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MEMOIRS OF THE

Institute of
Scientific and
Industrial
Research

OSAKA UNIVERSITY

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Foreword

The Institute of Scientific and Industrial Research (ISIR) was started as a part of Osaka University in 1939. Since then, the Institute has developed into one of the leading research organizations for science and engineering in our country.

We aim at the creation of new industries through Inter–Nanoscience, which integrates nanomaterial, IT nanotechnology, nano-biotechnology, energy, environmental engineering and information science to the next generations. At present (Mar.2006), ISIR has 28 research departments in the Institute and 4 divisions including 16 departments in the Nanoscience and Nanotechnology Center. Nanoscience and Nanotechnology Center is one of the leading research organizations in Japan for “Nanoscience and Nanotechnology” which is key technology now and future. ISIR keeps making a progress for the development of “Honorable Science” and “Advantageous Technology”.

This publication "Memoirs of the Institute of Scientific and Industrial Research (ISIR)" is our annual publication summarizing the scientific activities of ISIR. It has witnessed the sixty-five years' history of the Institute, since it was published in 1940. We report here information such as current research programs and recent findings of each laboratory, list of publications, financial supports from granting agencies, and all other scientific activities. We hope this annual publication will be useful and stimulating for all researchers and young scientists outside as well as inside our Institute.

Tomoji Kawai

Director,

The Institute of Scientific
and Industrial Research

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, in response to the strong requests from the industrial community of the Kansai area in Japan. The original buildings were constructed in Sakai supported financially by an association of leading private enterprises in Osaka. ISIR moved to the present place in Suita Campus in 1968. For more than half a century, ISIR has been very active as a University-associated research Institute, and dedicated to the advance of basic and applied sciences, especially in the fields of electronics, computer science, metallurgy, inorganic chemistry, organic chemistry, biochemistry, and radiation science. The Institute also has been developing industrial applications of the results obtained by staff members.

In April 1995, ISIR was reorganized in order to respond effectively to the highly developed science and technology in this country. It has modified its structure to expand basic original research, and to promote interdisciplinary programs based on the three major fields: material sciences, information sciences, and biological sciences. A new building was constructed in 2001 and in 2003 in response to the increased number of scientists and the development of Nanotechnology, respectively. At present, ISIR has 28 research departments in the Institute and 4 divisions including 16 departments in the Nanoscience and Nanotechnology Center. The Nanotechnology and Nanoscience Center has started in April 2002. In April 2005, Materials Science and Technology Research Center for Industrial Creation has started in order to promote technology transfer from ISIR to the industry. At the same time, ISIR has established AIR-office (Academia Industry Relations Office) to make the most of our fruits of research for industries.

The number of staff scientists is 127 in total, including full professors, associate professors, and assistant professors. Ages and Alma Maters of professors and research staff are shown below. In almost all the large national universities in this country, most of the faculties are graduates of their own university. However, more than half of the staff scientists in ISIR were graduated from other universities. This is a characteristic of ISIR, and contributes to promoting scientific activities of the Institute.

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
 Structure Ceramic Materials
 Advanced-Energy Materials

Organic Molecular Science

Regulatory Bioorganic Chemistry
 Organic Fine Chemicals
 Organic Molecular Materials
 Molecular Excitation Chemistry
 Synthetic Organic Chemistry
 Analytical Molecular 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

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****Nanotechnology Process Foundry****Materials Analysis Center****Materials Science & Technology Materials Research Project**

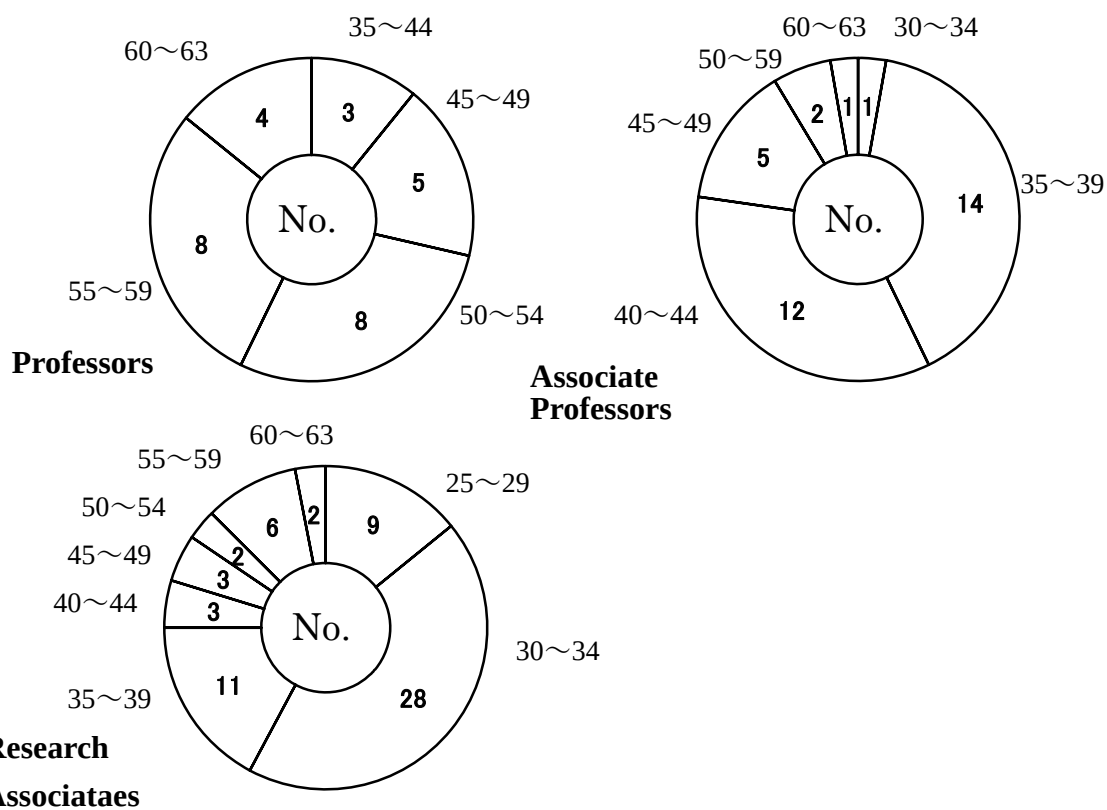
Research Center for Industrial Creation Hard Materials Research Group
Soft Materials Research Group

