hasegawa and H. Asahi: Reliability of Compound Semiconductors (ROCS) Workshop, Monterey, California, USA.

Growth and characterization of Fe nanostructures on GaN (poster), Y. Honda, S. Hayakawa, S. Hasegawa and H. Asahi: 4th Vacuum and Surface Sciences Conference of Asia and Australia, Matsue, Japan.

Ferromagnetism and Luminescence of Diluted Magnetic Semiconductors GaGdN and AlGdN (invited), S. Emura, M. Takahashi, H. Tambo, T. Nakamura, Y.K. Zhou, S. Hasegawa and H. Asahi: Materials Research Society Fall Meeting, Boston, MA, USA.

Field emission characteristics of GaN nanorods grown on Si by MBE (poster), S. Hasegawa, J. U. Seo and H. Asahi: International Symposium on Core University Program between Japan and Korea, Awaji, Hyogo, Japan.

Magnetic properties of GaCrN nanorods (poster), Y. K. Zhou, H. Tambo, S. Emura, S. Hasegawa and H. Asahi: International Symposium on Core University Program between Japan and Korea, Awaji, Hyogo, Japan.

Contributions to International Conferences and Journals

- | | |
|----------|--|
| H. Asahi | 2008 International Conference on Solid State Devices and Materials
(Program Committee member) |
| H. Asahi | 20th International Conference on Indium Phosphide and Related
Materials
(International Steering Committee member) |
| H. Asahi | 15th International Conference on Molecular Beam Epitaxy
(International Advisory Committee member) |
| H. Asahi | Second International Symposium on Growth of III-Nitrides
(International Advisory Committee member) |
| H. Asahi | 4th Vacuum and Surface Science Conference of Asia and Australia
(Program Committee member) |
| H. Asahi | International Conference on Functional Materials for Advanced
Technology
(International Organizing Committee member) |
| H. Asahi | 16th International Colloquium on Scanning Probe Microscopy
(Publication Committee member) |
| H. Asahi | 2009 International Conference on Solid State Devices and Materials
(Program Committee member) |

H. Asahi	21st International Conference on Indium Phosphide and Related Materials (International Steering Committee member)
H. Asahi	Journal of Crystal Growth (Editor)
H. Asahi	Current Applied Physics (Editorial Board member)
H. Asahi	J. Materials Science: Materials in Electronics (Editorial Board member)
H. Asahi	Journal of Ceramic Processing Research (Editor)
H. Asahi	Journal of Physics: Condensed Matter (Advisory Editorial Board member)
H. Asahi	e-Journal of Surface Science and Nanotechnology (Advisory Board member)

Publications in Domestic Meetings

The Japan Society of Applied Physics	12 papers
PASPS Symposium	3 papers
Electronic Materials Symposium	1 paper

Grant-in-Aid for Scientific Research (B) (2)

H. Asahi	Study on Room Temperature Ferromagnetic Nitride Semiconductor Nanostructures and Application to Nanospintronics Devices	¥2,300,000
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Grant-in-Aid for Scientific Research on Priority Areas

H. Asahi	Study on Fabrication of InN-Based Long Wavelength Circular Polarized Semiconductor Lasers	¥3,900,000
Y.K. Zhou	Experimental Study on Quantum Nanostructures of Insoluble Impurity Doped Semiconductors	¥2,300,000

Grant-in-Aid for Creative Scientific Research

H. Asahi	Development of properties and functionalities by precise control of rare-earth doping (Y. Fujiwara)	¥28,000,000
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Department of Handai Multi-Functional Nanofoundry

Professor:	Tomoji KAWAI
Professor:	Seiichi TAGAWA
Professor:	Hirotarou MORI
Specially appointed researcher:	Akio TAKAOKA (Professor emeritus)
	Hirotooshi FURUSHO
	Naoko KAJIMURA
	Tomoki NISHIDA
	ChunLin CHEN
	Lin-Yen LIN
	Naoko YAMADA
	Masakazu MURASUGI
	Hideto OHNISHI
	Akihiro OSHIMA
	Akira Kitajima (2008.5.1-)
Supporting staff	Yasuo NAKAMURA
	Naomi YANAMORI
	Yoshihiko INOUE
	Keiko TOYA (2008.4.21-12.31)
	Norio SUNAGAWA
	Keiko ENMI
	Chie MATSUMOTO

Outlines

Handai Multi-Functional Nanofoundry was founded in Mission of Nanotechnology Network Japan, supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. The purpose to start up the Nanofoundry is to establish a platform supporting Nanotechnology research and development, especially, for researchers outside of Osaka University. Nanofoundry started from April 2007, and our efforts resulted in supporting 85 research themes in 2008.

The Mission of Nanotechnology Network Japan was organized to respond to the requests that researchers belonging to public / private universities or companies hope to realize and to respond to researchers finding opportunity to use special facilities and equipments for their nanotechnology research and development program.

Institute of Science and Industrial Research (ISIR), Osaka University has played an important role in Nanotechnology fields by providing individual technologies and information. Our Nanofoundry supported lots of researchers inside / outside of Osaka University through “Nanofabrication”, “Molecular and thin film fabrication” and “Characterization & analysis”.

Focuses of Handai Multi-Functional Nanofoundry are shown below.

- (1) Innovation by integrated and speedy nanotechnology support consisting of “Fabrication (top-down and bottom-up)”, “Observation and Measurement”.
- (2) Creation of advanced interdisciplinary nanotechnology through integrated research and development of inorganic and organic materials, metals,

- semiconductor materials, and biomaterials.
- (3) Fostering of scientists in the field of advanced interdisciplinary nanotechnology.

Current Research Project

Bring-up Handai Multi-Functional Nanofoundry

The 85 research themes have been supported in this project in 2008. Considering they have been applied for by researchers in the universities, companies, and national institutes, we are able to see that Nanofoundry activates clearly nanotechnology field. Nanofoundry has been founded to support nanotechnology researchers through nanofabrication, molecular and thin film fabrication, characterization and analysis. These supports are divided into following four types. (a) Technical consulting, (b) Collaborative research, (c) equipment use, and (d) Technical supports.

Break-through toward Multi-functional Nanotechnology R&D

Nanofoundry support advanced nanotechnology research and development as well as fundamental study. The research on functional integration and system building based on nanomaterials is acceptable in the Nanofoundry.

Fusion between Top-down and Bottom-up Nanotechnologies

For top-down and bottom-up nanotechnologies, a lot of useful equipments such as FIB, EB drawing and PLD, and so on, are in operation. The fusion between top-down and bottom-up nanotechnologies will bring much important progress on nanotechnology in the near future.

International Conferences

Micro- and Nano- Fabrication of Fluorinated- Polymers by means of SR and FIB (invited), *A. Oshima, T.Urakawa, N.Fukutake, Y.Takasawa, K.Okamoto, S.Seki, T.Katoh, M.Washio, S.Tagawa: The 9th RadTech China, Hangzhou, China, April 8-11, 2008.

Fabrication of the hybrid PEM consists of perfluoro-sulfonic acid and sulfonated PS-g-FEP using EB-grafting (invited), *A.Oshima, Y.Satoukiko SATO, Y.Oshima, F. Shiraki, N.Mitani, K.Fujii, M.Ito, M.Washio: RADTECH UV&EB 2008, Chicago, USA, May 4-7, 2008.

Microfabrication of nano - scale pattern on crosslinked PTFE using focused ion beam (poster), *N.Fukutake, T.Urakawa, Y.Takasawa, A.Oshima, M.Washio, K.Okamoto, S.Tagawa: he 2nd Asia - Pacific Symposium on Radiation Chemistry (APSRC-2008), Tokyo, Japan, August 29-September 1, 2009.

Surface Modification of Polymeric Materials Using Ultra Low Energy Electron Beam Irradiation (poster), *A.Oshima, Y.Takasawa, N.Fukutake, T.Urakawa, F.Shiraki, M.Washio: he 2nd Asia - Pacific Symposium on Radiation Chemistry (APSRC-2008), Tokyo, Japan, August 29-September 1, 2008.

Nano- and Micro- Fabrication of Polymeric Materials Using Beam Technology (invited),
 *A. Oshima, M. Washio, S. Tagawa: 8th International Symposium on Ionizing
 Radiation and Polymers (IRaP2008), Angra dos Reis, Brazil, October, 12-17, 2008.

Nano-fabrication of Fluoropolymers using Focused Ion Beam (poster), *N.Fukutake,
 T.Urakawa, Y.Takasawa, T.Gowa, T.Takahashi, Y.Hirano, M.Washio, A.Oshima,
 K.Okamoto, S.Tagawa: FLUOROPOLYMER2008, South Carolina, USA, October 19-22,
 2008.

Fabrication of Micro- and Nano-Structures of Crosslinked Polytetrafluoroethylene by
 Means of Focused Ion Beam, *A.Oshima, N.Miyoshi, N.Fukutake, Y.Takasawa,
 Y.Matsui, K.Okamoto, S.Seki, M.Washio, S.Tagawa: The IUMRS International
 Conference in Asia 2008(IUMRS-ICA 2008), Nagoya, Japan, December 9-13,
 2008 .

Introduction of Handai Multi-Functional Nanofoundry (poster), N.Yanamori,
 Y.Nakamura, Y.Inoue, A.Kitajima, *H.Onishi, K.Enmi, M.Murasugi: The 2nd SANKEN
 Internatinal Symposium, Osaka, Japan, January 22, 2009.

Publications in Domestic Meetings

Society of Polymer Science, Japan	2 papers
Japan Radioisotope Association	1 paper
Japanese Society of Radiation Chemistry	2 papers
Chemical Society of Japan	1 paper

Sponsorship

Grant-in-Aid for Scientific Research (Young Scientists) (B)

A. Oshima	¥1,820,000
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Entrusted Research

T. Kawai	MEXT	Mission of Nanotechnology Network Japan	¥147,000,000
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Open Laboratory

Professor (concurrent, manager): Yoichi YOSHIDA
Professor (concurrent): Katsuaki SUGANUMA
Professor (concurrent): Hidekazu TANAKA
Technical Staff: Kimihiro NORIZAWA
Supporting Staff: Kayoko OHASHI

Outlines

Open Laboratory supports the comprehensive research for creative and advanced academic research on materials and devices, which should become the foundation of scientific and technological development on nanotechnology.

Current Research Project

On 2008, the following 17 researchers used Open Laboratory.

Prof. Yasufumi FUJIWARA	Graduate School of Engineering
Prof. Kiichi FUKUI	Graduate School of Engineering
Prof. Yoshihisa INOUE	Graduate School of Engineering
Prof. Kazuyoshi ITOH	Graduate School of Engineering
Prof. Tomoyuki KAKESHITA	Graduate School of Engineering
Prof. Ryoichi NAKATANI	Graduate School of Engineering
Prof. Yusuke MORI	Graduate School of Engineering
Prof. Kazuyoshi IKUTA	Research Institute for Microbial Diseases
Prof. Naoyuki TANIGUCHI	Research Institute for Microbial Diseases
Prof. Yoshimitsu YAMASAKI	Graduate School of Medicine
Prof. Hirotaro MORI	Research Center for Ultra-High Voltage Electron Microscopy
Prof. Tadashi ITOH	Promotion of Research on Nanoscience and Nanotechnology
Prof. Tomoji KAWAI	Institute of Scientific and Industrial Research
Prof. Hikaru KOBAYASHI	Institute of Scientific and Industrial Research
Assoc. Prof. Shun'ichi KURODA	Institute of Scientific and Industrial Research
Prof. Seiichi TAGAWA	Institute of Scientific and Industrial Research
Prof. Kazuhiko MATSUMOTO	Institute of Scientific and Industrial Research

Radiation Laboratory

Professor, Director: Yoichi YOSHIDA
Professors Seiichi TAGAWA, Goro ISOYAMA, Tetsuro MAJIMA
Associate Professors: Ryuko KATO, Yoshihide HONDA, Mamoru FUJITSUKA,
Takahiro KOZAWA, Kiyohiko KAWAI, Jinfeng YANG
Assistant Professors: Toshiji IKEDA, Norio KIMURA, Kazuo KOBAYASHI,
Sachiko TOJO, Shigeru KASHIWAGI, Akinori SAEKI,
Takashi TACHIKAWA
Specially Appointed Assistant Professors: Masanori SAKAMOTO, Takafumi KONDO
Technical Staff: Tamotsu YAMAMOTO
Support Staff: Ritsuko NAGAO

Outline

The Radiation Laboratory was newly established in the fiscal year 2002 in the Nanoscience and Nanotechnology Center as a successor of the *Radiation Laboratory*, which was a facility directly attached to the Institute but had been reorganized to be part of the center, for operating experimental equipment previously owned by the *Radiation Laboratory*. The main pieces of the equipment are the 40 MeV L-band electron linear accelerator (linac), the 150 MeV S-band electron linac, the 40 MeV RF-gun electron linac, and the ^{60}Co γ -ray irradiation facility. Among them, the L-band linac and the γ -ray irradiation facility are open to users in Osaka University. The staff of the Radiation Laboratory is composed of the full-time members, who are a technician from the Technical Division and a secretary, and concurrent members from the Division of Beam Science for Nanotechnology of the center and the Division of Beam Science and Technology as well as related Departments of the institute. They run the Radiation Laboratory and care for outside users.

Achievement

L-band linac

The L-band electron linac has four operation modes, which are transient, steady, single-bunch, and multi-bunch modes, in combination with either the short or long pulse duration of injected electrons and operation of the sub-harmonic buncher or not, and has ability to accelerate an electron beam up to the maximum energy 40 MeV and the highest charge per bunch 91 nC in the single bunch operation mode or the maximum current injected from the electron gun 30.6 A in the transient mode at the repetition rate 60 pulses per second at maximum. The machine time of the L-band linac in the fiscal year 2008 is as follows; 120 days including 21 days for maintenance are allocated in the first term and 118 days including 18 days for maintenance in the latter term. The operation days in the year are 204 days in total and the operation time is 2,400 hours. In this fiscal year, in order to enhance operational stability of the klystron, we replaced the

thyatron system.

S-band linac

The S-band linac can accelerate an electron beam of the nominal energy 100 MeV and a peak current 0.2 A at the repetition rate 30 Hz, and it has been used for production of the slow positron beam.

RF-gun linac

The laser-photocathode RF electron linac, which constructed with a photocathode rf gun and a magnetic bunch compressor, is one of the S-band accelerators in ISIR to generate a low-emittance, femtosecond-bunch electron beam with the maximum energy of 40 MeV. The femtosecond electron beam is used mainly to study the ultrafast reactions or phenomena in material by means of femtosecond pulse radiolysis. In 2008, the following researches were carried out:

- (1) Development of femtosecond pulse radiolysis,
- (2) Study on the electron-beam-induced reactions in femtosecond time scale,
- (3) Electron beam modulation for the radiation therapy of cancer, and
- (4) Research on the attosecond electron beam generation.

^{60}Co γ -ray irradiation facility

The ^{60}Co γ -ray irradiation facility is equipped with two irradiation rooms with different areas and irradiation experiments are conducted using three high-intensity ^{60}Co sources. In this fiscal year, the facility was widely used not only by members of our institute but also by those coming from the Graduate School of Science, the Graduate School of Engineering, the Research Institute for Microbial Diseases, Radioisotope Research Center, and the Faculty of Medicine. The number of research subjects is increasing recently and the facility was extensively used over the university and the total utilization time is about 2,950 hours, which is longer than a value in last year. The maintenance of the irradiation facility was carried out for safety operation.

Join-use

The number of joint-use this fiscal year is 21 subjects from this institute, 15 subjects from other faculties and institutes of the university, and 6 subjects proposed by groups including members of other universities and institutes, and these are added up to 42 subjects in total.

We held a workshop on “New Development of the Radiation Laboratory and Beam Science” on February 2-3, 2009 at the conference hall of the Icho-Kaikan. In addition, we held the annual meeting for presenting results obtained in the fiscal year 2008 on March 4, 2009 at the Joint-Project room of the institute. We received more than 220 visitors to the Radiation Laboratory.

Radiation safety management

The number of radiation users in ISIR is 162 persons in the fiscal year 2008. Education and training courses for the users was held on April 8-10, 2008 at the MO Hall in the Convention Center of Osaka University. An education and training course for new users was held on May 8, 2008 at the Joint-Project room of the institute.

Electron Microscope Laboratory

Professor, Director: Katsuaki SUGANUMA

Outlines

Electron microscope laboratory was established in 1951 and contributed to micro structural investigation in ISIR. From 2004 the facility belongs to the nano-science and nanotechnology center of ISIR, and is supporting nanoscale structural observations and structure analyses of advanced nano-materials.

This laboratory has a 300 kV high-resolution analytical electron microscope with a field emission gun, and a scanning electron microscope. These electron microscopes serve to make atomic scale structural observations, nano-area electron diffraction analyses, and nano-area chemical analyses of materials in response to each research division.

Achievements

In the year of 2006, the 300kV TEM served as an important equipment for the nano-structure characterization researches of 7 laboratories in ISIR with operation times as many as 224.

Electronic Processing Laboratory

Professor: Hajime ASAH
Associate Professor: Shigehiko HASEGAWA
Associate Professor: Takuya MATSUMOTO
Associate Professor: Koichi SUDOH
Associate Professor: Kenzo MAEHASHI
Assistant Professor: Yi-Kai ZHOU

Outlines

Electronic Processing Laboratory was established as a sort of device fabrication work-shop in 1991. The aim of this laboratory is to contribute to the development of nanotechnology and related researches by setting up the equipment and systems for fabrication, required commonly for the researches related to the areas such as photonic and electronic materials, molecular device materials and organic device materials and by improving process technology for various device materials.

The equipment and systems are a small-size clean room, a double crystal X-ray diffractometer, an atomic force microscope, a digital optical microscope, a photolithography system, a sputter deposition system, a high vacuum evaporation system, an electron beam evaporation system, a reactive ion etching system, a focused ion beam system, a crystal cleaving system, a wire bonding system and personal computers for data analysis

This laboratory is utilized for experimental researches of surface structure analysis and electrode formation, for the measurements of electronic and other properties of various materials and also for the fabrication of photonic, electronic and molecular devices. Guidance to the users to the equipments and systems as well as the daily maintenance and repair of them were conducted. In the year of 2008, the equipment and systems were used over 270 times from 11 laboratories and facilities.

Nanofabrication Shop

Professor, Director: Hiroyuki NOJI
Technical Staffs: Kimiaki TANIHATA, Shouichi SAKAKIHARA,

Outlines

Nanofabrication Shop was established in 2005 in order to promote nanotechnology-related research by use of equipments and special skills for nanotechnology researchers and students belonging to ISIR. In addition, this shop fabricates nano-devices for the ISIR researchers and develops devices for researchers who want to apply those devices for their own experiments.

Activities

Micro-fabrication room was set upon rebuilding of ISIR. Now we can do efficiently wet and dry processes, EB lithography and photolithography in the same place.

On demand fabrication requests

We have received requests from 12 laboratories in ISIR. Total number of their requests reached 77.

Practice seminar of fabrication and application of micro-devices

We have held a practice seminar. The content was making artistic objects utilizing micro-fabrication techniques. It took 1 day and was held 2 times. Total participants were 10 people.

Participation in “nanotech 2009”

We demonstrated a making process of micro droplets in the booth of Nanotechnology Center in the international nanotechnology exhibition and conference “nanotech 2009” which was held on 18th to 20th of February in 2009.

Materials Analysis Center

Professor Director:	Yoshio ASO
Associate Professor:	Takeyuki SUZUKI
Technical Staff:	Takanori TANAKA Tsuyoshi MATSUZAKI
Support Staff:	Yoshio TAKAI Misayo IMAI

Outlines

The Materials Analysis Center was founded in 1977, whose project includes (1) analysis of samples provided from other research sections in ISIR and (2) original research for developing novel synthetic methods using a molecular catalyst.

Current Research Programs

Iridium-catalyzed oxidation: development and applications

Development of catalytic reaction using clean oxidant is one of the most important themes in modern organic synthesis. In addition, desymmetrization of *meso* diols is the efficient methods for the synthesis of chiral building blocks. This time we have developed the catalytic asymmetric synthesis for the key intermediate of ottelione and scyphostatin by using desymmetrization of *meso* diols, which are a potent antitumor and a inhibitor of sphingomyelinase. The appropriate selections of cooxidant, base, and protecting group are important to obtain high yield and selectivity in this reaction.

Publications

Original Papers

Chiral dinuclear vanadium(v) catalysts for oxidative coupling of 2-naphthols, Takizawa, S.; Katayama, T.; Kameyama, C.; Onitsuka, K.; Suzuki, T.; Yanagida, T.; Kawai, T.; Sasai, H.: Chem. Commun., (2008) 1810-1812.

Dual activation in oxidative coupling of 2-naphthols catalyzed by chiral dinuclear vanadium complexes, Takizawa, S.; Katayama, T.; Somei, H.; Asano, Y.; Yoshida, T.; Kameyama, C.; Rajesh, D.; Onitsuka, K.; Suzuki, T.; Mikami, M.; Yamataka, H.; Jayaprakash, D.; Sasai, H: Tetrahedron, 64 (2008) 3361-3371.

International Conferences

Iridium-catalyzed Oxidative Dimerization, Tishchenko Reaction and Oxidative Desymmetrization (poster), *T. Suzuki, G. Kazem, N. K. Mangu, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Development of Dinuclear Vanadium Catalysts and Acid-Base Organocatalysts for Enantioselective Reactions via Dual Activation Mechanism (poster), *S. Takizawa, K. Matsui, T. Katayama, N. Inoue, D. Rajesh, S. Hirata, K. Kiriya, T. Suzuki, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Publications in Domestic Meetings

The Chemical Society of Japan

4 papers

Sponsorship**Other Research Fund**

T. Suzuki KRI Corp.

¥300,000

Materials Science & Technology Research Center for Industrial Creation (MSTeC)

Outline

Materials Science & Technology Research Center for Industrial Creation (MSTeC) was founded in April 2005 for contributing to the creation of new industry through the complementary cooperation with Institute of Multidisciplinary Research for Advanced Materials, Tohoku University. This center consists of two projects: P1 Materials Research Project and P2 Human Interface Research for Safety and Security Project which are divided to four groups: G1 Hard Materials Research Group, G2 Soft Materials Research Group, G3 Medical Sciences Research Group, and G4 Human Interface Research Group.

Director: Prof. T. Majima

P1 Materials Research Project

G1 Hard Materials Research Group: Group leader: Prof. H. Nakajima

G2 Soft Materials Research Group: Group leader: Prof. T. Majima

P2 Human Interface Research for Safety and Security Project

G3 Medical Sciences Research Group: Group leader: Prof. Y. Yoshida

G4 Human Interface Research Group: Group leader: Prof. M. Numao

Achievements

- Development of controlling the pore morphology in lotus-type porous metals
- Development of a new lotus-type porous materials and their application
- Development of on-demand printing circuit technology with nanopaste
- Development of lead-free electronic packaging technology
- Basic Research of High-Tc Superconductors
- Crystal growths and characterizations of useful quantum functional materials
- Laser-induced functionalized chemistry and its application
- Functional nano-scale wires using biomolecular building blocks
- Development of multifunctional asymmetric catalysts and multifunctional asymmetric organocatalysts
- Excited radicals for the preparation of nanomaterials
- Development of spiro chiral ligands for novel Pd catalyzed enantioselective reactions
- Identification of the enzymatic properties of the erythrocyte S1P transporter.
- Identification of the S1P transporter that regulates the migration of cardiac precursors.
- Elucidation of intracellular membrane dynamics as well as interaction between host cells and bacteria by using electron tomography.
- The Research of new possibility of the radiation therapy
- Dynamic optical modulation of electron beam using the Digital micro mirror device for high-performance intensity modulated radiation therapy
- Sophistication and application of knowledge sharing software called OntoGear for secure, safe, and creative manufacturing support.
- The adaptive interface by the sensor network and machine learning.
- Research on bio-applications of novel nano structures and on integrated operation of the interfaces.

Materials Research Project

Outline

The Materials Research Project is composed of two groups with research fields: Hard Materials (such as metals, semiconductors and ceramics) and Soft Materials (such as organic molecules, polymers, and biomolecules). We actively make joint researches with Institute of Multidisciplinary Research for Advanced Materials in Tohoku University and private enterprises. The development of high-degree materials can be obtained by highly advanced processes with new functional materials and their characterization.

In Hard Materials Group, the purpose is to develop novel processing of porous materials which controlled by nanostructure, microstructure and shape design. In addition, this group focuses on the identification of interconnection process, and on the development of new materials for environmental electronics packaging, as well as on basic research of useful quantum functional materials such as high-temperature superconductors.

In Soft Materials Group, the achievement of design, synthesis, assembly, and construction of functional organic molecules, polymers, and biomolecules is conducted for development of new functional molecules and materials based on elucidation of photoelectronic function, molecular recognition, catalytic reaction, high-ordered structure, and combination of multi-functions.

Achievements

- Development of controlling the pore morphology in lotus-type porous metals
- Development of a new lotus-type porous materials and their application
- Development of on-demand printing circuit technology with nanopaste
- Development of lead-free electronic packaging technology
- Basic Research of High-Tc Superconductors
- Crystal growths and characterizations of useful quantum functional materials
- Laser-induced functionalized chemistry and its application
- Functional nano-scale wires using biomolecular building blocks
- Development of multifunctional asymmetric catalysts and multifunctional asymmetric organocatalysts
- Excited radicals for the preparation of nanomaterials
- Development of spiro chiral ligands for novel Pd catalyzed enantioselective reactions

Hard Materials Research Group

Professor:	Hideo NAKAJIMA, Katsuaki SUGANUMA, Yoichi ANDO
Designated Associate Professor:	Shunkichi UENO
Assistant Professor:	Keiichi MURAI
Graduate Students:	Mitsuru KAWAZOME

Outline

The main purpose of this department is to investigate physics of materials and develop novel processing of the materials. The department has undertaken the following several topics of the metallic materials science and engineering.

Lotus-type porous materials developed by this department are unique materials which exhibit extraordinary superior mechanical strength. The materials are fabricated by unidirectional solidification using gas solubility gap at their melting point. Main issues are to develop a new simple and safety fabrication process for lotus-type porous materials and to fabricate new lotus-type porous materials. In this year, we have established a simple fabrication method for controlling the pores morphology by addition of oxide powders during the solidification.

We focus on the identification of interconnection process, and on the development of new materials for environmental electronics packaging. We are conducting the development of on-demand printing circuit technology with nanopaste, and of lead-free interconnection technology. We also conduct basic research of useful quantum functional materials such as high-temperature superconductors and spin Hall insulators, by focusing on growths of high-quality single crystals and top-notch transport measurements.

In addition, with the discovery of new iron-based high-T_c superconductors in 2008, we have started to new efforts to grow single crystals of iron-pnictide superconductors and to precisely control their carrier concentrations.

Current Research Programs

1. Development of controlling the pore morphology in lotus-type porous metals

A method for controlling pore diameter of lotus-type porous metals is achieved by addition of oxide powder during the solidification. The pore diameter of lotus-type porous nickel can be controlled below 100 micrometer using decomposition of moisture in argon atmosphere. In that mechanism, the oxygen atom reacts with liquid nickel and nickel oxide is formed during the solidification. Number of formed nickel oxide acts as nucleation sites for pore formation then, the number of pores increases and the pore size decreases. The same effect can be achieved by addition of nickel powder during the solidification. The pore diameter and porosity of the lotus-type porous nickel are well controlled by the amount and diameter of the nickel powder.

2. Development of a new lotus-type porous materials and their application

In the formation mechanism of lotus-type porous materials during the unidirectional

solidification, the convection in the liquid phase is an important factor for formation of pores at solid-liquid interface. The convection in the liquid phase can be controlled by high static magnetic field. The effect of high magnetic on the formation of pores is examined. Furthermore, a coating method for SiC layer on lotus-type porous copper is developed using Ultrasonic-based Coating Method. These research and development are conducted as collaborative research with Institute of Multidisciplinary Research for Advanced Materials, Tohoku University.

3. Development of on-demand printing circuit technology with nanopaste

Wiring printing method is one of the key issues on fine patterning of circuits with nanopastes. A variety of processes have potentials and each method has its own advantages. Ink-jet is one of major processes for electronics patterning. There are key technologies, i.e., control of Ag nanopaste suitable for wiring, ink-jet process suitable for fine pitch patterning, properties of patterned circuits and optimization, and practical applications. A new type of inks for wiring metallic Ag lines was developed. In this year, the electrical property and microstructure change of a Ag ink printed on two types of commercial papers, normal and surface coated papers, were examined. When printing circuit wiring on papers, it is necessary to avoid deterioration of the papers from heat required for curing. Comparing with normal papers, the surface coated papers provided the better electrical conductivity and the sound microstructural feature for the printed circuits.

4. Development of lead-free electronic packaging technology

Establishment of lead-free plating technology and whisker countermeasures is one of the critical problems remaining to be solved for lead-free electronics packaging. A new approach to prevent the Sn whisker, by surface treatment on Sn plating, was proposed. In this year, Sn whisker growth behavior of pure Sn plating and metal layer/Sn plating samples during 55°C/85% and 85°C/85% relative humidity (RH) exposure and thermal fatigue tests were investigated. Ni, Au and Pd layers with the thickness from 50nm to 200nm were deposited on matte Sn plating by flash-coating process. Ni, Au and Pd metal layer on Sn plating significantly suppressed the Sn whisker formation under the severe thermal and humid conditions.

With the breakthrough of the replacement of silicon by a wide band-gap semiconductor, such as SiC and GaN with high operating temperature and voltage in power semiconductor devices, the design and synthesis of adhesive die attach materials (applied to adhere a die to a substrate) are also undergoing a revolution. Among these attaching materials, silver-based material is expected to be an excellent candidate due to its high thermal and electrical conductivity. In this year, a new type of Ag nanorods paste was developed. The Ag nanorods paste can be sintered to form porous die attach layer between chip and substrates. Thermal cycles between -40 to 300°C with up to 500 cycles have no serious degradation effect on the shear strengths of Cu/Ag nanorods paste/Cu joints.

5. Basic Research of High-Tc Superconductors

The mechanism of the high-Tc superconductivity remains one of the most challenging problems in modern condensed-matter physics. This program focuses on the physics of the high-Tc cuprate materials to understand why superconductivity occurs in these

materials at notably high temperatures, the answer to which might help us find a blueprint for “room-temperature” superconductors. In addition, with the discovery of new iron-based high-T_c superconductors in 2008, we have started to new efforts to grow single crystals of iron-pnictide superconductors and to precisely control their carrier concentrations.

Publications

Original Papers

In Vitro Corrosion Resistance of Lotus-type Porous NI-free Stainless Steels, K. Alvarez, S.K. Hyun, S. Fujimoto, H. Nakajima: J. Mater. Sci.: Mater. Med., 19 (2008) 3385-3397.

Magnetization Process of Lotus-type Porous Metals, H. Onishi, S.K. Hyun, H. Nakajima, S. Mitani, K. Takanashi, K. Yakushiji: J. Appl. Phys., 103 (2008) 093539(5pages).

Fabrication of Lotus-type Porous Metals through Hydride Decomposition, H. Nakajima: Adv. Eng. Mater., 10 (2008) 816-819.

Effects of Heating Rate, Holding Temperature and Holding Time on Porosity and Pore Morphology of Aluminum Foams by Powder Metallurgy Process, H. Seki, S. Sasaki, M. Otsuka, H. Nakajima: J. Jpn. Inst. Metals, 72 (4) (2008) 278-284.

Evaluation of physical Properties of Porous Metals with Unidirectional Pores, H. Nakajima, M. Tane, K. Nakata, S. Fujimoto, T. Ichitsubo, T. Tanaka, and Y. Yamada: Tetus to hagane, 13 (6) (2008) 368-374.

Development of High-Performance Heat Sink with use of Lotus-type Porous Copper, H. Chiba, T. Ogushi, and H. Nakajima: J. HTSJ, 47 (2008) 11-15.

Peculiar elastic behavior of Ti-Nb-Ta-Zr single crystals, M. Tane, S. Akita, T. Nakano, K. Hagihara, Y. Umakoshi, M. Niinomi, H. Nakajima: Acta Mater., 56 (12) (2008) 2856-2863.

Equal-channel Angular Extrusion Process of Lotus-type Porous Copper, S. Suzuki, H. Utshunomiya, H. Nakajima: Mater. Sci. Eng. A, 490 (1-2) (2008) 465-470.

Shrinking of hollow Cu₂O and NiO nanoparticles at high temperatures, R. Nakamura, D. Tokozakura, J.-G. Lee, H. Mori, H. Nakajima: Acta Mater., 56 (18) (2008) 5276-5284.

Fabrication of Lotus-Type Porous Al-Si Alloys Using the Continuous Casting Technique, J.S. Park, S.K. Hyun, S. Suzuki, H. Nakajima: Metal. Mater. Trans. A, 40 (2) (2009) 406-414.

Plastic Deformation of Lotus-type Porous Copper through ECAE Process, S. Suzuki, H. Utunomiya, H. Nakajima: Journal of the JRI Cu, (47) (2008) 93-100.

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Kim, K.S. Kim, K. Suganuma: Materials Chemistry and Physics, 114 (2009) 333-338.

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The root causes of the "black pad" phenomenon and avoidance tactics, K. Suganuma, K.S. Kim: JOM, 60 (2008) 61-65.

Effects of Ag and Cu addition on microstructural properties and oxidation resistance of Sn-Zn eutectic alloy, J.E. Lee, K.S. Kim, M. Inoue, J. Jiang, K. Suganuma: J. Alloys and Compounds, 454 (2008) 310-320.

Quantum Phase Transition in the Magnetic-Field-Induced Normal State of Optimum-Doped High-T_c Cuprate Superconductors at Low Temperatures, F. F. Balakirev, J. B. Betts, A. Migliori, I. Tsukada, Y. Ando, and G. S. Boebinger: Phys. Rev. Lett., 102 (1) (2009) 17004/1-4.

Mapping of the formation of the pairing gap in Bi₂Sr₂Ca₂CuO_{8+δ}, K. K. Gomes, A. N. Pasupathy, A. Pushp, C. Parker, S. Ono, Y. Ando, G. Gu, and A. Yazdani: J. Phys. Chem. Solids, 69 (12) (2008) 3034-3038.

Implication of the Mott-limit violation in high-T_c cuprates, Y. Ando: J. Phys. Chem. Solids, 69 (12) (2008) 3195-3198.

Appearance of universal metallic dispersion in a doped Mott insulator, S. Sahrakorpi, R. S. Markiewicz, H. Lin, M. Lindroos, X. J. Zhou, T. Yoshida, W. L. Yang, T. Kakeshita, H. Eisaki, S. Uchida, S. Komiya, Y. Ando, F. Zhou, Z. X. Zhao, T. Sasagawa, A. Fujimori, Z. Hussain, Z. X. Shen, and A. Bansil: Phys. Rev. B, 78 (10) (2008) 104513/1-6.

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Effects of Static Magnetic Field and Gas Atmosphere on Solidification of Silicon by Electromagnetic Levitation (poster), *S. Ueno, H. Kobatake, H. Fukuyama, S. Awaji and H. Nakajima: International Conference on Advanced Structural and Functional

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Uncertainty Measurement in SCHF-DT Method Using Lotus-type Porous Copper (poster), *H. Chiba, T. Ogushi, H. Nakajima, S. Ueno, K. Torii and T. Tomimura: 4th International Conference on Diffusion in Solids and Liquids, Barcelona, Spain, July 9-11, 2008.

Accuracy Verification of Steady State Comparative-Longitudinal Heat Flow Method Using Specimen of Different Thickness for Measuring Thermal Conductivity of Lotus-Type Porous Metals (poster), *H. Chiba, T. Ogushi, H. Nakajima, S. Ueno, K. Torii, T. Tomimura, F. Ono: 1st International Symposium on Thermal Design and Thermophysical Property for Electronics, Tsukuba, Japan, June 18-20, 2008.

Contributions to International Conferences and Journals

H. Nakajima	Sixth International Conference on Porous Metals and Metal Foaming Technology (MetFoam2009) (International Advisory Board Member)
H. Nakajima	High Temperature Materials and Process (Editorial Board Member)
H. Nakajima	Diffusion and Defect Data (Editorial Board Member)
H. Nakajima	Materials Science Foundations (Editorial Board Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	5th International Conference on Diffusion in Solids and Liquids (Organizing Committee Member)
H. Nakajima	International Conference on Eco-Materials Processing and Design 2010 (Organizing Committee Member)
H. Nakajima	3rd International Symposium on Cellular Metals for Structural and Functional Applications (Program Committee)
H. Nakajima	International Conference on Advanced Structure and Functional Materials Design (Organizing Committee Member)
H. Nakajima	THERMEC 2009 International Conference on Advanced Materials (International Advisory Board Member)
K. Suganuma	TMS Annual Meeting, Committee of Phase Stability, Phase Transformation, and Reactive Phase Formation in Electronic Materials
K. Suganuma	TMS Annual Meeting, Committee of Phase Stability, Phase Transformation, and Reactive Phase Formation in Electronic Materials IV
K. Suganuma	Electronic Components and Technology Conference (ECTC), Materials Processing Committee
Y. Ando	9th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors (Japan Committee)

Y. Ando

12th Sanken International Symposium (Conference Chair)

Publications in Domestic Meetings

The Japan Institute of Metals	4 papers
Japan Institute of Electronics Packaging	1 paper
Physical Society of Japan	9 papers
Others	1 paper

Sponsorship

Grant-in-Aid for Scientific Research (C)

S. Ueno	Formation mechanism of high ordered porous ceramics and its application for catalyst support	¥100,000
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Entrusted Research

K. Suganuma	JEITA	Prevention of tin whiskers	¥8,479,000
K. Suganuma	Research and Development Association for Future Electron Devices	Development of hybrid Ag nano pastes applicable for SiC device packaging	¥14,700,000

Other Research Fund

K. Suganuma	C. Uyemura & Co., Ltd.	Understanding of whisker formation mechanism on Sn plating	¥420,000
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Soft Materials Research Group

Professor: Tetsuro MAJIMA, Hiroaki SASAI
Specially Appointed Research Associate: Masanori SAKAMOTO,
Kazuhiro TAKENAKA (~2008.12.15)
Ramalingan CHENNAN (2009.2.1~)

Outlines

Achievement of design, synthesis, assembly, and construction of functional organic molecules, polymers, and biomolecules is conducted for development of new functional molecules and materials based on elucidation of photoelectronic function, molecular recognition, catalytic reaction, high-ordered structure, and combination of multi-functions.