Human Interface Research for Safety and Security Project

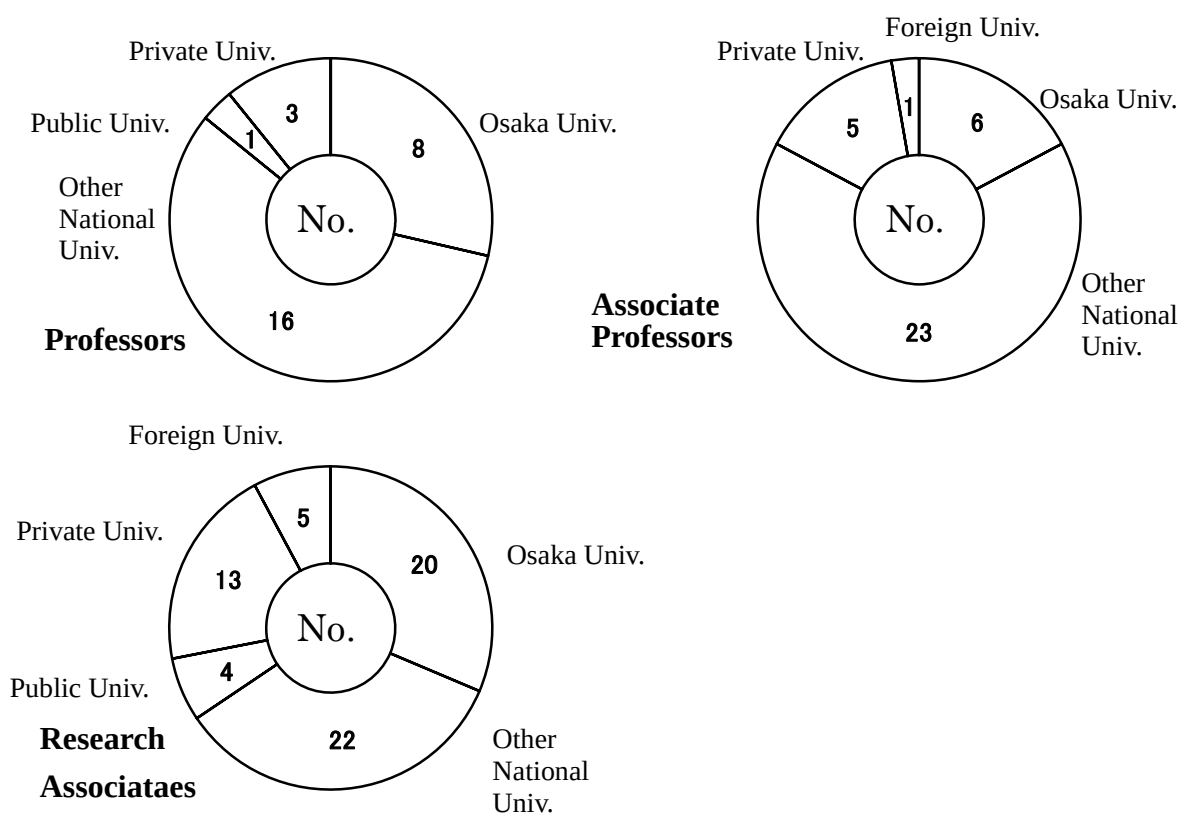
Medical Sciences Research Group
Human Interface Research Group

Service Facilities**Workshop****Office of Information Network****Laboratory for Radio-Isotope Experiments****Library****Academia Industry Relations Office****Public Relations Office**

Staffs' Age (years old) –As of 3.30.2006



Staffs' Alma Mater –As of 3.30.2006



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 cannot be in the position for more than four years. The Director as of March 31, 2006 is Professor Tomoji Kawai.

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 shown in the next page.

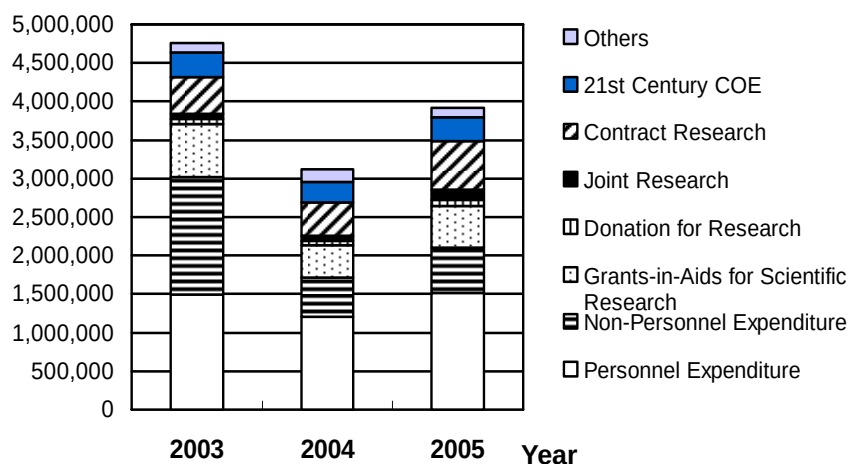
In 2002, the following project has been selected as a 21st Century Center of Excellence (COE) program from the Ministry of Education, Culture, Sports, Science and Technology.

Field: Interdisciplinary, Multi and New Fields

Program Title: Towards Creating New Industries Based on Inter-Nanoscience

Program Leader: Professor Tomoji Kawai (Division of Advanced Materials Science and Technology, ISIR)

Budget (Unit:Kilo yen)



Grants-in Aid for Scientific Research of Ministry of Education, Culture, Sports, Science and Technology are delivered to researchers and the total budget in 2005 is 550,601,000 yen.

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
2003	1,500 (2)	24,300 (20)	10,250 (13)	6,480 (5)
2004	1,111 (2)	30,811 (23)	3,950 (7)	4,352 (8)
2005	2,200 (3)	12,440 (16)	10,830 (14)	13,930 (10)

Division Year	Biological Science	Quantum Beam Science and Technology	Nanoscience and Nanotechnology center	Others	Total
2003	8,350 (9)	2,000 (3)	11,050 (14)	1,000 (1)	64,930 (67)
2004	3,833 (5)	1,111 (2)	9,010 (12)	1,480 (18)	55,658 (77)
2005	1,833 (3)	0 (0)	25,690 (18)	1,950 (6)	68,873 (70)

4) Cooperative Research

Cooperative Researches and Contract Researches in the fiscal year 2005-2006 are as follows: Cooperative Researches are carried out with 44 organizations. The budget for the fiscal year 2005-2006 is 131,709,000 yen. Contract Researches are 56. The budget for the fiscal year 2005-2006 is 631,971,000 yen.