Current Research Project

Two-laser-guided Three-dimensional Microfabrication and Processing in Flexible Polymer Matrix

The direct three-dimensional (3-D) fabrication of metal nanoparticles (Nps) in the polymer matrices is the attracting technique due to its potential applications to 3-D wiring for microelectronics, photonic-crystal waveguides, and other photonic devices. The two-color two-laser excitation method (sequential excitation using two lasers with different wavelengths) is the choice for the direct 3-D processing since the reactive species, such as excited radicals and molecules in the higher excited states, can be selectively generated in the cross-point of the two lasers.

By using the two laser beams with different wavelengths, we demonstrate the 3-D writing of a gold nanoparticle (AuNP) array with a line width of few micrometres inside the ablative polymer matrices without any surface damage. It is discovered that the irradiation of two laser beams causes novel photo-induced phenomena (laser-guided formation of the AuNP array and microcavity (tunnel) formation).

Direct Observation of Growing Process and Photoreactivity of Au Clusters at the Single-Cluster Level

Noble-metal clusters, composed of several tens of atoms, have attracted considerable attention for a variety of reasons, ranging from a fundamental scientific interest in nanoscopic materials to technological applications. The discrete states of noble-metal clusters along with the fluorescence have led to the investigation of the behavior and reactivity of these metal clusters by using the spectroscopic techniques. In this study, we have fabricated Au clusters (Au_n , n = atom number) by using a photochemical method in a polymer matrix and concurrently investigated the photoreactivity of newly formed clusters by using single-molecule fluorescence spectroscopy.

The proposed approach gives us an opportunity to achieve a better understanding of the following two topical aspects of Au_n , that is, growth and photoreactivity. 1) We have successfully captured the optical characteristics of individual Au_n during its growth. It has been revealed that Au_n composed of a different number of atoms were fabricated

during the formation/growth process, and the distribution was significantly biased towards the stable clusters. The study aims at providing a new insight into the growing process of a cluster. 2) We have discovered the reversible and irreversible quenching of fluorescence from ligand-free Au_n by O_2 for the first time. Electron transfer played an important role in the fluorescence quenching of Au_n .

Enantioselective Oxidative Cyclization Catalyzed by Pd-SPRIX Complexes

Recently, catalytic reactions via Pd(IV) intermediates generated from a Pd(II) precursor by the action of a powerful oxidant have been accomplished. Compared to the impressive development of enantioselective reactions through the Pd(0)/Pd(II) catalytic cycle, only minimal attention has been devoted to exploring asymmetric Pd(II)/Pd(IV) catalysis. We have found that spiro bis(isoxazoline) compounds (SPRIXs), which are remarkably stable under oxidative conditions, serve as effective chiral ligands in Pd(II)/Pd(IV) catalytic enantioselective transformations. Thus, cyclization of enyne derivatives proceeds in the presence of the Pd-SPRIX catalyst and a hypervalent iodine oxidant to give lactones bearing a bicyclo[3.1.0]hexane skeleton with up to 95% ee. It is noteworthy that no enantioselectivity is observed with general phosphine or oxazoline containing chiral ligands.

Novel enantioselective Pd(0)/Pd(II) catalysis using SPRIX ligands was also accomplished. Thus, Pd-SPRIX-catalyzed oxidative cyclization of 2-allylphenols afforded optically active chromene derivatives, which were valuable architectural platform for many biologically active substances.

Asymmetric Synthesis of Chiral Hybrid Spiro (Isoxazole–Isoxazoline) Ligands

Preparation of novel chiral spiro (isoxazole–isoxazoline) ligands without a tedious optical resolution was examined. Diastereoselective intramolecular double nitrile oxide cycloaddition of the key dioxime derived from bis(2,2,2-trifluoroethyl) malonate and the enantiomerically pure alcohol gave the desired ligands.

Development of Novel Chiral Molecules Based on Spirocholactams

New functional chiral molecules were prepared from spirocholactams which were readily available via an enantioselective palladium-catalyzed intramolecular double N-arylation. Optically pure spirocholactams were converted into diammonium salts as a novel chiral phase transfer catalyst and bis(amine-phosphine) as an effective chiral ligand by conventional synthetic methods.

Publications

Original Papers

Intramolecular Excimer Formation and Photoinduced Electron Transfer Process in bis-1,8-Naphthalimide Dyads Depending on the Linker Length, D. W. Cho, M. Fujitsuka, A. Sugimoto, and T. Majima: J. Phys. Chem. A, 112 (31) (2008) 7208-7213.

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Photodecomposition Profiles of β -Bond Cleavage of Phenylphenacyl Derivatives in the Higher Triplet Excited States during Stepwise Two-Color Two-Laser Flash Photolysis, M. Yamaji, X. Cai, M. Sakamoto, M. Fujitsuka, and T. Majima: *J. Phys. Chem. A*, 112 (45) (2008) 11306-11311.

Properties of Excited Radical Cations of Substituted Oligothiophenes, S. Samori, M. Fujitsuka, and T. Majima: *J. Phys. Chem. A*, 112 (45) (2008) 11312-11318.

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Iodine-Doped TiO_2 Photocatalysts. Correlation between Band Structure and Mechanism, S. Tojo, T. Tachikawa, M. Fujitsuka, and T. Majima: *J. Phys. Chem. C*, 112 (38) (2008) 14948-14954.

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Charge transfer in DNA assembly: effects of sticky end, Y. Osakada, K. Kawai, M. Fujitsuka, and T. Majima: *Chem. Commun.*, (2008) 2656-2658.

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α -Bond Dissociation of *p*-Phenylbenzoyl Derivatives in the Higher Triplet Excited State during Two-color Two-laser Flash Photolysis, M. Yamaji, X. Cai, M. Sakamoto, M. Fujitsuka, and T. Majima: J. Phys. Chem. A, 113 (9) (2009) 1696-1703.

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Charge Transfer in DNA (invited), T. Majima: 2008 KOREA-JAPAN Symposium on Frontier Photoscience, Jeju, Korea, Sep. 27, 2008.

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Photochemical Fabrication of 3D Metal Nanoparticles in Polymer Matrix (invited), T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

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Emission Mechanism of Doubly Orth-Linked Quinoxaline/Diphenylfluorene or *cis*-Stilbene/Fluorene Hybrid Compounds Based on the Transient Absorption and Emission Measurements during the Pulse Radiolysis (poster), Y. Wei, S. Samori, S. Tojo, M. Fujitsuka, J.-S. Lin, *C.-T. Chen, and T. Majima: 5th Asian Photochemistry Conference, Beijing, China, Nov. 1-4, 2008.

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Development of TiO₂ Photocatalyst: Real-Time Single Molecule Imaging of TiO₂ Photocatalytic Reactions (invited), T. Majima: The 10th International Symposium on Eco-materials Processing and Design, Xi'an, China, Jan. 13-16, 2009.

Single Molecule Imaging of the TiO₂ Photocatalytic Reactions (invited), T. Majima: 2009 Korea-Japan Workshop on Photocatalysis and Solar Conversion, Pohang, Korea, Jan. 20, 2009.

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Real-Time Single-Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species Generated on TiO₂ Photocatalysts (poster), K. Naito, T. Tachikawa, M. Fujitsuka, and *T. Majima: The 12th SANKEN International Symposium 2007 / SANKEN Nanotechnology Symposium / SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

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SANKEN MSTEC Symposium, Suita, Japan, Jan. 22, 2009.

Development of New TiO₂ Photocatalyst (invited), T. Majima: The 1st Hanyang-Osaka Symposium on Fusion-Tech based Materials, Seoul, Korea, Feb. 27, 2009.

Approach Toward Efficient Photo-electronic Devices by Supramolecular Chemistry (invited), *M. Fujitsuka, A. Sugimoto, and T. Majima: The 1st Hanyang-Osaka Symposium on Fusion-Tech based Materials, Seoul, Korea, Feb. 27, 2009.

Real-Time Single-Molecule Imaging of the Spatial and Temporal Distribution of Reactive Oxygen Species Generated on TiO₂ Photocatalysts (invited), T. Majima: Asian Academic Seminar 2008 on "Frontiers in the Photocatalysis and Photochemistry of Advanced Materials" Kawasaki, Japan, Mar. 2-6, 2009.

Charge Transfer in DNA (invited), T. Majima: Kyudai International Symposium on Photo and Supramolecular Chemistry, Fukuoka, Japan, Mar. 7, 2009.

Catalytic Enantioselective Synthesis of Spiro lactams via an Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, H. Sasai: Third International Conference on Advanced Organic Synthesis Directed toward the Ultimate Efficiency and Practicability, Shiga, Japan, May 26-27, 2008.

Novel Enantioselective Reactions Catalyzed by Palladium(II)-Spiro Bis(isoxazoline) Complex (poster), *H. Sasai, S. Takizawa, K. Takenaka, T. Tsujihara, R. N. Nadas, G. B. Bajracharya, P. S. Koranne, K. Onitsuka: International Symposium on Homogeneous Catalysis (ISHC-16), Florence, Italy, July 6-11, 2008.

Chiral Dinuclear Vanadium(V) Catalyst for Dual Activation of 2-Naphthols in Oxidative Couplings, *H. Sasai, S. Takizawa, T. Katayama: 6th International Vanadium Symposium, Lisbon, Portugal, July 17-19, 2008.

Enantioselective Synthesis of Spiro lactams via the Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, H. Sasai: The First International Symposium on Process Chemistry (ISPC 08), Kyoto, Japan, July 28-30, 2008.

Novel Catalytic Enantioselective Reactions Promoted by a Pd-SPRIX Complex (invited), *H. Sasai: 3rd International Conference on Cutting-Edge Organic Chemistry in Asia, Hangzhou, China, October 19-23, 2008.

Novel Catalytic Enantioselective Reactions Promoted by Palladium(II)-Spiro Bis(isoxazoline) Complex (invited), *H. Sasai: 11th International Symposium on Natural Product Chemistry, Karachi, Pakistan, October 29-November 1, 2008.

Enantioselective Synthesis of Spiro lactams via the Intramolecular Double Buchwald-Hartwig Reaction (poster), *K. Takenaka, N. Itoh, K. Sugimoto, H. Sasai: UK/Japan Joint Symposium on Asymmetric Catalysis, Kyoto, Japan, December 8-9,

2008.

Novel Catalytic Enantioselective Reactions Promoted by Pd-SPRIX Complexes (invited), *H. Sasai: UK/Japan Joint Symposium on Asymmetric Catalysis, Kyoto, Japan, December 8-9, 2008.

Iridium-catalyzed Oxidative Dimerization, Tishchenko Reaction and Oxidative Desymmetrization (poster), *T. Suzuki, G. Kazem, N. K. Mangu, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Novel Enantioselective Reactions Catalyzed by Palladium(II)-Spiro Bis(isoxazoline) Complex (poster), T. Tsujihara, G. B. Bajracharya, P. S. Koranne, R. N. Nadaf, *K. Takenaka, S. Takizawa, K. Onitsuka, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Enantioselective Synthesis of Spiro lactams via the Intramolecular Double Buchwald–Hartwig Reaction (poster), *K. Takenaka, N. Itoh, K. Sugimoto, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Development of Dinuclear Vanadium Catalysts and Acid-Base Organocatalysts for Enantioselective Reactions via Dual Activation Mechanism (poster), *S. Takizawa, K. Matsui, T. Katayama, N. Inoue, D. Rajesh, S. Hirata, K. Kiriya, T. Suzuki, H. Sasai: The 12th SANKEN International Symposium, Osaka, Japan, January 22, 2009.

Contributions to International Conferences and Journals

T. Majima	2007 Korea-Japan Symposium on Frontier Photoscience (Conference Chair)
T. Majima	2 nd Asia-Pacific Symposium on Radiation Chemistry (APSRC-2008) (Organizing Committee)
T. Majima	10 th International Symposium on Eco-materials Processing and Design (Organizing Committee)
T. Majima	Langmuir Symposium in Beijing 2008 (Organizing Committee)
T. Majima	2009 Korea-Japan Workshop on Photocatalysis and Solar Conversion (Organizing Committee)
T. Majima	1 st Hanyang-Osaka Symposium on Fusion-Tech based Materials' (Organizing Committee)
T. Majima	Langmuir, American Chemical Society (Senior Editor)

Publications in Domestic Meetings

The 30th Japan Photobiology and Photomedicine Meeting	1 paper
Photochemistry Meeting 2008	8 papers
The 23rd symposium on Biofunctional Chemistry	1 paper
The 51th Radiation Chemistry Meeting	2 papers
The 89th Japan Chemical Society Meeting	7 papers
Annual Meeting of The Chemical Society of Japan	12 papers
Symposium on Organic Reaction	2 papers

Symposium on Organometallic Chemistry	2 papers
Symposium on Organic Synthesis	1 paper
Annual Meeting of The Pharmaceutical Society of Japan	1 paper
Conference on Combinatorial Chemistry	1 paper
Symposium on Molecular Chirality	1 paper

Sponsorship

Grand-in-Aid for Scientific Research (S)

T. Majima	Nanoscience of Photofunctionalized DNA	¥8,840,000
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Grand-in-Aid for Basic Scientific Research

T. Majima	Construction of devices for photoelectronic conversion using photochemical control of Tobacco Mosaic Virus supramolecules	¥800,000
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Grant-in-Aid for Scientific Research on Priority Areas

H. Sasai	Development of Chiral Organocatalyst with Synergistic Effect	¥2,300,000
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Grand-in-Aid for Encouragement of Young Scientists

M. Sakamoto	Research for the fabrication of three-dimensional metal nanoparticle array using the two-color two-laser beams	¥520,000
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Other Research Fund

T. Majima	Sekisui Chemicals Co.	Super hydrophilicity by TiO ₂ photocatalytic reaction	¥400,000
T. Majima	Matsushita Electric Industrial Co.	Study on highly reactive nanostructured TiO ₂ photocatalysts	¥1,732,500
T. Majima	TOYOTA Co.	Hydrogen absorbing alloys with high surface area produced by photoreduction	¥5,000,000
H. Sasai	Meiji Seika Kaisha		¥1,000,000
H. Sasai	Daiso Co.		¥1,200,000
H. Sasai	Nissan Chemical Industries		¥400,000
H. Sasai	Nagase ChemteX Co.		¥1,000,000

Human Interface Research for Safety and Security Project

Outline

Human Interface Research for Safety and Security Project is one of two main projects of Materials Science & Technology Research Center for Industrial Creation, MSTeC, which is the newly established cooperative organization with ISIR and the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University from 2005. This project aimed for developing the sustainable technology of human interface for safety and security. This project contains two groups: 1) medical sciences research group and 2) human interface research group. Main research subjects are xenobiotic exporters as novel drug targets, next generation intensity modulated radiation therapy, sophistication and application of knowledge sharing software called OntoGear for secure, adaptive interface by the sensor network and machine learning, and bio-application of nano-structured materials.

Achievements

- Identification of the enzymatic properties of the erythrocyte S1P transporter.
- Identification of the S1P transporter that regulates the migration of cardiac precursors.
- Elucidation of intracellular membrane dynamics as well as interaction between host cells and bacteria by using electron tomography.
- The Research of new possibility of the radiation therapy
- Dynamic optical modulation of electron beam using the Digital micro mirror device for high-performance intensity modulated radiation therapy
- Sophistication and application of knowledge sharing software called OntoGear for secure, safe, and creative manufacturing support.
- The adaptive interface by the sensor network and machine learning.
- Research on bio-applications of novel nano structures and on integrated operation of the interfaces.

Medical Sciences Research Group

Professor: Yoichi YOSHIDA, Akihito YAMAGUCHI,
Specially Appointed-
Assistant Professor: Tsuyoshi NISHI (-2008.7.15), Takafumi KONDOH (-
2009.1.15),
Mitsuko NISHINO (2008.9.1-)

Outlines

We are focusing on the development of the medical science and technologies for the radiation cancer therapy and for the transporter oriented drug. One of our main research object is the development of the beam modulation technology about high spatial resolution and high speed control by a photo cathode RF gun for high-performance radiation cancer therapy, development of the femtosecond pulse radiolysis observing ultra-fast radiation induced reaction in the human body to search for new possibility of the radiation therapy, and the theoretical study of a new irradiation effect by the ultimate short pulse radiation. Another main research objective of our group is understands the mechanism of basic biological processes that are important for normal cellular functions. Especially we are focusing on the transporters that are contributing the secretion of the lipid mediators to develop the transporter oriented drugs and are trying to understand the physiological roles of the xenobiotic transporters. And our new focus is the electron tomographic reconstruction of clathrin coated endocytic intermediates in nerve terminals that lack dynamin 1.

Current Research Programs

The Research for new possibility of the radiation therapy

New possibility of the radiation cancer therapy was searched. Femtosecond pulse radiolysis with a laser-photocathode RF gun LINAC is developed for observation of the first radiation induced reaction in human body. The femtosecond pulse radiolysis system was developed. And we succeeded in the observation of the hydration electron generation process induced by an electron beam by femtosecond pulse radiolysis. For elucidation of effects by a heavy ion beam, an original unique ion beam pulse radiolysis system is developed. By the latest study, the new therapy principle was studied theoretically as a collective ionization by the ultimate short pulse radiation.

Dynamic optical modulation of electron beam using the Digital micro mirror device for high-performance intensity modulated radiation therapy

To realize more safety and effective cancer therapy, and optical modulation technology of the electron beam was developed for high-performance intensity modulated radiation therapy using a laser photo cathode RF gun LINAC. The radiation therapy of cancer is developing to un-uniform irradiation, for concentrating dose to a cancer tumor and reducing dose to normal tissue. In recent year, since diagnosis devices are developing, and small cancer less than 1 mm is able to find at early stage. Fine spatial resolution is required in the radiation cancer therapy of next generation. Moreover, motion of the human body cannot stop completely. It is necessary for the control of the beam to follow an involuntary motion. For fine un-uniform irradiation

and for fast following to the involuntary motion, optical modulation of electron beam using the Digital Micro Mirror Device (DMD) was studied on a photocathode RF gun electron LINAC. Optical modulation and dynamic control of electron beam were succeeded using the DMD.

Identification of the novel S1P transporter protein and the enzymatic properties of the erythrocyte S1P transporter.

Intercellular signal transduction is the important system for the communication between the cells in the highly organized living organism. Lipophilic and amphiphilic compounds such as steroid hormones and lipid mediators are one of the most popular signaling molecules. However, little is known about how are these molecules exported from the cells. We are trying to identify the secretion mechanism and to isolate the transporters that are directly transporting these amphiphilic molecules.