5) International Research Projects

Tomoji Kawai (Director of the operating organization)	Core University Program (CUP) between Japan and Korea (Joint Research Projects under the Bilateral Programs between JSPS and KOSEF).
Tohru Sekino (Coordinator)	"New Processing and Nanostructure/Property Relationship for Multi-functional Ceramic Materials" (in the field of Ceramic Materials Technology) Hanyang University (Counter Core University in Korean Side)
Hiroshi Katayama-Yoshida	JSPS Core-to-Core Program-Integrated Action Initiative- "Computational Nano-Materials Design"
Riichiro Mizoguchi	Japan Partnering Award (The Biotechnology and Biological Sciences Research Council in Britain) "Advanced Scientific Discovery Tools for Bioinformatics"

6) Symposia, Seminars, Workshops and Lectures

International Seminar on Core University Program between Japan and Korea (CUP Seminar) was held on February 3 - 5 (Nagaoka, Niigata) in conjunction with the Joint 21st Century COE Symposium between Nagaoka University of Technology and ISIR, Osaka University. Among the whole presented papers, 75 oral and posters were presented for the CUP seminar including 8 invited lecturers from Finland, Slovakia, New Zealand, Taiwan and China.

The 23rd International Conference on Defects in Semiconductors (ICDS-23)
(Jul 24-29, 2005)

The third international school and conference on spintronics and quantum
information technology (Spintech III) (Aug 1 -5, 2005)

International Symposium on Biological Membrane Transport 2005 (Aug 8-10, 2005)

The workshop on membrane export proteins (No. 1/ '05-'06) (Oct 14 2005)

The First SANKEN-Chungnam National University Joint Symposium on Advanced Materials Science(Nov.1-2,2005)

Towards Creating New Industries Based on Inter-Nanoscience (Nov 18-19 2005)

A 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. In 2005, the symposium was held on November 29. The topics were “Interdisciplinall Advanced Researches for Creating Knowledges”.

The workshop on membrane export proteins (No. 2/ '05-'06)(Jan 27 2006)

The 4th International Symposium on Nanoscience and Nanotechnology Center was held on Jan.30 - Feb.1st, 2006 at the Icho-kaikan, Osaka University. In this symposium, invited lectures by 44 researchers including 12 outstanding researches and ISIR as well as 60 posters were presented. The number of participants was about 250. Especially, special session of "Perspective toward Collaboration and Cooperation" was organized on the last day of the symposium to encourage the interdisciplinary collaboration.

Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams (SIS-2006) (Feb 8-9 2006)

The workshop on membrane export proteins (No.3/ '05-'06)(Mar 17 2006)

Other Lectures and Seminars

8 Apr 2005	Maurice Goeldner (Louis Pasteur Strasboug, Professor)	Photochemical Control of Protein Activities
11 Apr 2005	Micael L. Klein (University of Pennsylvania, U.S.A, Professor)	Coarse grain models for the simulation of Soft Matter and Biomaterials
25 Apr 2005	SHOONTHORNPHISAJ	Feature-Based Ensemble

	Nuanwan (Kasetsart University, Thai, Assistant Professor)	Classifiers Using Native Bayes for Web Pages Classification
16 May 2005	Shunkichi Ueno (Tokyo Institute of Technology, Researcher)	Development of Functional Oxide Materials
17 May 2005	Keiji Suzuki (Tohoku University, Prof. Emeritus)	Structural analysis of amorphous materials by neutron diffraction
20 Jul 2005	Yves Rubin (University of California, Los Angeles, USA, Professor)	The Inside and Out of Fullerene Chemistry
11 Aug 2005	Hendrik W. van Veen (Department of Pharmacology, University of Cambridge, University Senior Lecturer)	Novel insights into the mechanisms of ATP-binding cassette multidrug transporters
12 Aug 2005	Vassilis Koronakis (University of Cambridge, Professor)	Bypassing the periplasm – Mechanism and structural studies of the tripartite type I engines for drug efflux and protein export
12 Aug 2005	Robert H. Edwards (Department of Neurology and Physiology, UCSF and the Department of Neurology, Columbia University, Professor)	The dendritic release of neurotransmitter
19 Aug 2005	Chien –Tien Chen (National Taiwan Normal University, Professor)	New Dimensions of Vanadyl and Oxometallic Complex in Catalysis and Catalytic Site-selective DNA Photocleaveages
26 Aug 2005	Chien –Tien Chen (National Taiwan Normal University, Professor)	Dibenzosubereone and Aza-based Templates in Catalysis, Chirochromic Optical Switches, and OLED Applications
2 Sep 2005	Hideki Hayashida (N.E. Chemcat Corporation)	Investment decision under uncertainty
6 Sep 2005	Makio Uwaha (Nagoya University, Associate Professor)	Lectures on Crystal Growth
7 Sep 2005	Michael M. Haley (University of Oregon, USA, Professor)	Carbon-rich pi-Electronic Structures for Novel Applications
9 Sep 2005	Yoshinori Moriyama (Okayama University, Professor)	A novel type transporter of mammalian
20 Sep 2005	Michael M. Haley (University of Oregon, USA, Professor)	Carbon-rich pi-Electronic Structures for Novel Applications

26 Sep 2005	Makio Uwaha (Nagoya University, Associate Professor)	Lectures on Crystal Growth
26 Sep 2005	Jens K. Nørskov (Technical University of Denmark, Professor)	Heterogeneous catalysis from first principles
28 Sep 2005	Makio Uwaha (Nagoya University, Associate Professor)	Lectures on Crystal Growth
29 Sep 2005	Michael M. Haley (University of Oregon, USA, Professor)	Chemistry of Metallabenzenes and Valence Isomers: New Ligands, New Metals, New Insights
10 Nov 2005	Michiel Sprik (University of Cambridge, Professor)	DENSITY FUNCTIONAL SIMULATION OF REDOX REACTIONS IN SOLUTION
11 Nov 2005	Michiel Sprik (University of Cambridge, Professor)	DENSITY FUNCTIONAL COMPUTATION OF ELECTRONIC ABSORPTION SPECTRA IN SOLUTION
14 Nov 2005	Byeang Hyeon Kim (POSTEC, Korea, Professor)	Chemical Modification of Nucleic Acid
14 Nov 2005	Hiroshi Hiratsuka (Gunma University, Professor)	Dynamics of Organic Silicon Compounds in the Excited State
14 Nov 2005	Minoru Yamaji (Gunma University, Professor)	Beam-induced Bond Dissociation Reactions
15 Nov 2005	Cornelia Bohne (University of Victoria, Canada, Professor)	Photochemistry using Supramolecular Systems
16 Nov 2005	Werner Nau (International University Bremen, Germany, Professor)	Flexibility of Biomolecules by Fluorescence and Advancing New Screening Technologies
21 Nov 2005	Nathan Newman (Arizona State University, USA, Professor)	Development of ferromagnetic III-N semiconductor materials for spintronic applications
30 Nov 2005	John A. Robinson (Institute Organic Chemistry, University of Zurich, Professor)	Protein Epitope Mimetics in Inhibitor Design
6 Dec 2005	Hong-bin Zha (Center for Information Science, Peking University, China, Professor)	3D modeling and face animation
14 Dec 2005	Ung Chan Yoon (Department of Chemistry, Pusan National University, Professor)	SET-Promoted Photocyclization Reactions of Silicon Substituted Polydonor-Phthalimides
19 Dec 2005	Ferdi Aryasetiawan (National Institute of Advanced)	Beyond the Local Density Approximation: The GW method I