To analyze the transporter activity of the amphiphilic compounds, we develop the assay to measure the S1P transport activity in rat erythrocyte inside-out vesicles (IOVs). S1P was transported into the IOVs in the presence of ATP and apparent K_m is 21 μ M and 130 μ M for S1P and ATP, respectively. This transport activity was partially blocked with glyburide and bafilomycin A1 and was completely inhibited by vanadate. Moreover, the other ABC transporter and ATPase inhibitor or ionophores were not affected to the S1P transport activity. Interestingly, this ATP-dependent S1P uptake was also supported with non-hydrolyzable ATP analogue, AMP-PNP, suggesting this transporter do not require the ATP hydrolysis for the activity. These results indicated that erythrocyte S1P transporter is a new class of membrane transporter.

We are also trying to identify the S1P transporter molecules by analyzing the function of the orphan transporters. Recently, we identify the S1P transporter in MFS-type orphan transporter family. Functional defect of this S1P transporter, *spns2*, caused cardiac bifida phenotype in zebrafish. Over-expression of *spns2* in the cells, that accumulate the S1P inside the cells, showed the time-dependent export of the S1P from the cells. This is a first transporter that plays a central role in a S1P signaling pathway *in vivo*.

Electron tomographic reconstruction of clathrin coated endocytic intermediates in nerve terminals that lack dynamin 1.

Dynamin is a GTPase implicated in the fission reaction of endocytosis. Of the three dynamin genes present in mammalian genomes, the dynamin 1 gene is the one selectively expressed in neurons, where dynamin 1 represents a very abundant protein. Dynamin 1 is highly concentrated in nerve terminals where it participates in the endocytosis of synaptic vesicles. We have found that nerve terminals of dynamin 1 KO mice are characterized by a variable, activity-dependent, accumulation of clathrin-coated endocytic intermediates. We report here detailed 3D reconstructions of nerve terminals exhibiting a very prominent accumulation of such structures by electron tomography. The most striking feature is the presence of branched tubular networks capped by clathrin-coated buds, with only few buds originating directly from the outer profile of the plasma membrane. Some clathrin-coated buds appear to originate from deep tubular invaginations of the plasma membrane containing an evagination of the adjacent cell. The branched tubular necks of clathrin-coated pits in dynamin 1 KO

synapses emphasize the important partnership of dynamin with membrane tubulating proteins.

Publications

Original Papers

Dynamic Optical Modulation of an Electron Beam on a Photocathode RF Gun: Toward Intensity-Modulated Radiation Therapy (IMRT), T. Kondoh, H. Kashima, J. Yang, Y. Yoshida, S. Tagawa: Radiat. Phys. Chem., 77 (2008) 1142– 1147.

Effects of emittance and space-charge in femtosecond bunch compression, K. Kan, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: Nucl. Instrum. Methods A, 597 (2008) 126–131.

Reactions of Solvated Electrons with Imidazolium Cations in Ionic Liquids, K. Takahashi, T. Sato, Y. Katsumura, J. Yang, T. Kondoh, Y. Yoshida, R. Katoh: Radiat. Phys. Chem., 77 (2008) 1239– 1243.

Molar Absorption Coefficient and Radiolytic Yield of Solvated Electrons in Diethylmethyl(2-methoxy)ammonium bis (trifluoromethanesulfonyl)imide Ionic Liquid, A. Asano, J. Yang, T. Kondoh, K. Norizawa, R. Nagaishi, K. Takahashi, Y. Yoshida: Radiat. Phys. Chem., 77 (2008) 1244– 1247.

Picosecond Pulse Radiolysis: Dynamics of Solvated Electrons in Ionic Liquid and Geminate Ion Recombination in Liquid Alkanes, J. Yang, T. Kondoh, K. Norizawa, R. Nagaishi, M. Taguchi, K. Takahashi, R. Katoh, S. V. Anishchik, Y. Yoshida, S. Tagawa: Radiat. Phys. Chem., 77 (2008) 1233– 1238.

Study on the Reaction of Chlorophenols in Room Temperature Ionic Liquids with Ionizing Radiation, A. Kimura, M. Taguchi, T. Kondoh, J. Yang, Y. Yoshida, K. Hirota: Radiat. Phys. Chem., 77 (2008) 1253– 1257.

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Secreted indole serves as a signal for expression of type III secretion system translocators in enterohaemorrhagic *Escherichia coli* O157:H7, H. Hirakawa, T. Kodama, A. Takumi-Kobayashi, T. Honda and A. Yamaguchi: Microbiology, 155 (pt2) (2009) 541-550.

The Sphingolipid Transporter Spns2 Functions in Migration of Zebrafish Myocardial Precursors, A. Kawahara, T. Nishi, Y. Hisano, H. Fukui, A. Yamaguchi and N. Mochizuki: Science, 323 (5913) (2008) 524-527.

An Atg4B mutant hampers the lipidation of LC3 paralogues and causes defects in autophagosome closure, N. Fujita, M. Hayashi-Nishino, H. Fukumoto, H. Omori, A. Yamamoto, T. Noda and Y. Tamotsu: Mol Biol Cell., 19 (11) (2008) 6451-6459.

Physiological functions of drug efflux systems in Gram-negative bacteria: Their roles in bacterial drug resistance and virulence, K. Nishino and A. Yamaguchi: Jpn. J. Chemother., 56 (4) (2008) 443-452.

Virulence and Drug Resistance Roles of Multidrug Efflux Pumps in *Escherichia coli* and *Salmonella*, K. Nishino and A. Yamaguchi: Bioscience and Microflora, 27 (3) (2008) 75-85.

AcrS/EnvR Represses the Expression of the *acrAB* Multidrug Efflux Genes in *Escherichia coli*, H. Hirakawa, A. Takumi-Kobayashi, U. Theisen, T. Hirata, K. Nishino and A. Yamaguchi: J. Bacteriol., 190 (18) (2008) 6276-6279.

AcrAB Multidrug Efflux Pump Regulation in *Salmonella enterica* serovar Typhimurium by RamA in Response to Environmental Signals, E. Nikaido, K. Nishino and A. Yamaguchi: J. Biol. Chem., 283 (35) (2008) 24245-24253.

Role of Xenobiotic Transporters in Bacterial Drug Resistance and Virulence, K. Nishino and A. Yamaguchi: IUBMB Life, 60 (9) (2008) 569-574.

Cell- and stimulus-dependent heterogeneity of synaptic vesicle endocytic recycling mechanisms revealed by studies of dynamin 1-null neurons., M. Hayashi, A. Raimondi, E. O'Toole, S. Paradise, C. Collesi, O. Cremona, S. M. Ferguson, P. De Camilli.: Proc. Natl. Acad. Sci. U S A, 105 (6) (2008) 2175-2180.

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A selective role of dynamin 1 in synaptic vesicle endocytosis, M. Nishino-Hayashi, Pietro De Camilli, Protein, Nucleic Acid and Enzyme, 53 [16] (2008) 2225-2230

Physiological functions of drug efflux systems in Gram-negative bacteria: Their roles in bacterial drug resistance and virulence, K. Nishino, A. Yamaguchi, Japanese Journal of Chemotherapy, 56 (2008) 443-452

Virulence and Drug Resistance Roles of Multidrug Efflux Pumps in *Escherichia coli* and *Salmonella*, K. Nishino and A. Yamaguchi, Bioscience and Microflora, 27 (2008) 75-85

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The molecular mechanism of multidrug recognition and active transport by the multidrug transporter, A. Yamaguchi, Transporter Science, (2008) 305-320

Patents

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A. Yamaguchi, tokugan2008-245177

International Conferences

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Femtosecond Photocathode Electron Source (poster), J. Yang, K. Kan, T. Kondoh, K. Tanimura, Y. Yoshida, J. Urakawa: The 11th European Particle Accelerator Conference(EPAC'08), Genoa, Italy, June 23-27, 2008.

Collective Ionization by Attosecond Electron Bunches (poster), A. Ogata, T. Kondoh, K. Norizawa, J. Yang, Y. Yoshida: The 11th European Particle Accelerator Conference(EPAC'08), Genoa, Italy, June 23-27, 2008.

Pulse Radiolysis Study of Ion-Species Effects on the Solvated Electrons in Alkyl Ammonium Ionic Liquids, T. Kondoh, A. Asano, J. Yang, K. Norizawa, K. Takahashi, M. Taguchi, R. Nagaishi, R. Katoh, Y. Yoshida: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Breaking Time-Resolution Limits in Pulse Radiolysis, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida, S. Tagawa: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Pulse Radiolysis Study of Trapped Electron in $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ Single Crystal (poster), K. Norizawa, T. Kondoh, J. Yang, A. Ogata, Y. Yoshida: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Observation of Optical Reflection Change due to Electron Pulse Irradiation in GaAs for Femtosecond Electron Pulse Measurement (poster), K. Kan, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 2nd Asia Pacific Symposium on Radiation Chemistry, Waseda, Tokyo, Japan, Aug. 29-Sep. 1, 2008.

Development of Heavy Ion Beam Pulse Radiolysis in a Single Ion Nano-track (poster), T. Kondoh, J. Yang, K. Kan, Y. Yoshida, K. Norizawa, H. Shibata, M. Taguchi, S. Kurashima, T. Kojima and K. Hirota: The 4th Handai Nanoscience and Nanotechnology International Symposium, Sep. 29-Oct. 1, 2008.

Study of Electron-induced Ultrafast Phenomena in GaAs for Femtosecond Electron Measurement (poster), K. Kan, J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 4th Handai Nanoscience and Nanotechnology International Symposium, Sep. 29-Oct. 1, 2008.

Femtosecond Pulse Radiolysis for Study of Nanofabrication Process (poster), J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 4th Handai Nanoscience and Nanotechnology International Symposium, Sep. 29-Oct. 1, 2008.

Femtosecond reaction analysis based on a femtosecond electron beam and a femtosecond laser light (poster), J. Yang, T. Kondoh, K. Norizawa, Y. Yoshida: The 12th Sanken International Symposium, Jan. 22, 2009.

Optical Modulation of Electron Beam by Digital Micromirror Device for Radiation Therapy based on Photocathode RF Gun (poster), T. Kondoh, H. Kashima, J. Yang, K. Kan, K. Norizawa, A. Ogata, Y. Yoshida, S. Tagawa: The 12th Sanken International Symposium, Jan. 22, 2009.

Optical Absorption Spectrum of Hydrated Electron in MgSO₄ Aqueous Solution (poster), K. Norizawa, T. Kondoh, J. Yang, Y. Yoshida: The 12th Sanken International Symposium, Jan. 22, 2009.

AcrAB multidrug efflux pump regulation in *Salmonella enterica* serovar Typhimurium in response to indole (poster), I. Shirosaka, E. Nikaïdo, K. Nishino and A. Yamaguchi: 12th Sanken International Symposium/7th nanotechnology center international symposium/2nd MSTEC international symposium/1st Sanken Alliance Symposium(22 Jan. 2009, Osaka).

Sphingosine-1-phosphate (S1P) Release From Erythrocytes Mediated By ATP-dependent Transporter (poster), N. Kobayashi, N. Kobayashi, T. Nishi and A. Yamaguchi: 12th Sanken International Symposium/7th nanotechnology center international symposium/2nd MSTEC international symposium/1st Sanken Alliance Symposium(22 Jan. 2009, Osaka).

Electron Tomography Revealed the Endoplasmic Reticulum as a Cradle for Autophagosome Formation (poster), M. Hayashi-Nishino, N. Fujita, T. Noda, A. Yamaguchi, T. Yoshimori and A. Yamamoto: The American Society for Cell Biology 48th Annual Meeting, San Francisco, 2008.13-17 December.

AcrAB multidrug efflux pump regulation in *Salmonella enterica* serovar Typhimurium by RamA in response to environmental signals, K. Nishino, E. Nikaïdo and A. Yamaguchi: The Awaji International Forum on Infection and Immunity, Awaji Island(10 Sep. 2008, Hyogo).

Regulatory network of multidrug efflux pumps reveals their physiological role in *Salmonella* virulence, K. Nishino and A. Yamaguchi: Gordon Research Conference (6-11 Jul. 2008, MA, USA).

Molecular Design of the Carbenicillin Hyper-Resistance AcrB Multidrug Exporter in *Escherichia coli* (poster), A. Iwata, N. Kobayashi, S. Murakami and A. Yamaguchi: 22nd Annual Symposium of The Protein Society (July 19-23, 2008, San Diego, California USA).

Structure and Mechanism of the Tripartite Multidrug Exporter, A. Yamaguchi: The Joint 4th AOHUPO(Asian Oceania Human Proteome Organisation) and 2nd PRICPS(Pacific Rim International Conference on Protein Science) (22-26 Jun. 2008, Carins Convention Center, Australia).

Zebrafish spinster2 involved in the migration of myocardial precursors is a novel regulator in sphingosine-1-phosphate (S1P) signaling (poster), A. Kawahara, T. Nishi, A. Yamaguchi and N. Mochizuki: 8th International Meeting on Zebrafish development & Genetics (Jun 25-29, 2008, Madison, USA).

Regulatory Network of Multidrug Transporters Reveals their Physiological Role in *Salmonella* Virulence, K. Nishino and A. Yamaguchi: American Society for Microbiology 108th General Meeting (1-5 Jun. 2008, Boston Convention and Exhibition Center, Boston, Massachusetts).

Regulation of the AcrAB Multidrug Efflux Pump in *Salmonella enterica* by RamA in Response to Environmental Signals, E. Nikaido, K. Nishino and A. Yamaguchi: American Society for Microbiology 108th General Meeting (1-5 Jun. 2008, Boston Convention and Exhibition Center, Boston, Massachusetts).

Contributions to International Conferences and Journals

A. Yamaguchi Journal of Bacteriology (Editorial Board Member)

Publications in Domestic Meetings

Particle Accelerator Society of Japan	4 papers
The third Takasaki Advanced Radiation Research Symposium	1 paper
Japanese Society of Radiation Chemistry	4 papers
RF gun meeting	4 papers
The Chemical Society of Japan	1 paper
82 th Japanese Society for Bacteriology	4 papers
Biochemistry and Molecular Biology 2008	7 papers
The 56 th Japanese Society of Chemotherapy, Western Japan Division	1 paper
46 th The Biophysical Society of Japan	1 paper
61 th Japanese Society for Bacteriology, the Kansai Division	1 paper
12 th Spring-8 Symposium	1 paper
30 th Membrane-Drug Interaction Symposium	7 papers
The 60 th Annual Meeting of the Japan Society for Cell Biology	1 paper
The 56 th Japanese Society of Chemotherapy	1 paper
The 82 th Japanese Association for Infectious Diseases	1 paper

Sponsorship

Grant-in-Aid for Scientific Research (S)

A. Yamaguchi	Structures, functions, regulations and physiological roles of xenobiotic exporters	¥21,580,000
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Grant-in-Aid for Scientific Research (A)

Y. Yoshida	Research on Equivalent velocity spectroscopy for Sub-femtosecond and Attosecond Pulse Radiolysis	¥10,790,000
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Entrusted Research

A. Yamaguchi	National Institute of Biomedical Innovation	Development of novel inhibitors that counteract infectious diseases by drug resistant bacteria	¥93,000,000
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Cooperative Research

Y. Yoshida	National Institute of Radiological Sciences	The research about the beam control for the particle beam cancer therapy.
Y. Yoshida	Sumitomo Heavy Industries, LTD	Research on photocathode RF gun and high brightness electron beam.
Y. Yoshida	Japan Atomic Energy Agency Takasaki	The research about the ion beam induced chemical reaction process by the ion pulse radiolysis.
Y. Yoshida	Japan Atomic Energy Agency Kansai	Basic research for application of femtosecond electron beam driven by high intensity laser.

Human Interface Research Group

Professor: Masayuki NUMAO (Group leader), Riichiro MIZOGUCHI,
Hidekazu TANAKA (2008.4.1-)

Specially Appointed Professor: Sunao TAKAFUJI

Specially Appointed Assistant Professor: Ken-ichi FUKUI, Makoto NAKAZAWA,
Nam Goo CHA (2008.9.1-)

Outlines

Our research interests are foundation software systems and its basis device for development of safe and reliable technology, which include intelligent sensor data analysis methods, knowledge sharing technology for manufacturing support, prediction of new industry, and Nanoinprint Lithography known as an advantaged forming technique for an integrated circuit.

Current Research Project

Study on Data Mining Technique for Mechanical Evaluation for Solid-type Energy Device (Fukui, Numao)

- 1) We improved clustering accuracy of Acoustic Emission waves that are observed from damage on a fuel cell by applying recently developed kernel method to Self-Organizing Map.
- 2) Methodology to analyze combination of latent AE wave pattern in terms of complex network analysis was studied. Also we confirmed the network structure dynamically changes followed by damage progress.

Research on knowledge sharing technology for secure, safe, and creative manufacturing support (Takafuji, Mizoguchi)

- 1) A software, which is called OntoGear, to externalize functional knowledge of an artifact on designing has achieved to the level of practical use by sophisticating the functionality and incorporating way knowledge contents.
- 2) Applied research onto failure knowledge management, service science, etc by using OntoGear has also proceeded, and has partially resulted in good evaluation by a manufacturing company.

Research on the strategic new industry prediction accompanying change of industrial structure (Nakazawa)

- 1) We analyzed patent descriptions about Lithium rechargeable battery as an application of intellectual property map.
- 2) We discussed the methodology for research management to capture future trend by analyzing the scenario paper predicting the future's market.

Molding nano gold foil using Nanoinprint Lithography (NIL) (Cha, Tanaka)

- 1) Nano pattern of 10 nm can be made by NIL at a low cost. As a result, eight million boxes or more of three dimensions of 400 nm gold cube were actually accumulated on

one substrate.

Publications

Original Papers

Compilation to Visualize the Dynamic Clusters by the Adapted Self- Organizing Network, Ken-ichi Fukui, Kazumi Saito, Masahiro Kimura, Masayuki Numao: Transactions of the Japanese Society for Artificial Intelligence, 23 (5) (2008) 319-329.

Technical Knowledge Management Platform Based on Ontology Engineering and XML Technology, Sunao Takafuji, Yoshinobu Kitamura, Riichiro Mizoguchi: Transactions of the Japanese Society for Artificial Intelligence, 23 (6) (2008) 424-436.

International Conferences

Sequence-based SOM: Visualizing Transition of Dynamic Clusters, Ken-ichi Fukui, Kazumi Saito, Masahiro Kimura, Masayuki Numao: IEEE 8th International Conference on Computer and Information Technology (CIT), Sydney, Australia, July 8-11, 2008.

Publications in Domestic Meetings

The Japanese Society for Artificial Intelligence	5 papers
The Solid State Ionics Society of Japan	1 paper
The Japan Society of Mechanical Engineers	1 paper
Japanese Society for the Science of Design	1 paper
Seminar hosted by Institute of Multidisciplinary Research for Advanced Materials, Tohoku University	1 paper

Sponsorship

Grant-in-Aid for Scientific Research on Exploratory Research

M. Nakazawa	Research on the strategic new industry prediction accompanying change of industrial structure	¥800,000
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Other Research Fund

S. Takafuji	Justsystem Corporation	Research on knowledge sharing by utilization of both ontology engineering and natural language processing	¥6,500,000
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Post-Silicon Materials and Devices Research Alliance

Outline

“Post-Silicon Materials and Devices Research Alliance” was started to attempt strategic development of the post-silicon materials and devices as a cooperative research project with Institute of Multidisciplinary Research for Advanced Materials, Tohoku University in fiscal year 2006 and further with Research Institute for Electronic Science, Hokkaido University and Chemical Resources Laboratory, Tokyo Institute of Technology in fiscal year 2007. This alliance consists of three research groups; Molecular Nano-Electronics research group, New Functional Nano-Electronics research group and Molecular Nano-Mechanics & Bio-Mechanics research group

This Post-Silicon Alliance is being run under the Steering Committee of 4 member Institutes. The Committee members from ISIR are Prof. H. Asahi (Chair), Prof. A. Yamaguchi, Prof. T. Kawai, Prof. Y. Hirotsu, and Prof. Y. Aso. The members of this Post-Silicon Alliance from ISIR are as follows.