	Industrial Science and Technology, Research Institute for Computational Sciences, Senior Researcher)	Beyond the Local Density Approximation: The GW method II
20 Dec 2005	Ferdi Aryasetiawan (National Institute of Advanced Industrial Science and Technology, Research Institute for Computational Sciences, Senior Researcher)	Merging first-principles and model approaches Determining Hubbard U from first-principles
2 Feb 2006	Jochen Blumberger (University of Pennsylvania, Researcher)	Computation of redox properties of transition metal ions in aqueous solution and proteins using ab initio MD
6 Feb 2006	Hak-Min Kim (Korean Institute of Machinery & Materials, Director)	R&D Activities of KIMM (Korean Institute of Machinery & Materials)
6 Feb 2006	Bo-Young Hur (Korea, Gyeongsang National University, Professor)	Recent Development of Foamed Metals
8 Feb 2006	Young Do Kim (Hanyang University, Korea, Professor)	Fabrication and Consolidation Behavior of W-Cu Nanocomposite Power
9 Feb 2006	Miguel Angel Miranda Alonso (Instituto de Tecnologia Quimica UPV-CSIC, Universidad Politecnica de Valencia, Prof)	Cycloreversion of oxetane radical ions
10 Feb 2006	Peter Sturm (INRIA Rhone-Alpes)	Generic Models and Algorithms for Omnidirectional Vision
24 Feb 2006	B.S. Murty (Indian Institute of Technology, Profesor)	Nanocomposites by Non-equilibrium Processing
13 Mar 2006	Silvia Picozzi (University L'Aquila, Research Associate)	Towards Si-based spintronics: a first-principles overview on Mn-doped group IV semiconductors
13 Mar 2006	Hannes Jonsson (University of Iceland, Professor)	Prediction of material properties using DFT calculations: Some successes and failures - as well as improvements with a self-interaction correction
13 Mar 2006	Junji Endoh (FK Optics Laboratory, Ltd., Senior Research Scientist)	Principal and application of holography
20 Mar 2006	Peter Henderson (University of Leeds, Professor)	The molecular mechanisms, structure and regulation of membrane transport proteins in

7) Public Information Activity

Public information activity of ISIR in 2005 is as follows:

- Bulletin of ISIR (2005 (in both Japanese and English)
- Memoirs of the Institute of Scientific and Industrial Research, Osaka University (Vol.62 2005 (in English)
- Annual Report of ISIR (2005 (in Japanese)
- SANKEN News Letters, 25-27(in Japanese)
- Report on SANKEN TECHNO SALON (2005 (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 2005 is 523. The details are described in the part of activity of divisions and facilities.

9) Scientific Awards

H. Goto	Best Poster Prize (International Symposium on Surface Science and Nanotechnology)
Y. Hirotsu	Tanigawa-Harris Award (The Japan Institute of Metals)
M. Ishimaru	Young Scientist Award (The Japanese Society of Microscopy)
A. Hirata	Young Scientist Award (The Japan Institute of Metals)
Kawai Laboratory	TEPIA Excellent Best Video Award (The Machine Industry Memorial Foundation)
Kawai Laboratory	Ministry of Economy, Trade and Industry Prize (Japan Industrial Film Council and Mainichi Daily News)
H. Motoda	Encouragement Award (Japanese Society for Artificial Intelligence)
T. Washio	Encouragement Award (Japanese Society for Artificial Intelligence)
K. Nakatani	Japan IBM Award (IBM Japan)
Y. Ie	Research Planning Award (The Society of Synthetic Organic Chemistry, Japan)
R. Mizoguchi	The Okawa Publications Prize (The Okawa foundation)

R. Mizoguchi	Encouragement Award (Japanese Society for Artificial Intelligence)
Y. Kitamura	JSAI Annual Conference Award (The Japanese Society for Artificial Intelligence)
K. Tanizawa	Japan Bio-venture Grand Prize (Fuji Sankei Business i)
S. Kuroda	Japan Bio-venture Grand Prize (Fuji Sankei Business i)
S. Kuroda	The San-Gaku Kan Award in Chugoku Area 2005 (Category University-originated Venture Company)(Chugoku Bureau Economy, Trade and Industry(METI), Japan)
K. Nishino	Young Scientist Award (<i>Science/</i> AAAS and GE Healthcare)
H. Hirakawa	Student Travel Grant Award (105th American Society for Microbiology General Meeting)
M. Inoue	ICEP Awards Outstanding Paper of the 2004 Conference (Japan Institute of Electronics Packaging)

2. Education

ISIR accepts graduate students (about 200) 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, 2006 is as follows.

G.S. Course	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Course	37	54	17	8	14	5	135
Doctor Course	23	36	7	4	8	0	78
Total	60	90	24	12	22	5	213

Number of students who had obtained Master's or Doctor's Degree in 2005 is as follows.

Field \ Degree	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Degree	15	31	4	5	7	0	62
Doctor Degree	8	11	0	2	2	0	23
Total	23	42	4	7	9	0	85

3. International Exchange

1) Exchange Agreement

Academic Exchange Agreements are now concluded with the following 13 organizations.

- Faculty of Natural Science, Otto-Von-Guericke University, Magdeburg (Germany)
- University of Maryland at COLLEGE PARK (U.S.A.)
- Basic Science Research Institute, Pukyong National University (Korea)
- Research Center Juelich (Germany)
- University College London (U.K.)
- Hanyang University (Korea)
- College of Engineering, Gyeongsang National University (Korea)
- College of Natural Sciences, Pusan National University (Korea)
- College of Natural Science, Chungnam National University (Korea)
- College of Science, National Taiwan University (Taiwan)
- Pacific Northwest National Laboratory (U.S.A.)
- French National Center for Scientific Research (France)
- Rwth Aachen University(Germany)

2) Foreign Researchers and Students

Number of foreign researchers and students staying in ISIR as of March 31, 2006 is 64 in total. Details are: Associate Professors (1), Research Associates (6), Visiting Researchers (1), Part-time Employee (29), Research Students (6), Graduate Students (Doctor Course) (15), (Master Course) (6). Their nationalities are : Korea (21), China (13), India (11), Viet Nam (6), Egypt (2), Mongolia(2), Bangladesh (2), Romania(1), U.K(1), Taiwan (1), Iceland(1), Thailand (1), Philippines (1), Morocco(1) Foreign visitors in 2005 are as follows:

U.S.A. (27), Korea (10), Germany (5), Portugal (3), France(2), Poland (2), Singapore (2), Canada (1), Netherlands (1), Australia (1), China(1), Mongolia(1) Total (56).

3) International Conferences and Symposiums

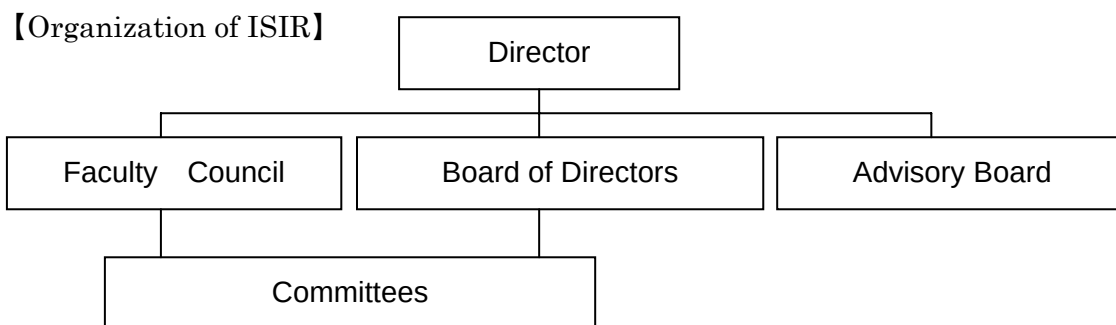
Number of presentations (plenary, invited, oral and poster in various international conferences and symposia) by staff of ISIR is 959 in total.

Number of ISIR staffs who have been working as committee members of International Conferences or Editorial Board of international academic journals are 208 in total. For more details, see the part of activity of divisions and facilities.

4. Concluding Remarks

(1) Organization and Management System

As time passes, our organization had been reshaping. At present (March.2006), ISIR has 28 departments in the Institute and 4 divisions including 16 departments in the Nanoscience and Nanotechnology Center. In the Institute, brilliant staff together from wide-range fields, these professors, associate professors and research associates do research and have scientific communication among scientists. By the 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.



(2) Budget and Facilities

Necessary facilities and equipments for researches have been installed to a considerable level. A new building was constructed in 2001 and in 2003 to the increased number of scientists and the development of Nanotechnology, respectively. Nanoscience and Nanotechnology Center started in April 2002. However reconstruction of an old first research building is necessary for the next advance and development of the Institute. Sufficient research budget has been obtained for the

Institute compared with other research institutes.

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. The COE budget has been one of the important resources for the Institute for exploiting new and interdisciplinary research through basic science and technology.

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 to release effective.

(3) Graduate and Undergraduate Education

The Institute has about 200 graduate students and undergraduate students coming from various departments such as Science and Engineering, and also researchers for special training with “Nano Science”. Considering the situation of Osaka University and objective of ISIR, we should support the undergraduate education to some extent.

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 who don't have only highly skill and knowledge but also pregnant humanity.

(4) Contribution to Societies

Presentation of scientific meetings and publications of research achievements by the Institute members have been highly evaluated. Joint research and development with industry has been made through the efforts of individual professors and through *Sanken Techno Salon* started in 1998. Mutual understanding between the Institute and industries is obtained to considerable extents by the *Salon*. Through workshops, we will be able to transfer our industrial seeds for new technology and exchange ideas for new materials.

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

(5) International Exchange

In the 21st century as information technology develops at a tremendous speed, globalization is also advancing. At present (March, 2006), 64 foreign researchers and

students join in the Institute. Our Institute consider International Exchange is one of indispensable element we are trying to open the door widely to invite more researchers and students from other countries. 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.

(6) Future Plan and Prospect

In 1998, Future Planning Committee was established in the Institute. Future plan of the Institute has been discussed in this Committee and summarized in annual report which can be seen in the Home Page of ISIR (<http://www.sanken.osaka-u.ac.jp/>). Since April 2004, by the change of their structure to National University Agencies, all the committee systems have been reconstructed to promote research and education activities. Aiming to stay effective and relevant Institute for industries, we widely announce and release our results be the members of the Institute towards all over the world. 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

- Thermodynamic study of atomic steps and nanostructures on crystal surfaces
- Molecular fluorescence of organic films by STM-induced luminescence spectroscopy
- Crystal growth, characterization and device application of new semiconductors including Tl-III-V, III-V nitrides, magnetic III-V semiconductors and quantum nanostructures
- Control of the physical properties of carbon nanotubes and the application of bio sensors
- 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 interface for organic-molecular electronics and materials design from the first principles

Department of Quantum Molecular Devices

Professor:	Hiroshi IWASAKI
Associate Professor:	Koichi SUDOH
Research Associates:	Toshiyuki ADACHI, Hongwen LIU
Post Doctoral Fellow:	Shanmugam KUMARAN
Graduate Students:	Hitoshi KURIBAYASHI, Hiroomi GOTO, Koji MIYAZATO, Yuki MORIKAGE, Noritsune ANAN
Under Graduate Students:	Nobuyasu HORI, Mahito YAMAMOTO
Support Staff:	Fumi TOGAI

Outlines

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 atomic steps on crystal surfaces with UHV- scanning tunneling microscopy (STM), behaviors of surface/interface structures under non-equilibrium conditions such as crystal growth and phase separation, crystal growth and applications of biomolecules by atomic force microscopy (AFM), physical modeling and simulation of mesoscale structures and luminescent organic films by STM-induced luminescence spectroscopy.

Current Research Programs

Relaxation of Two-Dimensional Structures on SrTiO₃(001) Surfaces

Relaxation kinetics of two-dimensional structures on SrTiO₃(001) surfaces have been studied, using ultrahigh vacuum STM. Real-time STM observation of thermal relaxation of unit-cell deep holes and Gaussian shaped steps, which are fabricated by STM nanofabrication, has been performed. By analyzing the observations, the rate limiting process is determined to be terrace diffusion of ad molecules.

Study on Growth Mechanism of Protein Crystals

Investigations to obtain physical understanding on relationship between growth conditions and growth morphology of protein crystals were performed. For needle-shaped orthorhombic “form I” lysozyme crystals, the growth mechanism was studied by AFM. Moreover, evolution of an apex composed of four {101} planes of tetragonal lysozyme crystals was studied by AFM.