(1) Molecular Nano-Electronics Research Group)

Prof. Y. Aso (Group Leader), Prof. T. Kawai, Prof. S. Tagawa

(2) New Functional Nano-Electronics Research Group)

Prof. K. Matsumoto (Group Leader), Prof. H. Asahi, Prof. K. Tanimura, Prof. H. Kobayashi

(3) Molecular Nano-Mechanics & Bio-Mechanics Research Group)

Prof. N. Kato (Group Leader), Prof. H. Noji, Prof. K. Nakatani, Prof. T. Washio

Achievements

- Development of functionalized molecular wires and solution-processable organic semiconductors
- Single molecular DNA sequencing by STM and the development of Gating Nanopore system
- Nanometer-scale charge dynamics in π -conjugated polymer film containing donor and acceptor
- Coherent transport and Coulomb blockade transport in carbon nanotube device
- Diameter-controlled growth of GaGdN nanorod and magnetooptical properties of GaDyN
- Formation of sp^3 -bonded carbon nanostructures by femtosecond laser excitation of graphite
- Development of complete metal removal method from SiC surfaces by dilute HCN solutions
- Crystal structure of the association complex of 14-3-3 protein and cotylenin
- Development of fluorescent energy transfer based ATP sensor protein for living cell imaging
- Development of DNA based supramolecular optical switch
- Development of matrix completion method for data estimation in quantum experiments

Molecular Nano-Electronics Research Group

Professor: Yoshio ASO (Group Leader), Seiichi TAGAWA, Tomoji KAWAI

Outlines

We have been focusing our research on the design, synthesis, and properties of (1) novel extended conjugation systems as active materials for organic electronic devices and (2) nano-scale conjugated molecules for promising functional molecular wires. (Aso)

Using time-resolved microwave conductivity (TRMC) which enables us to measure nano-scale electric conductivity in organic semiconductors, we elucidated the optoelectronic properties, i.e. photoconductivity in pi-conjugated polymer containing donor and acceptor. (Tagawa)

With the aim of developing a biosensor or a high-speed DNA sequencer, we develop a gating nanopore structure comprising nanoelectrodes combined with solid-state nanopores. This device structure has one pair of electrodes arranged in parallel with the nanopores and another pair arranged orthogonally. (Kawai)

Current Research Projects

Organic Electronics Materials

We have designed difluorodioxocyclopentene-annelated thiophene, carbonyl-bridged bithiazole monomer units and synthesized their based conjugated oligomers. Some of these electronegative oligomers revealed high field-effect electron mobility and air stability. Solution-processable n-type materials have also been accomplished by introducing lipophilic 3-hexylthiophene into the electronegative pi-conjugated oligomeric backbone. The branched-oligothiophene/perylenebisimide or naphthalenebisimide linkage molecules showed highly efficient photo-induced electron transfer, and their thin films exhibited good performance as active materials for organic photovoltaic devices.

Molecular Electronics Materials

The cyclopentathiophene with a spiro-type substituted dioctylfluorene has been designed as a monomer unit for encapsulated molecular wire, and then a series of their oligomers up to 12-mer were synthesized. The electronic absorption spectra of oxidized species of these insulated oligothiophenes showed complete blocking of pi-dimer formations unlike usual oligothiophenes. We have also achieved the synthesis of the encapsulated thiophene 6-mers with terminal thiol anchor groups for gold electrodes as well as with terminal ethynyl anchor groups for silicon electrodes. For certain connection of molecular wires with metal electrodes and efficient carrier injection, we have developed tetraphenylmethane tripodal anchor units with selenium functional groups. Their monolayers on a gold electrode revealed the effectiveness of selenol functional groups as well as the three-armed structure.

Charge carrier dynamics in single crystal rubrene

The charge carrier mobility and its generation efficiency in regioregular and regiorandom poly(3-hexylthiophene) (P3HT) films upon exposure to light pulses are studied by flash-photolysis time-resolved microwave conductivity and transient

absorption spectroscopy. For the full experimental determination of alternating current mobility without electrodes, we incorporated a perylenecarboxydiimide (PDI) derivative into the films not only to increase the photoconductivity but also estimate the quantum efficiency of charge generation by kinetic tracing of PDI radical anions. We discuss the mobility, quantum efficiency, decay of charge carriers, and film morphology observed by an X-ray diffraction and an atomic force microscope with various PDI concentrations. It is found that the three-dimensional mobility mainly attributed to the positive charges on regioregular P3HT is decreased from 0.12 to 0.070 cm²/Vs by addition of PDI which disturbs the intermolecular pi-stacking, while that on regiorandom P3HT shows an almost constant value of 0.006 cm²/Vs. The quantum efficiency in regioregular P3HT reveals a peak at 6 mol % PDI for 355-nm excitation. The reason for the appearance of the peak is examined by changing excitation wavelength and inspecting the steady-state absorption and fluorescence spectra. The methodology and findings obtained by utilizing the additive as both an acceptor and a probe is proved to be useful for the investigations on optoelectronic properties of wide varieties of organic semiconductors.

Fabrication of gating nanopore

We succeeded in producing the gating nanopore with a minimum diameter of 40 nm by 19 nanofabrication processes. In order to investigate whether a nanoparticle can be identified via electrical measurement, a nanostructure combining a gating nanopore and a micro-fluid was produced. A gold nanoparticle with a diameter of 40 nm was passed through the nanopore, and the time dependence of electric current between nanoelectrodes was measured. An electric signal originating from the gold nanoparticle was observed.

Identification of single nanoparticle via electrical measurement

We developed the microfluidics-integrated mechanically controllable break junction for ultra-fast single-molecule identification via the transverse electron transport. Electrical detection of individual gold nanoparticles in the microfluidics is accomplished by probing tunneling current across the nanogap electrodes whose gap size precisely controlled to the particle size at a sub-picometer resolution. Transverse electric field slows down the particle flowing through the electrode nanogaps via the electrostatic electrode-particle interactions.

Publications

Original Papers

Synthesis, Structure, and Properties of 2,5,8,11,14,17-Hexamethyltriphenylene [2,1-b:3,4-b':6,5-b'':7,8-b''':10,9-b''':11,12-b''']hexathiophene, M. Endou, Y. Ie, and Y. Aso, *Heterocycles*, 76[2] (2008) 1043-1048.

Dendritic Oligothiophene Bearing Perylene Bis(dicarboximide) Groups as an Active Material for Photovoltaic Device, Y. Ie, T. Uto, N. Yamamoto, and Y. Aso, *Chem. Commun.*, [10] (2009) 1213-1215.

Electrodeless Determination of Charge Carrier Mobility in Poly(3-hexylthiophene) Films Incorporating Perylenediimide as Photoconductivity Sensitizer and Spectroscopic

Probe, A. Saeki, S. Ohsaki, S. Seki, and S. Tagawa, *J. Phys. Chem. C* 112 (2008) 16643-16650

Long-Lived Hole Stabilized at a Triphenylamine Core and Shielded by Rigid Phenylazomethine Dendrons: A Pulse Radiolysis Study, A. Saeki, S. Seki, N. Satoh, K. Yamamoto, and S. Tagawa, *J. Phys. Chem. B* 112 (2008) 15540-15545.

Prominent Electron Transport Property Observed for Triply Fused Metalloporphyrin Dimer: Directed Columnar Liquid Crystalline Assembly by Amphiphilic Molecular Design, T. Sakurai, K. Shi, H. Sato, K. Tashiro, A. Osuka, A. Saeki, S. Seki, S. Tagawa, S. Sasaki, H. Masunaga, K. Osaka, M. Takata, and T. Aida, *J. Am. Chem. Soc.* 130 (2008) 13812-13813.

Mobility and Dynamics of Charge Carriers in Rubrene Single Crystals Studied by Flash-Photolysis Microwave Conductivity and Optical Spectroscopy, A. Saeki, S. Seki, T. Takenobu, Y. Iwasa, and S. Tagawa, *Adv. Mater.* 20 (2008) 920-923.

Intra-Molecular Mobility of Charge Carriers Along Oligogermane Backbones Studied by Flash Photolysis Time-Resolved Microwave Conductivity and Transient Optical Spectroscopy Techniques, S. Seki, A. Saeki, A. Acharya, Y. Koizumi, S. Tagawa, and K. Mochida, *Radiat. Phys. Chem.* 77 (2008) 1323-1327.

Electrode-Less Measurement of Conductivity Transients in Poly(n-alkylthiophene)s Induced by 193nm Photoexcitation, A. Saeki, S. Ohsaki, Y. Koizumi, S. Seki, and S. Tagawa, *J. Photopolym. Sci. Technol.* 21 (2008) 559-562.

Amphiphilic Molecular Design as a Rational Strategy for Tailoring Bicontinuous Electron Donor and Acceptor Arrays: Photoconductive Liquid Crystalline Oligothiophene-C₆₀ Dyads, W.-S. Li, Y. Yamamoto, T. Fukushima, A. Saeki, S. Seki, S. Tagawa, H. Masunaga, S. Sasaki, M. Takata, and T. Aida, *J. Am. Chem. Soc.* 130 (2008) 8886-8887.

Superstructure-Dependent Optical and Electrical Properties of an Unusual Face-to-Face, π -Stacked, One-Dimensional Assembly of Dehydrobenzo[12]annulene in the Crystalline State, I. Hisaki, Y. Sakamoto, H. Shigemitsu, N. Tohnai, M. Miyata, S. Seki, A. Saeki, and S. Tagawa, *Chem. Eur. J.* 14 (2008) 4178-4187.

Visualization of the Detailed Structure of Plasmid DNA, Hiro. Tanaka, S. P. Mielke, C. J. Benham, and T. Kawai, *JOURNAL OF PHYSICAL CHEMISTRY B*, 112[51] (2008) 16788-16792.

Enhancement of Oxide VLS Growth by Carbon on Substrate Surface, T. Yanagida, A. Marcu, H. Matsui, K. Nagashima, K. Oka, K. Yokota, M. Taniguchi, and T. Kawai, *JOURNAL OF PHYSICAL CHEMISTRY C*, 112[48] (2008) 18923-18926.

Electrical resistivity of individual molecular-assembly nanowires of amphiphilic bis-tetrathiafulvalene macrocycle/2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-p-quinodimethane charge transfer complex characterized by point-contact current-imaging atomic force

microscopy, R. Tsunashima, Y. Noda, Y. Tatewaki, S. Noro, T. Akutagawa, T. Nakamura, T. Matsumoto, and T. Kawai, APPLIED PHYSICS LETTERS, 93[17] (2008) 173102(1-3).

Fabrication of 0.5 nm electrode gaps using self-breaking technique, M. Tsutsui, M. Taniguchi, and T. Kawai, APPLIED PHYSICS LETTERS, 93[16] (2008) 163115(1-3).

Mechanism and control of sidewall growth and catalyst diffusion on oxide nanowire vapor-liquid-solid growth, K. Nagashima, T. Yanagida, K. Oka, Hide. Tanaka, and T. Kawai, APPLIED PHYSICS LETTERS, 93[15] (2008) 153103(1-3).

Measurement Environment Dependency of Single Molecule Conductance, M. Taniguchi, K. Morimoto, M. Tsutsui, and T. Kawai, CHEMISTRY LETTERS, 37[9] (2008) 990-991.

Self-organized functional lipid vesicle array for sensitive immunoassay chip, H. Y. Lee, B. K. Lee, J. W. Park, H. S. Jung, J. M. Kim, and T. Kawai, ULTRAMICROSCOPY, 108[10] (2008) 1325-1327.

Local Heating in Metal-Molecule-Metal Junctions, M. Tsutsui, M. Taniguchi, and T. Kawai, NANO LETTERS, 8[10] (2008) 3293-3297.

Control of device characteristics of ambipolar organic field-effect transistors using the hydroxyl in organic insulator, H. Kawaguchi, M. Taniguchi, and T. Kawai, SYNTHETIC METALS, 158[8-9] (2008) 355-358.

Growth atmosphere dependence of transport properties of NiO epitaxial thin films, K. Oka, T. Yanagida, K. Nagashima, Hide. Tanaka, and T. Kawai, JOURNAL OF APPLIED PHYSICS, 104[1] (2008) 013711(1-4).

Mechanism of critical catalyst size effect on MgO nanowire growth by pulsed laser deposition, T. Yanagida, K. Nagashima, Hide. Tanaka, and T. Kawai, JOURNAL OF APPLIED PHYSICS, 104[1] (2008) 016101(1-3).

Thermodynamic stability of single molecule junctions, M. Tsutsui, K. Shoji, K. Morimoto, M. Taniguchi, and T. Kawai, APPLIED PHYSICS LETTERS, 92[22] (2008) 223110(1-3).

Metallic nature of metal-molecule interface formed by Au-Se bonds, K. Yokota, M. Taniguchi, Hiro. Tanaka, and T. Kawai, PHYSICAL REVIEW B, 77[16] (2008) 165416(1-5).

Crucial role of interdiffusion on magnetic properties of in situ formed MgO/Fe₃-delta O₄ heterostructured nanowires, A. Marcu, T. Yanagida, K. Nagashima, K. Oka, Hide. Tanaka, and T. Kawai, APPLIED PHYSICS LETTERS, 92[17] (2008) 173119(1-3).

Effect of the heterointerface on transport properties of in situ formed MgO/titanate heterostructured nanowires, K. Nagashima, T. Yanagida, Hide. Tanaka, S. Seki, A.

Saeki, S. Tagawa, and T. Kawai, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130[15] (2008) 5378-5382.

Transverse Field Effects on DNA-Sized Particle Dynamics, M. Tsutsui, M. Taniguchi, and T. Kawai, NANO LETTERS, 9[4] (2009) 1659-1662.

Nonvolatile Bipolar Resistive Memory Switching in Single Crystalline NiO Heterostructured Nanowires, K. Oka, T. Yanagida, K. Nagashima, Hide. Tanaka, and T. Kawai, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 131[10] (2009) 3434-3435.

Control of threshold voltage and hysteresis in organic field-effect transistors, H. Kawaguchi, M. Taniguchi, and T. Kawai, APPLIED PHYSICS LETTERS, 94[9] (2009) 093305(1-3).

Nanoarrays of tethered lipid bilayer rafts on poly(vinyl alcohol) hydrogels, B. K. Lee, H. Y. Lee, P. Kim, K. Y. Suh and T. Kawai, LAB ON A CHIP, 9[1] (2009) 132-139.

Review Papers

Development of Electron-Transporting Conjugated Oligomers Based on Fluorination Reactions and Their Application to Organic Field-Effect Transistors, Y. Ie and Y. Aso, J. Syn. Org. Chem. Jpn., 66[5] (2008) 504-514 (in Japanese).

Development of Novel Organic n-Type Semiconductors Based on Fluoroalkyl Annelation, Y. Aso and Y. Ie, Manufacturing & Technology, 60[3] (2008) 73-76 (in Japanese).

Nanometer-Scale Dynamics of Charges Generated by Radiations in Condensed Matter, A. Saeki and S. Tagawa, Pure Appl. Chem. 81 (2009) 45-60.

Electrostatic force microscopy of nano-scale adsorbates on a insulating solid surface – application to biological molecules, T. Matsumoto, F. Yamada, E. Satho-Mikamo, A. Takagi, and T. Kawai, Journal of The Surface Science Society of Japan 29 (2008) 246-252 (in Japanese).

Nanoscale imaging of surface charges by scanning probe microscopy, T. Matsumoto and T. Kawai, Journal of the Clay Science Society of Japan 47 [1] (2008) 1-8 (in Japanese).

Development of time-resolved electrostatic force detection using scanning probe microscopy, T. Matsumoto and T. Kawai, MICROSCOPY 43 [2] (2008) 149-151 (in Japanese).

Books

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S. Tagawa Conference of Photopolymer Science and Technology 2008,
organizing committee

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The Chemical Society of Japan	5 papers
Symposium on Main Element Chemistry	1 paper
Symposium on Organic pi-Systems	2 papers
Symposium on Fundamental Organic Chemistry	3 papers
Symposium on Fluorine Chemistry	1 paper
The Society of Polymer Science, Japan	1 paper
The Japan Society of Radiation Chemistry	1 paper
The Japan Society of Applied Physics	26 papers
The Japan Physical Society	6 papers
Society for Molecular Science	4 papers
The Biophysical Society of Japan	1 paper
Society of Nano Science and Technology	2 papers
Others	1 paper

Sponsorship

Grant-in-Aid for Scientific Research (S)

S. Tagawa	Femtosecond Pulse Radiolysis Study on Time Profile of Radiation-Induced Processes in Nanoscopic Region	¥20,900,000
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Grant-in-Aid for Scientific Research (A)

T. Kawai	Creation of DNA nanostructure and the study of their properties	¥10,140,000
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Grant-in-Aid for Scientific Research on Innovative Areas

Y. Aso	Functions of Highly Elaborated pi-Space Based on Synthesis of Extended pi-Electron Systems and Application to Electronics	¥4,420,000
T. Kawai	Emergent Chemistry of Nano-scale Molecular System	¥9,880,000
T. Kawai	Program emergent chemistry beyond hierarchy in transition metal oxide Nano structure	¥19,890,000

Grant-in-Aid for Scientific Research on Priority Areas

Y. Aso	Development of Extended Conjugated Oligomers toward Construction of Charge-Transporting Hierarchical Structure	¥1,500,000
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Entrusted Research

Y. Aso	Japan Science and	Synthesis and Application of	¥4,999,000
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	Technology Agency	Novel Conjugated Oligomers as n-Type Semiconductors for Stable Operation	
S. Tagawa	JST CREST	Research on resist for ultrafine fabrication and development of process simulator	¥166,270,000
S. Tagawa	ASET	Research on reaction mechanism of chemically amplified resist	¥1,000,000
T. Kawai	MEXT (Ministry of Education, Culture, Sports, Science and Technology)	Handai Multi-Functional Nanofoundry	¥147,000,000
T. Kawai	NEDO (New Energy and Industrial Technology Development Organization)	Development of the high sensitivity gene polymorphism detection biochip system	¥6,600,000
T. Kawai	MEXT (Ministry of Education, Culture, Sports, Science and Technology)	Promotion of Novel Interdisciplinary Fields Based on Nanotechnology and Materials	¥6,470,000

New Functional Nano-Electronics Research Group

Professors: Kazuhiko MATSUMOTO (Group Leader),
Hajime ASAHI, Katsumi TANIMURA, Hikaru KOBAYASHI

Outline

New functional nano-electronics research group treated mainly the semiconductor and its material characteristics, physical evaluation, device performance, etc. are analyzed in details as follows:

The Synthesis and development of III-nitride semiconductor-based room temperature transparent ferromagnetic semiconductors with strong photoemission properties and their application to novel semiconductor nano-spintronics device fabrications are conducted. (Asahi)

Using the carbon nanotube as a treating material, the quantum functional device, field effect transistor, FET type bio sensor, electrochemical biosensor are developed. Also, the fundamental growth process, such as a chirality control, growth direction control are investigated. (Matsumoto).

The aim of our research is to establish the new methods to fabricate highly functional nano-electronic materials and structures by controlling modes of condensation via electronic excitation of solids. (Tanimura)

SiC is chemically stable, and thus, surface oxidation and etching do not occur by the conventional RCA cleaning method. Therefore, metal contaminants on SiC surfaces cannot be removed completely by the RCA method. In the case of the HCN cleaning method, on the other hand, cyanide ions form complex ions with metals, resulting in the removal of metal contaminants from SiC surfaces. (Kobayashi)

Current Research Projects

Magnet-optical properties of ferromagnetic semiconductor GaDyN

Transition-metal and rare-earth doped GaN magnetic semiconductors are gathering great interest as new functional materials to fabricate semiconductor spintronics devices because of their ferromagnetic properties and strong photo emission properties at room temperature. We have grown rare-earth Dy-doped GaN, GaDyN and observed room temperature ferromagnetism. We also conducted the MCD measurement and observed large enhancement of MCD signals and clear hysteresis suggesting “real” ferromagnetic semiconductors.

Diameter-controlled growth of GaGdN nanorod

To fabricate magnetic semiconductor nano-devices, we have investigated the formation of GaGdN nano-rod structures. GaCrN nano-rods were grown on n-Si (100) substrates with native oxide layer. It was found that the diameter of the GaGdN nano-rods can be controlled by changing the growth parameters, especially substrate temperature.

Fabrication of amperometric biosensors based on carbon nanotube-arrayed electrodes

Carbon nanotube (CNT) amperometric chips with 6 pneumatic micropumps by the combination of amperometric biosensors based on 12 CNT-arrayed electrodes and 3 microchannels are fabricated. By modifying the CNT electrodes by two kinds of antigens, two kinds of cancer marker, such as PSA and hCG can be detected in one chip. We conclude that microfluidic chips with CNT-arrayed electrodes are a promising candidate for the development of hand-held electrochemical biosensors.

Mechanism of Laser-Induced Surface-Bond Rupture on Semiconductor Surfaces

Local structural changes induced by fs-laser excitation for Si(111)-(7x7) surfaces have been studied by means of scanning tunnelling microscopy as a function of substrate temperatures. Thermal fluctuation of the surface-lattice systems and electronic excitation cooperate synergistically to enhance the bond-rupture rate dramatically. The mechanism can be analyzed in terms of a type of stochastic resonance, and provides an efficient tool to develop atomic-scale manipulation and nano-structure formation on semiconductor surfaces.

Photoinduced Graphite-to-Diamond Phase Transition

A novel sp^3 -bonded phase of carbons is formed by femtosecond laser excitation of Graphite, which has been identified experimentally by direct imaging of the irradiated surface by STM. Abinitio total energy calculation has confirmed the unique structure of “Diaphite” which is just an intermediate between graphite and hexagonal diamond structures. Ultrafast electron diffractometer has been newly developed to study the structural dynamics induced by fs-laser excitation with fs-temporal resolution.

Removal of metal contaminants from SiC surfaces by use of defect passivation etch-less cleaning method

SiC is chemically stable, and thus oxidation and etching do not proceed easily. Therefore, the conventional semiconductor cleaning method (i.e., RCA method) which removes contaminants by oxidation and etching cannot remove surface metals completely, and metals with $10^{11} \sim 10^{12}$ atoms/cm² concentration remain after cleaning. HCN solutions, on the other hand, remove metal contaminants by reaction of CN^- ions with metals resulting in the formation of cyanide-metal complex ions. The reactivity of CN^- ions is so high that cleaning can be performed at room temperature using extremely dilute HCN solutions. However, SiC surfaces are rough compared with Si surfaces. Consequently, metal contaminants present in tiny pores cannot be removed by the HCN cleaning, but can be removed by combination of the RCA and HCN cleaning methods.

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High-Performance Carbon Nanotube Field-Effect Transistors Using Low-Energy Ion Implantation, Kenzo Maehashi, Kohei Nishiguchi, Yasuhide Ohno, Koichi Inoue, Kazuhiro Yamamoto, and Kazuhiko Matsumoto, 2008 Device Research Conference (2008) Jun. 23 - 25, Santa Barbara, USA

High Sensitive Carbon Nanotube FET Biosensor with Micro Fluid System and AC Measurement System, Kazuhiko Matsumoto, Kenzo Maehashi, Yasuhide Ohno, and Yasuki Yamamoto, Ninth Int. Conf. on the Science and Application of Nanotubes (2008) June 29 - July 4, Montpellier, France

Room Temperature Operation of Carbon Nanotube Single-Hole Transistors Fabricated by Shadow Evaporation Methods, Yasuhide Ohno, Yoshihiro Asai, Kenzo Maehashi, Koichi Inoue, and Kazuhiko Matsumoto, 2008 Int. Conf. on Solid State Device and Materials (2008) Sept. 24 - 26, Tsukuba, Japan

Low-Energy Oxygen Ion Irradiation Effects on Carbon Nanotube Field-Effect Transistors with Passivation Films, Satoshi Nagaso, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, Kazuhiro Yamamoto, and Kazuhiko Matsumoto, 2008 Int. Conf. on Solid State Device and Materials (2008) Sept. 24 - 26, Tsukuba, Japan

HIGH-PERFORMANCE CARBON NANOTUBE FIELD-EFFECT TRANSISTORS FOR HIGH-SENSITIVE BIOSENSORS, Kenzo Maehashi and Kazuhiko Matsumoto, The IASTED International Conference on Nanotechnology and Applications (2008) Sept. 29 – Oct. 1, Crete, Greece

CARBON NANOTUBE FIELD-EFFECT TRANSISTOR BIOSENSORS WITH HIGH SIGNAL-TO-NOISE RATIO USING ALTERNATING CURRENT MEASUREMENT, Yasuki Yamamoto, Yasuhide Ohno, Kenzo Maehashi, and Kazuhiko Matsumoto, The IASTED International Conference on Nanotechnology and Applications (2008) Sept. 29 – Oct. 1, Crete, Greece

Ultrafast carrier dynamics on Si surfaces studied by time-resolved two-photon photoemission spectroscopy (Invited), K. Tanimura, 6th International Conference on Ultrafast Surface Dynamics, Kloster Banz, Germany, July 20-25, 2008

Ultrafast carrier dynamics in Si and on Si surfaces studied by time-resolved two-photon photoemission spectroscopy (Invited), K. Tanimura, Ultrafast Phenomena in Semiconductors and Nanostructure Materials XIII, San Jose, USA, January 25-28, 2009

Local bond rupture on Si surfaces induced by low-energy electron-beam excitation, J. Kanasaki and K. Tanimura, International workshop on “Low-Energy Electron Molecule Interaction:LEEMI-EIPAM’08, Roscoff, France, May 7-11, 2008.

Interlayer bond formation of graphite crystals induced by femtosecond laser excitation,

Kanasaki, E. Inami, K. Tanimura, and K. Nasu, 25th European Conference on Surface Science, Liverpool, UK, July 27-Aug.1, 2008.

Surface-carrier dynamics on Si(001)-(2x1): roles of electron transfer from bulk- to surface-electronic states, S. Tanaka and K. Tanimura, 25th European Conference on Surface Science, Liverpool, UK, July 27-Aug.1, 2008.

Hot-hole and hot-electron dynamics at Si surfaces studied by time-resolved twophoton photoemission spectroscopy, T. Ichibayashi and K. Tanimura, 6th International Conference on Ultrafast Surface Dynamics, Kroster Banz, Germany, July 20-25, 2008.

Image-potential induced surface-resonance states at Si(100)-(2x1), T. Ichibayashi and K.Tanimura, 25th European Conference of Surface Science, Liverpool, UK, July 27-Aug.1, 2008..

Ultrafast carrier dynamics in Si studied by time-resolved two-photon photoemission spectroscopy, T. Ichibayashi and K. Tanimura, 3rd International Conference on Photo-Induced Phase Transitions and Cooperative Phenomena, Osaka, Japan, Nov. 11-13, 2008.

Nitric acid oxidation of Si at 120°C to fabricate MOS Structure with excellent electrical characteristics, H. Kobayashi, 1st International Conference on Thin Films and Porous Materials, May 19-22, 2008, Zeralda, Algiers.

Surface cleaning and defect passivation by the use of cyanide solutions, M. Takahashi, 1st International Conference on Thin Films and Porous Materials, May 19-22, 2008, Zeralda, Algiers.

Low temperature nitric acid oxidation of Si (NAOS) for fabrication of gate oxides in LSI and TFT, H. Kobayashi, The 1st International Symposium on Hybrid Materials and Processing, Oct. 27-29, 2008, Busan, Korea.

One-step and two-step NAOS methods for fabrication of SiO₂/Si structure with excellent electrical characteristics, H. Kobayashi, 6th Solid State Surfaces and Interfaces, Nov. 24-27, 2008, Smolenice, Slovakia.

Semiconductor defect passivation etch-less cleaning method using HCN solutions with ppm order concentration, H. Kobayashi, 10th International Symposium on Eco-materials Processing and Design, Jan. 13-15, 2009, Xi'an, China.

Contributions to International Conferences and Journals

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|----------|---|
| H. Asahi | 2008 International Conference on Solid State Devices and Materials
(Program Committee member) |
| H. Asahi | 15th International Conference on Molecular Beam Epitaxy
(International Advisory Committee member) |
| H. Asahi | Second International Symposium on Growth of III-Nitrides
(International Advisory Committee member) |

H. Asahi	International Conference on Functional Materials for Advanced Technology (International Organizing Committee member)
H. Asahi	Journal of Crystal Growth (Editor)
H. Asahi	J. Materials Science: Materials in Electronics (Editorial Board member)
K. Matsumoto	International Conference on Solid State Device & Materials 2008(Program Sub-Committee Chair)
K. Matsumoto	MSS17 (Program Committee member)
K. Matsumoto	IEEE Nanotechnology (Associate Editor)
K. Matsumoto	Japanese Journal of Applied Physics (Editor)
H. Kobayashi	Applied Surface Science (Editor-in-Chief)
H. Kobayashi	2008 SSSI International Conference (Chairman of Science Committee)
H. Kobayashi	International Symposium on Eco-materials and Design (Session Chairman)
H. Kobayashi	4th Vacuum and Surface Science Conference of Asia and Australia (Publishing Committee)

Publications in Domestic Meetings

The Japan Society of Applied Physics	27papers
PASPS Symposium	3papers
Electronic Materials Symposium	1paper
International Conference on Solid State Device & Materials 2007	2papers
The Japan Physical Society	10papers
The Surface Science Society of Japan	1paper
Surface and Interface Spectroscopy	2papers

Sponsorships

Grant-in-Aid for Specially Promoted Research

K. Tanimura	Dynamical studies of photoinduced phase transitions	¥175,760,000
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Grant-in-Aid for Scientific Research on Priority Areas

H. Asahi	Study on Fabrication of InN-Based Long Wavelength Circular Polarized Semiconductor Lasers	¥3,900,000
K. Matsumoto	Development of carbon nanotube biosensor	¥37,000,000

Grant-in-Aid for Scientific Research (A)

K. Tanimura	Dynamical properties of excited semiconductor surfaces with two-dimensional features	¥2,300,000
H. Kobayashi	Low temperature fabrication of SiO ₂ /SiC structure by use of nano-pores formed with nitric	¥17,810,000

acid oxidation method

Grant-in-Aid for Scientific Research (B)

H. Asahi	Study on Room Temperature Ferromagnetic Nitride Semiconductor Nanostructures and Application to Nanospintronics Devices	¥2,300,000
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Grant-in-Aid for Creative Scientific Research

H. Asahi	Development of properties and functionalities by precise control of rare-earth doping (Y. Fujiwara)	¥28,000,000
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Entrusted Research

K. Matsumoto	Japan Science and Technology Organization CREST	Development of quantum nanodevices by controlling quantum interface	¥10,000,000
H. Kobayashi	Japan Science and Technology Organization	Low temperature formation of TFT gate oxide layers and lower power consumption by the nitric acid oxidation	¥62,400,000
H. Kobayashi	Japan Science and Technology Organization	Japan-Slovakia joint research project	¥2,500,000

Molecular Nano-Mechanics & Bio-Mechanics Research Group

Professors: Nobuo KATO (Group Leader), Hiroyuki Noji (Group Sub-Leader)
Kazuhiro NAKATANI, Takashi WASHIO

Outlines

With biomechanics of molecular motors, DNA, and other related materials, researches of this group aim at the development of devices functioning with self-organization on the basis of producing new material, nano light processing, nano measurement of extremely weak force, dynamic assessments of nano space. Kato group focused the attention on the photoresponsive gene expression with peptide nucleic acid and modulation of cell signaling by diterpenoid-based or peptide-mimetic type of small molecules. Noji group, in cooperation with the Nagai group of Research Institute for Electronic Science, Hokkaido University and Yoshida group of Chemical Resources Laboratory, Tokyo Institute of Technology, pushed forward a study about elucidation of the energy conversion mechanism of the ATP synthase with single molecule measurement technology and microdevices. Furthermore, they developed a fluorescent probe for ATP and measured dynamics of the ATP density in the cell. Nakatani group studied the photoresponsive molecular glue for DNA and realized the light control of the DNA double strand formation with photoswitchable molecular glue.

Current Research Projects

Crystal structure of the association complex of 14-3-3 protein and cotylenin

Cotylenin, a fungal metabolite originally described as a cytokinin-like bioactive substance against plants shows differentiation-inducing and antitumor activity in certain human cancers. We solved the crystal structure of cotylenin acting on a 14-3-3 regulatory protein complex. By comparison with the closely related, but non-anticancer agent fusicoicin, a rationale for the activity of cotylenin in human cancers has been demonstrated.

Intracellular ATP Imaging

With the aim of direct measurement of the intracellular [ATP] in individual cells, we have developed a ratiometric fluorescent ATP sensor protein. The ATP sensor protein was successively expressed in a culture cells such as a human cultured cell and bacteria cells. When apoptosis was induced in human cells, a large decrement in intracellular [ATP] level was reproducibly observed several seconds before the morphologic change of cell, which is characteristic of apoptosis, indicating the intracellular [ATP] drop is a trigger of apoptosis. This project has been done under the frame of the collaboration with Nagai lab in Hokkaido University.

Single-molecule Study on a Rotary Molecular Motor Protein

F₁-ATPase is a rotary molecular motor that makes 120° stepping rotation, each step driven by a single ATP hydrolysis reaction. Since the establishment of the single-molecule rotation assay, attempts have been made to resolve the rotary motion of F₁-ATPase into discrete steps of ATP hydrolysis in order to clarify how the rotation is coupled with the elementary reaction steps of ATP hydrolysis. In the collaboration work with Yoshida lab in Tokyo Institute of Technology, we has found a new reaction

intermediate of F₁-ATPas in the rotation assay at 4°C. Kinetic analysis shows that the intermediates state is relevant to ADP-releasing step.

Development of DNA based supramolecular optical switch

With photoswitchable molecular glue for DNA containing azobenzene photochromic moiety, we investigated the hybridization/dehybridization of DNA modified with pyrene fluorophore by replacing a DNA base pair. Pyrene is known to form an exciplex dimer when stacked with each other in solution and, as a result changes the fluorescence from monomer blue to excimer green emission. Upon photoisomerization from *trans* to *cis* or *vice versa* of azobenzene moiety of photoswitchable molecular glue for DNA, we observed reversible switching of DNA hybridization and emission of fluorescence.

Matrix completion for data estimation in quantum experiments

Results of quantum experiments are known to satisfy a mathematical property named positive semi-definiteness due to their background physical nature. This study worked on the development of a method and its algorithm to derive the estimation of the experimental results against the disturbance of condition fluctuations, uncertainty and missing values based on the mathematical property.

Publications

Original Papers

Identification of diterpene biosynthetic gene clusters and functional analysis of labdane-related diterpene cyclases in *Phomopsis amygdali*, T. Toyomasu, R. Niida, H. Kenmoku, Y. Kanno, S. Miura, C. Nakano, Y. Shiono, W. Mitsuhashi, H. Toshima, H. Oikawa, T. Hoshino, T. Daiiri, N. Kato, and T. Sassa, *Biosci. Biotechnol. Biochem.* 72 (2008) 1038-1047.

Enhanced anti-influenza A virus activity of (-)-epigallocatechin-3-O-gallate fatty acid monoester derivatives: Effect of alkyl chain length, S. Mori, S. Miyake, T. Nakaya, N. Kato, and K. Kaihatsu, *Bioorg. Med. Chem. Lett.* 18 (2008) 4249-4252.

Enhanced antitumor activities of (-)-epigallocatechin-3-O-gallate fatty acid monoester derivatives in vitro and in vivo, K. Matsumura, K. Kaihatsu, S. Mori, H. H. Cho, N. Kato, and S. H. Hyon, *Biochem. Biophys. Res. Commun.* 377 (2008) 1118-1122.

Biosynthetic gene-based secondary metabolite screening: A new diterpene, methyl phomopsenonate, from the fungus *Phomopsis amygdali*, T. Toyomasu, A. Kaneko, T. Tokiwano, Y. Kanno, Y. Kanno, R. Niida, T. Kawano, H. Oikawa, N. Kato, and T. Sassa, *J. Org. Chem.* 74 (2009) 1541-1548.

Identification and functional analysis of brassicicene C biosynthetic gene cluster in *Alternaria brassicicola*, A. Minami, N. Tajima, Y. Higuchi, T. Toyomasu, T. Sassa, N. Kato, and T. Daiiri, *Bioorg. Med. Chem. Lett.* 19 (2009) 870-874.

A structural rationale for selective stabilization of anti-tumor interactions of 14-3-3 proteins by cotylenin A, C. Ottmann, M. Wayand, T. Sassa, T. Inoue, N. Kato, A. Wittinghofer, and C. Oecking, *J. Mol. Biol.* 386 (2009) 913-919.

Correlation between the conformational states of F1-ATPase as determined from its crystal structure and single-molecule rotation, D. Okuno, R. Fujisawa, R. Iino, Y. Hirono-Hara, H. Imamura, and H. Noji, *Proc. Natl. Acad. Soc. U.S.A.* 105 (2008), 20722-20727.

Photo Gel-Sol/Sol-Gel Transition and Its Patterning of a Supramolecular Hydrogel as Stimuli-Responsive Biomaterials, S. Matsumoto, S. Yamaguchi, S. Ueno, H. Komatsu, M. Ikeda, K. Ishizuka, Y. Iko, K. V. Tabata, H. Aoki, S. Ito, H. Noji, and I. Hamachi, *Chemistry - A European Journal* 14 (2008), 3977-3986.

Loop-mediated isothermal amplification of a single DNA molecule in polyacrylamide gel-based microchamber, L. Lam, S. Sakakihara, K. Ishizuka, S. Takeuchi, H. F. Arata, H. Fujita, and H. Noji, *Biomed. Microdevices* 10 (2008) 539-546.