Step Dynamics in Relaxation of Micro-Structures on Crystalline Surfaces

Thermal relaxation of micro structures fabricated on Si substrates has been studied. By AFM observation of the sidewalls of deep trenches during relaxation, the dynamic behavior of atomic steps involved in rounding of sharp corners was revealed. Analysis based on a one-dimensional step flow model, it has been found that the observed step

behavior occurs when the mass transport on each terrace obeys a local mass conservation law.

Patterning of Biomolecules on Si by AFM Anodic Oxidation

Processes for micro-patterning of protein and DNA molecules on Si were developed based on the anodic oxidation technique of the Si surface by an AFM probe.

Study of Luminescent Organic Films by STM-induced Luminescence

The molecular luminescence of porphyrin films on a nanometer region has been studied. The spectra excited by tunneling electron injected from STM shows peaks which are nearly identical to photo luminescence peaks. It was found that the molecular fluorescence was strongly enhanced by the local plasmon excited by STM for noble metal substrates.

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H. Iwasaki, 8th International Conference on Atomically Controlled Surfaces, Interfaces, and Nanostructures, Stockholm, Sweden, Jun. 19-23, 2005.

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Morphology of Submonolayer CaF₂ Films on Vicinal Si(111) Surfaces (Poster), *K. Miyazato, K. Sudoh, and H. Iwasaki, International Symposium on Surface Science and Nanotechnology, Saitama, Japan, Nov. 14-17, 2005.

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Observation of Si (100) Surface Annealed in Hydrogen Gas Ambient by Scanning Tunneling Microscopy (Poster), *H. Kuribayashi, K. Sudoh, H. Iwasaki, M. Gotoh, R. Hiruta and R. Shimizu, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium (ISCOE-2005), Shiga, 9 - 10 March 2005.

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Fluorescence of Porphyrin Thin Films on Conductive Substrates by STL, H. W. Liu, R. Nishitani, T. Yoshinobu, K. Sudoh, H. Iwasaki, Y. Ie and Y. Aso, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques

(STM'05), Sapporo, July 3-8, 2005.

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Surface plasmon - Enhanced Molecular Fluorescence by STM (invited), H. W. Liu, Chinese Physical Society 2005 Fall (CPS2005), 18-20 September 2005, Wuhan, China

Publications in Domestic Meetings

The Japan Society of Applied Physics	2 papers
The Physical Society of Japan	5 papers
The Surface Science Society of Japan	1 paper

Academic Degrees

Master Degree of Engineering

Hiroomi GOTO	Thermal Relaxation of Two-Dimensional Structures on SrTiO ₃ (001)
Koji MIYAZATO	Growth of CaF ₂ Thin Films on Si(111)
Yuki MORIKAGE	Study on Structures and Nucleation of Si Nanocrystals in Amorphous SiO ₂

Bachelor Degree of Engineering

Nobuyasu HORI	Temperature Dependence of Surface Structures of Lysozyme Crystals
Mahito YAMAMOTO	Study on Si(111) Surfaces Covered by CaF ₂ and Au Films

Sponsorship

Grant-in-Aid for Young Scientists (B) (2)

K. SUDOH	Study on Macro-scale Shape Transformation of Three-Dimensional Crystalline Structures via Atomic Step Motion	¥2,100,000
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Other Research Fund

H. IWASAKI	Foundation for Biomedical Research and Innovation	¥5,000,000
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2,3-D Display of Cells and Its Application to Next Generation Analysis System

Department of Photonic and Electronic Materials

Professor: Hajime ASAH
Associate Professor: Shigehiko HASEGAWA
Research Associate: Shuichi EMURA
Post Doctoral Fellow: Shanthi SUBASHCHANDRAN
Research Technical Expert: Daivasigamani KRISHNAMURTHY
Graduate Students: Atsushi FUJIWARA, Moo-Seong KIM, Sung-Woo CHOI,
Shigeya KIMURA, Kanae UCHIDA, Satoru KOBAYASHI,
Shunsuke MATSUNO, Takeshi MATSUMOTO,
Atsushi YABUUCHI, Masatoshi TERAYAMA,
Masayuki HUNAKOSHI, Yoshiaki YAMAUCHI
Support Staffs: Noriko KIKUMOTO, Akiko WATANABE

Outlines

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 Programs

1. Crystal Growth and Properties of Diluted Magnetic Semiconductors

Diluted magnetic semiconductors, which have two characters of semiconductors and magnetic materials, are gathering 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 the room temperature ferromagnetism together with sharp PL emission for the rare-earth doped GaN, GaGdN and GaEuN. By the EXAFS measurement, we confirmed that the Cr, Gd and Eu atoms occupy the Ga site. Great advances in 2005 are the fabrication of the GaCrN/GaN/GaCrN trilayer structure tunnel diodes and the observation of tunnel magnetoresistance effect at 77 K as well as the successful growth of cubic phase GaCrN with room temperature ferromagnetism.

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

In 1995, we proposed new semiconductors TlInGaAs in which the bandgap energy is independent of temperature. We have succeeded in the growth of TlInGaAs by MBE and already realized the pulsed-current injection laser operation in TlInGaAs/InP DH laser diodes (LDs) at room temperature and confirmed the small temperature variation of lasing peak wavelength as small as 0.06 nm/K. We also confirmed the small temperature variation of the refractive index of TlInGaAs. We also proposed the TlInGaAsN/AlGaAs for both temperature-stable wavelength and threshold current LDs. In 2005, we have fabricated the TlInGaAs/InGaP/GaAs LDs and obtained room temperature laser operation. We also fabricated the TlInGaAs/TlInP/InP SCH LDs and obtained the reduction of threshold current and the small temperature variation of lasing peak wavelength in the wider temperature range.

3. 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 characteristics of electrons from GaN/metal samples, which is promising to fabricate the field emission 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 electron emission. In 2005, we have grown GaN/AlN superlattices on Si substrate to investigate the nano-rod formation process and made clear the appropriate GaN thickness to obtain the best electric field emission characteristics.

4. Nano-Observation and Characterization of Short-Channel MOSFET

The nano-structural and physical properties of the short-channel MOSFETs are studying with STM from various viewpoints. In 2005, we have conducted the STM observation on the cross section surfaces along the MOSFET channel width direction for the cross sectional cut samples and succeeded in the nano-scale characterization of the source/drain structures as well as the fluctuation of the gate side surface structures along the channel direction.

5. XAFS Characterization of New Functional Materials

XAFS is 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. Using this technique, we have characterized the atomic arrangements/coordination in new functional materials, GaCrN and GaGdN, and showed that the Cr (Gd) atoms substitutionally occupy group III sites. We also found the possibility of the occurrence of Jahn-Teller deformation around Cr atoms in GaCrN.