Genotyping by allele-specific L-DNA-tagged PCR, G. Hayashi, M. Hagihara, and K. Nakatani, *J. Biotechnol.* 135 (2008) 157-160.

Genotyping by allele-specific L-DNA-tagged PCR, G. Hayashi, M. Hagihara, and K. Nakatani, *J. Biotechnol.* 135 (2008) 157-160.

Synthesis of Dimeric 2-Amino-1,8-naphthyridine and Related DNA-Binding Molecules, K. Nakatani, H. He, S. Uno, T. Yamamoto, and C. Dohno, *Current Protocols in Nucleic Acid Chemistry* 2 (2008) 1-21.

DNA Labeling by Ligand Inducible Secondary Structure, T. Peng, H. He, M. Hagihara, and K. Nakatani, *ChemBioChem* 9 (2008) 1893-1897.

Ligand Binding to Tandem G-quadruplex from Human Telomeric DNA, L.-P. Bai, M. Hagihara, Z.-H. Jiang, K. Nakatani, *ChemBioChem* 9 (2008) 2583-2587.

Site-specific binding of chelerythrine and sanguinarine to single pyrimidine bulges in hairpin DNA, L.-P. Bai, Z. Cai, Z.-Z. Zhao, K. Nakatani, and Z.-H. Jiang, *Anal. Bioanal. Chem.* 392 (2008) 709-716.

Dimer of 2,7-diamino-1,8-naphthyridine for the detection of mismatches formed by pyrimidine nucleotide bases, A. Kobori, and K. Nakatani, *Bioorg. Med. Chem.* 16 (2008), 10338-10344.

RNA Aptamers That Reversibly Bind Photoresponsive Azobenzene-Containing Peptides, G. Hayashi, M. Hagihara, and K. Nakatani, *Chem. Eur. J.* 15 (2009) 424-432.

The effect of linker length on binding affinity of a photoswitchable molecular glue for DNA, C. Dohno, S. Uno, S. Sakai, M. Oku, and K. Nakatani, *Bioorg. Med. Chem.* 17 (2009) 2536-2543.

Synthesis and Reaction of DNA Oligomers Containing Modified Cytosines Related to Bisulfite Sequencing, Y. Oka, T. Peng, F. Takei, and K. Nakatani, *Org. Lett.* 11 (2009)

1377-1379.

Modeling Dynamic Substate Chains among Massive States, N. V. Phuong and T. Washio, *Intelligent Data Analysis* 12 (2008) 271-291.

International Conferences

Anti-influenza A virus activity of (–)-epigallocatechin-3-O-gallate fatty acid monoester derivatives, K. Kaihatsu, S. Mori, S. Miyake, T. Nakaya, and N. Kato, 21st International Conference on Antiviral Research, Canada, April 13-17, 2008.

Diterpene Cyclase Responsible for Fusicoccin Biosynthesis, T. Toyomasu, T. Dai, N. Kato, and T. Sassa, 7th US-Japan Seminar on the Biosynthesis of Natural Products Enzymology, Structural Biology, and Drug Discovery, La Jolla, California, USA, June 22-27, 2008.

Chemical ligation of epoxide-containing fusicoccins and peptide fragments induced by 14-3-3 protein surface, J. Ohkanda, T. Maki, A. Kawamura, and N. Kato, 9th Tetrahedron Symposium, San Francisco, USA, July 22-23, 2008.

Synthetic Method of 4-Carbamoylimidazolium 5-olate, C. Kondo, Y. Higuchi, M. Sunagawa, and N. Kato, The First International Symposium on Process Chemistry [ISPC 08], Kyoto, Japan, July 28-30, 2008.

Antitumor activity of (–)-epigallocatechin-3-O-gallate fatty acid derivatives, K. Kaihatsu, S. Sawada, and N. Kato, 11th Sanken International Symposium, Awaji, Japan, February 2-4, 2008.

Synthesis of Green Tea Catechin Derivatives and Evaluation of Their Anti-influenza Virus Activity, K. Kaihatsu, K. Matsumura, S. Mori, H. H. Cho, and S. H. Hyon, and N. Kato, The 8th International Conference of Anticancer Research, Greece, October 17-22, 2008.

Fusicoccin derivative (ISIR-005) suppression anchorage-independent growth of cancer cells through anoikis activation, Y. Honma, M. Akimoto, T. Sassa, and N. Kato, 20th EORTC-NCI-AACR Symposium on Molecular Targets and Cancer Therapeutics, Geneva, Switzerland, October 21-24, 2008.

Module assembly for protein surface recognition, *J. Ohkanda, The IUMRS International Conference in Asia 2008, Nagoya, Japan, December 9-11, 2008.

Mechanical modulation of ATP-binding and hydrolysis by single F1-ATPase molecule, *H. Noji, MPSA2008, Sapporo, Japan, August 29, 2008.

Single-molecule Imaging of the transport-vesicle formation mediated by COPII system reconstituted on a planar bilayer system, *H. Noji, The 17th CDB Meeting - Towards Synthesis of Cells, Kobe, Japan, October 14-15, 2008.

Single molecule studies on F1-ATPase molecular motor, *H. Noji, 16th International

Colloquium on Scanning Probe Microscopy, Izu-Atagawa, Japan, December, 13, 2008.

Femtoliter chamber for single-molecule and single-cell analysis, *H. Noji, 4th IEEE-NEMS09, Shinsen, China, January, 6, 2009.

Single molecule biophysics of F1-ATPase: Mechanical modulation of reaction rate constants and equilibrium constants by F1-ATPase, *H. Noji, 6th Asian Biophysics Association Symposium, HKUST, Hong Kong, January, 11, 2009.

Controlling Hybridization by Molecular Glue for DNA, K. Nakatani, International Conference in Organic Synthesis (ICOS-17), Daejeon Conference Center, Daejeon, Korea, June 23-27, 2008.

Synthesis and evaluation of photoresponsive molecular Glue for DNA, S. Uno, C. Dohno, M. Oku, S. Sakai, and K. Nakatani, International Conference in Organic Synthesis (ICOS-17), Daejeon Conference Center, Daejeon, Korea, June 23-27, 2008.

The fluorescent detection of single nucleotide difference using cytosine bulge hairpin primers, F. Takei, M. Hagihara, Y. Oka, and K. Nakatani, XXII IUPAC symposium on photochemistry, Kyoto, July 28-August 1, 2008.

Reversible control of DNA hybridization by a small synthetic ligand, C. Dohno, S. Uno, T. Yamamoto, S. Sakai, and K. Nakatani, International symposium on integrated synthesis, September 5-6, 2008.

Fluorescent Ligand as a molecular probe for the RNA structure, S. Umemoto, J. Zhang, C. Dohno, and K. Nakatani, Joint Symposium of 18th International Roundtable on Nucleosides, Nucleotides and Nucleic Acids (IRTXVIII) and 35th International Symposium on Nucleic Acids Chemistry, September 8-12, 2008.

The reaction of cytosine with bisulfite by base flipping from the duplex, Y. Oka, T. Peng, F. Takei, K. Nakatani, Joint Symposium of 18th International Roundtable on Nucleosides, Nucleotides and Nucleic Acids (IRTXVIII) and 35th International Symposium on Nucleic Acids Chemistry, September 8-12, 2008.

RNA aptamers that reversibly bind to photoresponsive peptide, G. Hayasi, M. Hagihara, and K. Nakatani, Joint Symposium of 18th International Roundtable on Nucleosides, Nucleotides and Nucleic Acids (IRTXVIII) and 35th International Symposium on Nucleic Acids Chemistry, September 8-12, 2008.

Recognition of Mismatched Base Pairs by Small Synthetic Ligands, K. Nakatani, International Symposium of Molecular Recognition of DNA: Biological Application, Kyoto University, September 18, 2008.

DNA sensing and architecture, K. Nakatani, RIKEN conference 2008 on Chemical Biology, Radisson Hotel Narita, November 12-15, 2008.

A Range Query Approach for High Dimensional Euclidean Space Based on EDM

Estimation, K. Kido, H. Kuwajima, and T. Washio, Proc. of the Eighth SIAM International Conference on Data Mining (SDM08), Edited by M. J. Zaki, K. Wang, C. Apte, and H. Park, (2008) 387-398.

A Fast Method to Mine Frequent Subsequences from Graph Sequence Data, A. Inokuchi and T. Washio, Proc. of 2008 Eighth IEEE International Conference on Data Mining, (2008) 303-312.

Feasibility of Graph Sequence Mining based on Admissibility Constraints, A. Inokuchi and T. Washio, Proc. of 3rd International Workshop on Data Mining and Statistical Science (DMSS2008), (2008) 1-4.

On Feasibility of Graph Spectrum-based Frequent Sub-graph Mining, K. Ohara, T. Washio, and D. V. Nguyen, Proc. of 3rd International Workshop on Data Mining and Statistical Science (DMSS2008), (2008) 9-11.

Isomorphism Identification by Using Graph Spectra and Its Application to Graph Mining, K. Ohara and T. Washio, Proc. of IASC2008: the Joint Meeting of 4th World Conference of the IASC and 6th Conference of the Asian Regional Section of the IASC on Computational Statistics & Data Analysis, (2008) 229 (Invited).

Contributions to International Conferences and Journals

N. Kato 27th Conference on Combinatorial Chemistry, Japan
(Organizing Committee)

Publications in Domestic Meetings

Japan Chemical Society	12 papers
Biophysical Society of Japan	11 papers
Japan Bioenergetics Group	4 papers
Symposium on Biofunctional Chemistry	3 papers
Japanese Society for Chemical Biology	2 papers
SORST Joint Symposium	2 papers
Supported Membrane Workshop	2 papers

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

H. Noji	Rotational mechanism of FoF1-ATP synthase	¥59,700,000
T. Washio	Establishment of Knowledge Mining and Modeling Principles for Large Scale Dimensional Time Series and Its Application to Commercial Ubiquitous Data	¥3,000,000

Grant-in-Aid for Scientific Research (S)

K. Nakatani	Regulation of DNA Structure and Function Based on the Stabilization of DNA Duplex	¥17,940,000
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Grant-in-Aid for Scientific Research (A)

H. Noji	Development of novel single molecule measurement method using ultra-small reaction chamber array	¥7,800,000
T. Washio	Development of Causal Structure Mining Method for Large Scale Dimensional Data and Construction of Knowledge Base on Gene Functional Relations	¥12,350,000
Entrusted Research		
N. Kato	Program for Promotion of Fundamental Studies in Health Sciences (NIBIO)	Development of new anti-cancer agents based on the differentiation-inducing diterpene glycoside ¥24,000,000

Department of Quantum Information Photonics

(Alliance Laboratory of ISIR, Osaka Univ. and RIES, Hokkaido Univ.)

Professor:	Shigeki TAKEUCHI
Visiting Professor:	Jeremy O'Brien (2009.1.16-)
Assistant Professor:	Ryo OKAMOTO
Assistant Professor:	Masazumi FUJIWARA (2009.1.1-)
Post Doctoral Fellow:	Hideaki TAKASHIMA
Visiting Researcher:	Lixin Xia (-2008.8.7)
Graduate Students:	Tomohisa NAGATA (Hokkaido Univ., Corporate Promotion Member) Takeshi ASAI (Hokkaido Univ., Corporate Promotion Member) Masato TANIDA (Hokkaido Univ., Corporate Promotion Member)
Research Student:	Kiyota TOUBARU
Supporting Staff:	Izumi KASAGI

Outlines

By using quantum nature of light, it is predicted that we can drastically enhance the performance of information processing (Quantum Computer), secure communication (Quantum Cryptography) and even sensing (Quantum Metrology). We carry on experimental researches into the realization and the application of ***the novel states of light***, by generating individual single photons and controlling the ***quantum correlation*** between these photons. Toward the perfect control of single photons, we investigate ***nano-scale photonic structures*** for optical quantum devices and single photon sources. Using those devices, we are constructing quantum optical systems and ***optical quantum circuits*** for quantum information processing, quantum metrology and quantum lithography. Our research topic also includes the generation and characterization of ***entangled photons, single molecular spectroscopy, and highly efficient single photon detectors***.

Current Research Project

- **Realization of the world-largest-class optical quantum circuit
– an Entanglement Filter –**

The ability to filter quantum states is a key capability in quantum information science and technology, where one-qubit filters, or polarizers, have found wide application. Filtering on the basis of entanglement requires extension to multi-qubit filters with qubit-qubit interactions. We have proposed such a device for photonic qubits (Phys. Rev. Lett. 2002), however, the technical requirements to build such a device, an optical circuit with two ancillary photons and multiple quantum gates, requiring both quantum interference and classical interference in several nested interferometers, have been

lacking.

We demonstrate an entanglement filter by combining two key recent technological approaches - a displaced-Sagnac architecture (Science 2007) and partially polarizing beam splitters (Phys. Rev. Lett. 2005). The entangling capability of the filter was verified, distinguishing it from classical ones. The optical quantum circuit is one of the world's largest quantum circuits in terms of both the number of quantum gates and classical interferences. This achievement indicates the potential for the development of various optical quantum circuits, and is expected to lead to highly significant developments in quantum computers and long-distance quantum cryptography.

- **Sensitivity of the phase measurement using quantum optical interferometer**

Quantum metrology promises greater sensitivity for optical phase measurements than could ever be achieved classically. We presented a theory of the phase sensitivity for the general case where the detection probability is given by an N photon interference fringe. We have found that the phase sensitivity has a complicated dependence on both the intrinsic efficiency of detection and the interference fringe visibility. Most importantly, the phase that gives maximum phase sensitivity is in general not the same as the phase at which the slope of the interference fringe is a maximum, as has previously been assumed. We determined the parameter range where quantum enhanced sensitivity can be achieved. In order to illustrate these theoretical results, we performed a four-photon experiment with the efficiency of 3/4 and the visibility of $82 \pm 6\%$ [an extension of our previous work (Science 2007)] and found a phase sensitivity 1.3 times greater than the standard quantum limit.

- **Coupling a microsphere resonator with a tapered fiber at a ultra low temperature**

We succeeded in controlling the coupling condition of a microsphere resonator and a tapered fiber at an cryogenic temperature (10K) for the first time as far as we know. The observed resonance width was 40MHz, which corresponds to the Q factor of 5×10^6 . This is a big step to realize nanophotonic devices to control the quantum states and quantum correlations of photons.

- **Measurement of the optical phase shift due to the resonance of fiber-microsphere system using polarization analysis.**

We established a novel method to measure the optical phase shift of a fiber-microsphere system. Since probe light can pass through our tapered fibers without depolarization, we measured Stokes parameter spectrum of the fiber-microsphere system and determined the phase shift spectrum. This novel method can be applied for the measurement of the phase shift of individual photons passing through the fiber-microsphere system with a small change, by replacing two photodiodes used in the system with photon counting modules.

Publications

Original Papers

Beating the standard quantum limit: phase super-sensitivity of N-photon interferometers, R. Okamoto, H. F. Hofmann, T. Nagata, J. L.. O'Brien, K. Sasaki and S. Takeuchi: New Journal of Physics, 10 (2008) 073033/1-073033/9.

Observing Quantum Correlation of Photons in Laguerre-Gauss Modes Using the Gouy Phase, D. Kawase, Y. Miyamoto, M. Takeda, K. Sasaki, and S. Takeuchi: Physical Review Letters, 101 (2008) 050501/1-050501/4.

An Entanglement Filter, R. Okamoto, J. L.. O'Brien, H. F. Hofmann, T. Nagata, K. Sasaki and S. Takeuchi: Science International, 323 (2009) 483-485.

Effect of high-dimensional entanglement of Laguerre-Gaussian modes in parametric downconversion,, D. Kawase, Y. Miyamoto, M. Takeda, K. Sasaki and S. Takeuchi: Journal of the Optical Society of America B, 26 (4) (2009) 797-804.

Review Papers

Toward the Realization of Optical Quantum Phase Gates Using Fiber Coupled Microsphere Resonators, Hideaki Takashima, Hideki Fujiwara, Keiji Sasaki, Shigeki Takeuchi, KOGAKU 37 [12] (2008) 686-691

Manipulation of the Quantum States of Photons – Optical Quantum Gates and Optical Quantum Circuits, Shigeki Takeuchi, The Review of Laser Engineering, 36 [8] (2008) 1-5

Realization of photonic quantum integrated circuit, Shigeki Takeuchi, Parity, 24 [1] (2009) 11-12

Patents

Tapered optical fiber with periodic structural modulations, Shigeki Takeuchi, 2009-028429

International Conferences

Observing quantum correlation of photons in Laguerre-Gaussmodes using the Gouy phase (invited), *S.Takeuchi, D.Kawase, Y.Miyamoto, M.Takeda, and K.Sasaki: 17th International Laser Physics Workshop(2008) Trondheim, Norway, Jun.30-Jul.4,2008.

Photon juggling for quantum information processing and quantum metrology (invited), S.Takeuchi: International Nano-Optoelectronic Workshop 2008, Lake Saiko and Shonan Village, Japan, Aug.2-15,2008.

Controlling photonic qubits using geometrical phase (invited), *D.Kawase, Y.Miyamoto, M.Takeda, K.Sasaki and S.Takeuchi: SPIE Optics + Photonics2008, San Diego, U.S.A, Aug.10-14,2008.

Demonstration of a non-local quantum filter (poster), *R.Okamoto, J.L.O'Brien, H.F.Hofmann, T.Nagata, K.Sasaki, and S.Takeuchi: The Ninth International Conference

on QCMC2008, Calgary, Canada, Aug.19-24,2008.

Analysis of errors in an optical Controlled-NOT gate (poster),
*T.Nagata,R.Okamoto,H.F.Hofmann,K.Sasaki, and S.Takeuchi: The Ninth International Conference on QCMC2008, Calgary, Canada, Aug.19-24,2008.

Optical Phase Shift Observed in a Resonance Mode of a Tapered-Fiber Coupled with a Microsphere Resonator (poster), *T.Asai, H.Takashima, H.Fujiwara, K.Sasaki, and S.Takeuchi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sep.29-Oct.1,2008.

Hong-Ou-Mandel Dip with Independence Heralding Single Photon Sources (poster),
*M.Tanida, T.Nagata, R.Okamoto,K.Sasaki, and S.Takeuchi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sep.29-Oct.1,2008.

Quantum information processing using photons (invited), S.Takeuchi: 4th Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Sep.29-Oct.1,2008.

Analysis of input-output characteristic of fiber-coupled microsphere laser using rate equations (poster), *H.Takashima, H.Fujiwara, S.Takeuchi, K.Sasaki, and M.Takahashi: EOS Annual Meeting 2008, Paris, France, Sep.28-Oct.2,2008.

Photon juggling for quantum information processing and quantum metrology (invited), S.Takeuchi: International Workshop on Fundamentals of Light-Matter Interaction, Recife, Brazil, Oct.20-22,2008.

Realization of non-local quantum filter (poster), *R.Okamoto, J.L.O'Brien, H.F.Hofmann, T.Nagata, K.Sasaki, and S.Takeuchi: International Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28,2008.

Beating standard quantum limit: The sensitivity of N photon interferometers (poster),
*R.Okamoto, J.L.O'Brien, H.F.Hofmann, T.Nagata, K.Sasaki, and S.Takeuchi: International Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28,2008.

Micro-sphere resonator coupled with a tapered for quantum information processing (poster), *T.Asai, H.Takashima, H.Fujiwara, K.Sasaki and S.Takeuchi: International Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28,2008.

Toward high-fidelity operation of linear-optics quantum gates (poster), *T.Nagata, R.Okamoto, H.F.Holger, K.Sasaki and S.Takeuchi: International Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28,2008.

Highly-pure heralding single-photon sources for linear optics quantum computation (poster), *M.Tanida, T.Nagata, R.Okamoto,K.Sasaki, and S.Takeuchi: International

Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28, 2008.

Toward large-scale optical quantum circuits-Activity of Hokkaido University Group,a sub-group of Imoto Team- (poster), S.Takeuchi: International Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28,2008.

Manipulation of optical quNits using geometrical phase (invited), *D.Kawase, Y.Miyamoto, M.Takeda, K.Sasaki and S.Takeuchi: International Symposium on Physics of quantum information processing, Nara, Japan, Nov.25-28,2008.

Photon juggling for quantum information processing and quantum metrology (poster), S.Takeuchi: Workshop on Information,Nano and Photonics Technology 2008, Kobe, Japan, Nov.27-28, 2008.

Optical quantum circuits and nano-phonic devices for quantum information and quantum metrology (invited), S.Takeuchi: The 10th RIES-Hokudai International Symposium on "綾" [aya] , Hokkaido, Japan, Dec.8-9,2008.

Evaluation of an entanglement filter (poster), *R.Okamoto, J.L.O'Brien, H.F.Hofmann, T.Nagata, K.Sasaki and S.Takeuchi: The 10th RIES-Hokudai International Symposium on "綾" [aya] , Hokkaido, Japan, Dec.8-9,2008.

Toward high-fidelity operation of linear-optics quantum gates (poster), *T.Nagata, R.Okamoto, H.F.Hofmann, K.Sasaki and S.Takeuchi: The 2nd International Symposium on Global COE Program of Center for Next-Generation Information Technology Based on Knowledge Discovery and Knowledge Federation(GCOE-NGIT2009), Hokkaido, Japan, Jan.20-21, 2009.

Toward high-fidelity operation of linear-optics quantum gates (poster), *T.Nagata, R.Okamoto, H.F.Hofmann, K.Sasaki and S.Takeuchi: The 12th SANKEN International Symposium Joint Meeting of The 7th SANKEN Nanotechnology Center Symposium The 2nd SANKEN MSTeC Symposium The 1st SANKEN Alliance Symposium, Osaka, Japan, Jan.22, 2009.

Quantum metrology using entangled photons (invited), *R.Okamoto, and S.Takeuchi: SPIE Photonics West (2009), San Jose, U.S.A, Jan.24-29, 2009.

Contributions to International Conferences and Journals

S. Takeuchi	(International Conference) SPIE Photonics + Optics, Quantum communications and Quantum Imaging (Program Committee member)
S. Takeuchi	(Scientific Journal) Nonlinear Optics Quantum Optics, Editorial Board Member

Publications in Domestic Meetings

The Physical Society of Japan	1 paper
The Japan Society of Applied Physics	1 paper
Quantum Information Technology Symposium	4 papers
Others	3 papers

Academic Degrees

Master Degree for Engineering

T. Asai	“A tapered fiber coupled with a microsphere resonator - the control of the coupling condition and its phase shift spectrum”
M. Tanida	“The study on the visibility of two-photon interferences between heralding single-photon sources”

Sponsorship

Grant-in-Aid for Scientific Research (A)

S. Takeuchi	Realization and application of spatio-temporally single mode single photon source using group velocity engineering.	¥ 1,710,000
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Other Research Fund

S. Takeuchi	MIC-SCOPE	Researches on the realization of Highly efficient solid state quantum phase gate for photons	¥13,187,000
S. Takeuchi	JST-CREST	Researches on the quantum logic gates for multiple photons	¥13,500,000
S. Takeuchi	Mitsubishi Electric		¥4,000,000

Intelligent Artificial Agents and Information Systems Inspired by Biological System Dynamics

Specially Appointed Associate Professor: Naoki ASAKAWA

Specially Appointed Assistant Professor: Yasushi HOTTA

Outlines

“Intelligent Artificial Agents and Information Systems Inspired by Biological System Dynamics” (“Yuragi Project”) forms the innovation center as the project of the “Formation of Innovation Center for fusion of Advanced Technologies”. In Yuragi Project, in cooperation with participating private companies, we seek to create new intelligent artificial agents and information systems that implement highly flexible functions currently unique to living organisms.

Our strategy for achieving this goal is first to elucidate the mechanisms of expressing function in biological systems via active applications of biodynamics, that is, to understand the intrinsic stochastic and fluctuating nature of biological systems. Specifically, we will measure and analyze “dynamical fluctuations” which make biological functions highly robust and flexible. From this, we will establish new applications based on the novel principles elucidated from biological energy conversion and information processing. Incorporating knowledge from such research, new nano-materials science, information systems science, and robotics will be established. We wish to contribute to the creation of new basic and applied sciences that are capable of responding to the needs of an increasingly information-driven society.

The key concept in Yuragi project is an attractor selection model, where attractor dynamics are modified by the environmental activity under the fluctuation. We reveal the structure of the attractor selection devices inspired by stochastic resonance model, and study the nature of such stochastic devices. Then, nano materials suitable for the attractor selection devices using fluctuation mechanism are developed with the process methods and functions. And also we will develop the novel techniques for the evaluation of dynamical fluctuations.

Current Research Project

Cooperative Dynamics of an Artificial Stochastic Resonant System

We have investigated cooperative dynamics of an artificial stochastic resonant system, which is a recurrent ring connection of neuron-like signal transducers (NSTs) based on stochastic resonance (SR), using electronic circuit experiments. The ring showed quasi-periodic, tunable oscillation driven by only noise. An oscillation coherently amplified by noise demonstrated that SR may lead to unusual oscillation features. Furthermore, we found that the ring showed synchronized oscillation in a chain network composed of multiple rings. Our results suggest that basic functions (oscillation and synchronization) that may be used in the central pattern generator of biological system are induced by collective integration of the NST element.

Noise-driven attractor switching device

Problems with artificial neural networks originate from their deterministic nature and inevitable prior learnings, resulting in inadequate adaptability against unpredictable, abrupt environmental change. Here we show that a stochastically excitable threshold unit can be utilized by these systems to partially overcome the environmental change. Using an excitable threshold system, attractors were created that represent quasiequilibrium states into which a system settles until disrupted by environmental change. Furthermore, noise-driven attractor stabilization and switching were embodied by inhibitory connections. Noise works as a power source to stabilize and switch attractors, and endows the system with hysteresis behavior that resembles that of stereopsis and binocular rivalry in the human visual cortex. A canonical model of the ring network with inhibitory connections composed of class 1 neurons also shows properties that are similar to the simple threshold system.

Publications

Original Papers

Cooperative Dynamics of an Artificial Stochastic Resonant System, Y. Hotta, T. Kanki, N. Asakawa, H. Tabata, and T. Kawai: Appl. Phys. Express, 1 (2008) 088002-1-088002-3.

Noise-driven attractor switching device, N. Asakawa, Y. Hotta, T. Kanki, T. Kawai, and H. Tabata: Phys. Rev. E, 79 (2009) 021902-1-021902-8.

Review Papers

Patents

Hysteresis Comparator, Y. Hotta, T. Kanki, N. Asakawa, T. Kawai, and H. Tabata: Japanese Patent Application Number, 2008-223036.

Methodology of Control-Signal Generation, Device and Control Device for Mobile object, Y. Hotta, T. Kanki, N. Asakawa, and T. Kawai: Japanese Patent Application Number, 2008-243521.

Comparator, Noise Generator, and Stochastic-Resonance Device, T. Kanki, Y. Hotta, N. Asakawa, T. Kawai, and H. Tanaka: Japanese Patent Application Number, 2008-259480.

Yuragi Oscillator, Yuragi Oscillator System, Device for Observation, and Control System Using Yuragi Oscillators, Y. Hotta, T. Kanki, N. Asakawa, T. Kawahara, T. Kawai, and H. Tabata: PCT/JP2008/064932

International Conferences

"Brain-inspired stochastic resonant devices using poly(3-alkylthiophene)s", N. Asakawa, Y. Hotta, T. Kanki, and T. Kawai, 18th Iketani Conference: "International Conference on Control of Super-Hierarchical Structures and Innovative Functions of Next-generation Conjugated Polymers", October 21-23, 2008 Awaji Yumebutai International Conference Center, Hyogo, Japan

Publications in Domestic Meetings

The Japan Society of Applied Physics

1 paper

The Society of Polymer Science, Japan

1 paper

Sponsorship**Entrusted Research**

T. Kawai	Ministry of Education, Culture, Sports, Science and Technology	Intelligent Artificial Agents and Information Systems Inspired by Biological System Dynamics	¥98,100,000
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Activities of Facilities

Workshop

Director Professor: Masayuki NUMAO

Technical Staff

Machine Shop: Michiaki KAKUICHI, Masayoshi OHNISHI

Glassworks: Hiroaki MATSUKAWA, Noriyuki OGAWA

Outline

A machine and carpentry shop and a glass factory, which are predecessors of the Workshop, were set up at the same time when the Institute of Scientific and Industrial Research was founded. The machine and carpentry shop and the glass factory were unified to be the Workshop when the Technical Division was established in 1982. Since research fields studied in the institute covers a wide range, many of experimental apparatuses requested to the Workshop are various and novel. The Workshop, which consists of the Machine Shop and the Glassworks, plays an important role in activities of the institute and contributes to them by making and providing such experimental apparatuses.

The Machine Shop performs design and trial manufacture of experimental apparatuses for science and engineering as well as production of experimental tools made of various metals. Requests of experimental apparatuses for ultra high vacuum or ultra low temperature are increasing recently and accordingly we work in closer cooperation with researchers asking such apparatuses from the design phase to respond to the requests and make apparatuses best fit to experimental purposes. A gate-type machining center was introduced in 2002, and a CNC lathe was introduced in 2009, so that we can answer to advanced and difficult requests from researchers. A corner of the machine shop for joint-use, called an open shop, is attached and we coach researchers in technique properly.

The Glassworks performs design and trial manufacture of experimental tools and apparatuses made of various kinds of glass. We develop apparatuses necessary and suitable for experiments and we also devote ourselves to our studies and establishment of technique for improving functions of conventional apparatuses and for providing safer and easier-to-use apparatuses. Since we are recently asked to work with ceramics, we are trying to obtain machines for it. A CNC plain grinding machine was introduced in 2009, so that we can answer to advanced and difficult requests from researchers.

Activities

We continued an open house of the Workshop for the Festival of Osaka University called Ichō-Sai. The machine shop showed machine tools, displayed experimental apparatuses being made. Glassworks showed a glass lathe and experimental apparatuses being made, displayed objects d'art associated with science, and also gave demonstrations of glass processing by handwork. At the manufacturing school from August 6 to 8, 2008 organized by the Technical Division, the workshop held two teaching courses at the Machine Shop and at Glassworks, titled respectively as "Let's make plates!" and as "Let's make the Cartesian Divers!", for elementary school and junior high school students and we taught them fun of manufacturing and interest of science.

We renewed a high-speed grinder unit of the Machine Shop and a CNC plain

grinding machine of the Glassworks. We also equipped with a CNC lathe and a drill grinder of the Machine Shop. Moreover we equipped with peripheral devices and tools for the machining center for precise machining.

The members of the Workshop organized and participated in the national technical meeting and the symposium on glass works for all the engineers and technicians of universities and national laboratories in Japan.

The Glassworks receives staff members of universities in the Kansai area for technical training in glass work and in 2008 it received persons from Kobe University, Osaka Prefecture University and coached them for handing skills and technique down to the next generation. In addition, we coach technique individually for the members of the Institute.

1. Number of jobs

Machine Shop: 210 jobs (254 jobs in the previous year).

Glassworks: 141 jobs (209 jobs).

2. Number of users in the open shop

Machine Shop: 50 users.

Glassworks: 10 users.

3. Number of visitors during Icho-Sai

Machine Shop: 20 persons.

Glassworks: 30 persons.

4. Number of persons being trained

Machine Shop: 13 persons.

Glassworks: 20persons, including 10 subjects from the outside.

Office of Information Network

Professor,Director:	Kazuhiko NAKATANI
Professor:	Yoichi ANDO
Associate Professor:	Yoshinobu KITAMURA
Assistant Professor:	Keun-Soo KIM
Technical Staffs:	Takanori TANAKA, Senjin AIHARA, Yuka OKUMURA
Supporting Staff:	Miyu SAKAMOTO

Outline

Office of Information Network was inaugurated in March, 1999, to organize the operation of the information network in ISIR, which had been started with support by volunteers, because of the rapid spread of the information network and the growth of its importance in the research environment. The information was constructed as a prototype by the departments in the division of Intelligent System Science in the late 1980's and has been expanded to the whole of ISIR with the development of ODINS (Osaka University Information Network System). Recently it has played an important role in ISIR to release/access the information available in the Internet. Office of Information Network is now supporting researchers and students on the variety areas.

Laboratory for Radio-isotope Experiments

Professor: Akihito YAMAGUCHI

Outline

This laboratory is specially designed for biochemical and molecular biological experiments using the radioactive compounds labeled with ^3H , ^{14}C , ^{32}P , ^{33}P or ^{35}S . The main equipments are liquid scintillation counters and a bioimaging analyzer. This laboratory is essential for the research in the field of biochemistry, molecular biology, and cell biology. Contributions of the facilities to the research projects are described in the section of each department. The use of radioisotopes is regulated with the national law for the prevention of radiation hazard. The facilities are inspected regularly with authorities and pass the required standard. Radioisotope users are mandatory to be educated every year to get the knowledge for the safe use of radioisotopes.

Library

Professor: Nobuo KATO
Staff: Yasuko ONO
Supporting Staff: Kuniko HAMANAKA

Outline

The ISIR Library houses technical books and journals for researchers. Most materials are on open shelves directly available to faculty and students. The library has two reading rooms and a workroom with photocopiers on the second floor of the administration building, and the storage facility on the first floor of the research building.

The library office offers the following services; orders for books, survey and inquiry of literature, Interlibrary Loan services, photocopy request, and so on.

Guide to the Library could be found on its home page
(<http://www.sanken.osaka-u.ac.jp/labs/lib-web/>).

(As of March 31, 2009)

	Number of books	Journals	Newspapers
Japanese	10071	201titles	4 titles
Foreign	35709	755titles	1 title

Academia Industry Relations Office

Director, Specially Appointed Professor: Hirokazu Shimizu, Ph.D.

Outlines

The Academia Industry Relations Office (AIR Office) of the Institute of Scientific and Industrial Research (ISIR), is dedicated to reinforcing collaboration between ISIR and the industrial community, thereby combining and developing research potential of the two sectors and promoting activities for new industrial creation and innovation. The AIR Office organizes a variety of activities to inform the industrial community of the ISIR's research efficiently through the interaction with the industrial community such as SANKEN Techno Salon (four times a year) and various Lectures events, and studies on prediction of new industry, novel system of new Industry generation, and intellectual property.

The major activities of AIR Office are: 1) A network development between ISIR and Industry, 2) Responding to inquiries from industry, 3) A liaison between academia and industrial research activities, 4) Creation of complementary opportunities for science and technology progress. AIR Office will make proposals for new business opportunity between academia and industry. New venture business activities and novel industrial products are the vision of AIR Office.

Achievements

Liaison between academia and industrial research activities and Responding to inquiries from industry

- 1) SANKEN Techno Salon: Quarterly seminar and get-together (July1, 2008, Aug.29, 2008, Oct.30, 2008 and Jan.28, 2009)
- 2) WEB site
- 3) WEB promotion through outsourcing
- 4) Patent Publicity: SANKEN Techno Salon (July1, 2008 and Aug.29, 2008), International Nanotechnology Exhibition (Feb.18-20, 2009)

Supporting Technology Transfer

Study groups for the new industry generation

New Seminar for Industry Sector

“New Materials Electronics – Quest for new industry –“, Dec.19, 2008

AIR-Office Seminar

1)“Trend of advanced semiconductor design from the aspect of Electronic Design Automation”, July14, 2008.

2)“Philosophy of intellectual property strategy and management”, Oct. 23, 2008.

3)“Strategic exploitation of research evaluation”, Feb. 23, 2009.

Coordination of industry-academia collaborative research and development projects supported by public assistance system

Interactive ISIR’s Laboratory Tour

4 times (July1, 2008, Oct.30, 2008, Feb.16, 2009 and Mar.12, 2009)

A network development between ISIR and Industry

Visiting industrial entities, Exhibition of ISIR activities at various meeting, and participating to the various academic meetings and symposiums.

Public Relations Office

Director Professor: Nobuo KATO
Support Staff: Noriko MATSUMOTO

Outline

Public Relations Office was opened on February 1, 2006. We provide the right information of our Research Institute for the public effectively. The major activities of Public Relations Office are: 1) To collect any required file to generate the basic plan of the publicity, 2) To support editing and issue the Memoirs of ISIR (annual report) and publications, 3) To collect any requires document for creating and editing of official WEB of ISIR, 4) To perform Press Release except the subjects related to the section of general affairs, 5) To collect and preserve of any press release related to ISIR.

Technical Division

Head: Takeshi ISHIBASHI

Outlines

The Technical Division was established in 1982 to deal with professional duties providing better service for researchers. In the ISIR organization, the technician group is independent of the management and the research groups. The organization was the first one among similar organizations established in the national universities of Japan. The Division consists of two groups: Group of Machine and Group of Measurement, in which each group has two sections: Section of Machine/Circuit, Section of Glass in Group of Machine and Section of Measurement/Information, Section of Analysis/Data in Group of Measurement. The technicians work at various places: the Materials Analysis Center, the Workshop, the Office of Information Network, the Electronic Processing Laboratory and the Nanotechnology Center. The Division gives not only high-quality service to research groups but technical training to the researchers and students. The annual report is published to help and encourage training and activities of the members of the Division. In addition, the Division has started the safety lecture for utilizing various machines in the ISIR since 2004. The Technical Division makes every effort to promote the ISIR more important development under an independent administration system.

Administrative Office (31-March , 2009)

Director : Noboru NAKATA

Facilities Planning Office

Staff : Aya NISHIDA

General Affairs Division

Staffs : Kazutaka TSUMURA
 Masahito KAWAZOE
 Kazuhisa YAMASAKI
 Akira KAMATANI

Supporting Staffs: Keiko KOJIMA
 Yukie YAMADA
 Sachiko MITSUMORI
 Kazumi HAYASHI

Research Cooperation Division

Staffs : Katsumi UEDONO
 Shigeo KASHIWAKURA
 Hiroaki HANAOKA
 Tetsuya MORI
 Yuji SORIHASHI
 Akemi KIDA
 Satoshi YAMAGUCHI

Supporting Staffs: Misako SHIMIZU
 Mari KONISHI
 Masako OSUGI
 Tamiko SHINDE
 Hiroko YAMAUCHI
 Misato KUBO
 Kumiko TERADA
 Mayuko TSUDA
 Ruri MAEKAWA
 Shigeo NAGAOKA