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XAFS Study on Site Occupation of Cobalt and Iron in Z-type ferrite, Ba₃C0₂-xFe₂₄+xO₄₁, Takashi Nakagawa, Masato Yuya, Takeshi Tachibana, Yukio Takada, Hiroaki Nitani, Shuichi Emura and Takao A. Yamamoto, J. Magn. Mater. 288 (2005) 366 – 373.

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Temperature-independent bandgap semiconductors, H. Asahi: in *Investigation Report on Optical Technologies Trend in 2004*, Optoelectronic Industry and Technology Development Association Technical Report (OITDA Japan, 2005) 23-27.

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S. Kimura, M. S. Kim, Y.K. Zhou, S. Emura, N. Hasuike and H. Harima, S. Hasegawa, M. Ishimaru, Y. Hirotsu and H. Asahi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Shiga, Japan, March 9-10, 2005.

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Improved light output characteristics of GaAs/InAs short-period superlattice quantum dot light emitting diodes by the insertion of InAlAs current blocking layer, *T. Shimada, J. Mori, S. Hasegawa and H. Asahi, 17th International Conference on Indium Phosphide and Related Materials, May 8-12, 2005, Glasgow, UK.

Growth and characterization of transition-metal-doped and rare-earth-doped III-Nitride based magnetic semiconductors, *H. Asahi, Y.K. Zhou, M.S. Kim, S. Emura, S. Shanthi, S. Kimura and S. Hasegawa, Wide Band Gap Ferromagnetic Semiconductor Workshop, Edinburgh, UK, May 15-19, 2005.

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Optical and magnetic properties of DyN/GaN superlattice and Dy-doped GaN, *Y. K. Zhou, S. W. Choi, M. S. Kim, S. Kimura, S. Kobayashi, S. Shanthi, S. Emura, S. Hasegawa and H. Asahi, The third international school and conference on spintronics and quantum information technology (Spintech III), August 1-5, 2005, Awaji, Japan.

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Crystal and electronic structures of the $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ -based materials, *H. Kobayashi, Y. Arachi, S. Emura, K. Tatsumi and T. Kamiyama, 15th International conference on Solid State Ionics, Baden-Baden, Germany, July 17 – 22, 2005

Structural analysis on high density H (D) absorbed nano-size Pd for hydrogen storage materials, *Y. Arachi, S. Huichimura, A. Omura, M. Nunogaki, T. Asai, S. Yamaura, A. Inoue and Y. Arata, 15th International conference on Solid State Ionics, Baden-Baden, Germany, July 17 – 22, 2005.

Li de-intercalation behavior of $\text{Li}_{1-y}\text{Ni}_{0.5}\text{Mn}_{0.5}\text{O}_2$ cathode material for Lithium-ion batteries, *Y. Arachi, H. Kobayashi, S. Emura, Y. Nakata and T. Asai, 10th European Conference on Solid State Chemistry, Sheffield, UK, August 29 – September 1, 2005

Hydrogen absorbing process in nano-composite Pd/ZrO₂ for hydrogen storage materials. *Yoshinori Arachi, Shuichi Emura, Akira Omura, Masanobu Nunogaki, T. Asai, Shinichi Yamaura, Akihisa Inoue, Yoshiaki Arata, MC7: Functional Materials for the 21st Century, Edinburgh, UK, July 5-8, 2005

Contributions to International Conferences and Journals

- | | |
|----------|---|
| H. Asahi | 14th International Conference on Molecular Beam Epitaxy
(Organizing Committee Vice-Chair, Program Committee Chair) |
| H. Asahi | 17th International Conference on Indium Phosphide and Related Materials
(International Steering Committee member, Program Committee member) |
| H. Asahi | The Third International School and Conference on Spintronics and Quantum
Information Technology (Spintech III) (Organizing Committee member) |
| H. Asahi | 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy
and Related Techniques (Publication Committee member) |
| H. Asahi | 2005 International Conference on Solid State Devices and Materials
(Program Committee member) |
| H. Asahi | 15th International Conference on Ternary and Multinary Compounds
(Program Committee member) |

H. Asahi	Fourth International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" (Organizing Committee member)
H. Asahi	18th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	2006 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	Japan. J. Appl. Phys. (Editor)
H. Asahi	Journal of Crystal Growth (Editor)
H. Asahi	Current Applied Physics (Editor)
H. Asahi	J. of Materials Science: Materials in Electronics (Editor)
H. Asahi	e-Journal of Surface Science and Nanotechnology (Advisory Board)
S. Hasegawa	14th International Conference on Molecular Beam Epitaxy (Program Committee member, Treasures Committee member)
S. Hasegawa	18th International Conference on Indium Phosphide and Related Materials (Local Arrangements Committee member)

Publications in Domestic Meetings

The Japan Society of Applied Physics	18 papers
The Physical Society of Japan	1 paper
The Surface Science Society of Japan	1 paper
Electronic Materials Symposium	2 papers

Academic Degrees

Master Degree of Engineering

K. Uchida	Study on Crystal Growth of GaN Nano-Rods on Si Substrate and Electric Field Emission
S. Kobayashi	Study on Crystal Growth and Characterization of Cubic Phase Ferromagnetic Cubic Semiconductors
A. Yabuuchi	Study on Nano-Characterization of Nano-Structure Devices by Scanning Tunneling Spectroscopy

Master Degree of Science

S. Matsuno	Study on Fabrication of GaCrN Quantum Dots by RF-MBE and their Characterization
T. Matsumoto	Study on Growth and Characterization of Tl-Containing Semiconductor Heterostructures

Doctor Degree of Engineering

M.S. Kim	Study on GaN-Based Diluted Magnetic Semiconductor and Their Nano-Spintronics Device Applications
T. Nakamura	Study on 1.3 μm Wavelength Range Laser Diodes for Metro/Access Optical Communication System
K. Iizuka	Development of New Surface Cleaning Method for III-V Compound Semiconductors and Basic Study on Self-Organized Quantum Dots

Sponsorship

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

S. Hasegawa	Nano-Magnetic Characterization of Diluted Magnetic Semiconductors by Spin-Polarized Scanning Tunnel Spectroscopy	¥1,500,000
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Entrusted Research

S. Hasegawa	Construction of STM Data Analysis System	¥3,150,000
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Department of Semiconductor Electronics

Professor:	Kazuhiko MATSUMOTO
Associate Professor:	Koichi INOUE
Research Associates:	Kenzo MAEHASHI, Yasuhide OHNO
Graduate Students:	Takafumi KAMIMURA, Hirokazu OZAKI, Daisuke KAMINISHI, Kazuki NARUMI, Yasuyuki FUJIWARA, Jun OKUNO,
Under Graduate Students:	Yoshihiro ASAI, Taiji KATSURA, Kohei NISHIGUCHI
Supporting Staff:	Saori KONO

Outlines

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) 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 single electron devices using carbon nanotubes are studied at present using thermal CVD method, Raman scattering spectroscopy, scanning probe microscopy, and photoluminescence spectroscopy.

Current Research Programs

Chirality Selected Growth of Carbon Nanotubes Using a Laser CVD Method

It is important to grow CNTs with the chirality suitable for the application to quantum devices. Since the laser resonance energy of CNTs depends on the chirality, CNTs with the specific chirality could be removed from the other nanotubes by the laser irradiation with the resonant wavelength in atmosphere. Conversely, we have developed a laser CVD method in which carbon nanotubes are grown by the decomposition of alcohol vapor under specific laser irradiation, and have successfully obtained CNTs bridging two electrodes only in the local irradiated area. In this method, it may be possible to promote the growth of CNTs with the specific chirality by the resonance effect.

Raman Scattering Spectra of Oxygen Ion-Implanted Carbon Nanotubes

It is known that CNTs usually shows p-type character in atmosphere. In order to obtain n-type CNTs, oxygen ions have been implanted into CNTs at 25 eV which is near to the exchange energy of C atoms in the graphene. In resonant Raman scattering spectra of the implanted samples, the characteristic shift of the resonance energies has been observed. The band structures and optical transition energies of CNTs randomly

doped with substitutional O atoms have been calculated theoretically. The shift of resonant energies can be explained due to the change of electronic band structures in CNTs.

Ultrasensitive Detection of DNA Hybridization using Carbon Nanotube Field-Effect Transistors

DNA hybridization has sensitively been detected using carbon nanotube field effect transistors (CNTFETs) in real time. Amino modified peptide nucleic acid (PNA) oligonucleotides at 5' end were covalently immobilized onto the Au surface of the back gate. For 11-mer PNA oligonucleotide probe, full-complementary DNA with concentration as low as 6.8 fM solution could be effectively detected. Our CNTFET-based biochip is a promising candidate for the development of an integrated, high-throughput, multiplexed DNA biosensor for medical, forensic and environmental diagnostics.

Formation of Carbon Nanotube Field-Effect Transistors with Top-Gate Structures on SiN Passivation Films

CNTFETs have been fabricated with SiN passivation films formed by catalytic chemical vapor deposition (Cat-CVD). The characteristics of CNTFETs can also be controlled by substrate temperature of SiN passivation film deposition. Because the CNTFETs are completely protected by the SiN passivation films from further effects of ambient gases, we have fabricated air-stable both p- and n-type CNTFETs with top-gate structures on SiN passivation films formed by Cat-CVD.

Publications

Original Papers

Peptide Nucleic Acid-Modified Carbon Nanotube Field-Effect Transistors for Ultra-sensitive Real-Time Detection of DNA Hybridization, Kagan Kerman, Yasutaka Morita, Yuzuru Takamura, Eiichi Tamiya, Kenzo Maehashi, and Kazuhiko Matsumoto: *Nanobiotechnology* 1 (2005) 065-070.

Position-Controlled Growth of Single-Walled Carbon Nanotubes by Laser-Irradiated Chemical Vapor Deposition, Y. Fujiwara, K. Maehashi, Y. Ohno, K. Inoue and K. Matsumoto: *Jpn. J. Appl. Phys.*, 44 (2005) 1581.

Raman Scattering of Single-Walled Carbon Nanotubes Implanted with ultra-Low-Energy Oxygen Ions, Y. Ohno, K. Inoue, T. Kamimura, K. Maehashi, K. Yamamoto and K. Matsumoto: *Jpn. J. Appl. Phys.*, 44 (2005) 1615.

Air-stable n-type carbon nanotube field-effect transistors with Si₃N₄ passivation films fabricated by catalytic chemical vapor deposition, D. Kaminishi, H. Ozaki, Y. Ohno, K. Maehashi, K. Inoue, K. Matsumoto, Y. Seri, A. Masuda and H. Matsumura: *Appl. Phys. Lett.*, 86 (2005) 113115-1.

Laser Resonance Chirality Selection in Single-Walled Carbon Nanotubes, Kenzo Maehashi, Yasuhide Ohno, Koichi Inoue, and Kazuhiko Matsumoto, AIP Conference Proceedings of 27th Int. Conf. on the Physics of Semiconductors 772 (2005) 1023.

Transport Properties of Charge Carriers in Single-Walled Carbon Nanotubes by Flash-Photolysis Time-Resolved Microwave Conductivity Technique, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, Kazuhiko Matsumoto, Akinori Saeki and Seiichi Tagawa, AIP Conference Proceedings of 27th Int. Conf. on the Physics of Semiconductors 772 (2005) 1041.

Air Stable n-type Top Gate Carbon Nanotube Field Effect Transistors with Silicon Nitride Insulator Deposited by Thermal Chemical Vapor Deposition, Atsuhiko Kojima, Mitsuyasu Shimizu, Chan Kyeong Hyon, Takafumi Kamimura, Masatoshi Maeda, Kazuhiko Matsumoto, Jpn. J. Appl. Phys. 44 (2005) L328-L330.

Room temperature single hole transistors by semiconductor carbon nanotube with artificial defects near carrier depletion, Takafumi Kamimura, Masatoshi Maeda, Kazue Sakamoto, Kazuhiko Matsumoto, Jpn. J. Appl. Phys. 44, (2005) 461-464

Electrical Heating Process for p Type to n Type Conversion of Carbon Nanotube Field Effect Transistor, Takafumi Kamimura, Kazuhiko Matsumoto, Jpn. J. Appl. Phys., 44, (2005) 1603-1605

Protein Sensor Using Carbon Nanotube Field Effect Transistor, Atsuhiko Kojima, Chan Kyeong Hyon, Takafumi Kamimura, Masatoshi Maeda, Kazuhiko Matsumoto, Jpn. J. Appl. Phys. 44 (2005) 1596-1598.

Growth Control of Carbon Nanotube using Various Applied Electric Fields for Electronic Device Applications, M. Maeda, C. K. Hyon, T. Kamimura, A. Kojima, K. Sakamoto, K. Matsumoto, Jpn. J. Appl. Phys. 44, (2005) 1585-1587

Non-contact Atomic Force Microscope Electrical Manipulation of Carbon Nanotubes and Its Application to Room Temperature Operating Single Electron Transistor Fabrication, Chan Kyeong Hyon, Atsuhiko Kojima, Takafumi Kamimura, Masatoshi Maeda and Kazuhiko Matsumoto, Jpn. J. Appl. Phys., 44, (2005) 2056-2060.

Nitrogen Doping of Single-Walled Carbon Nanotube by Using Mass-Separated Low-Energy Ion Beams, Kazuhiro Yamamoto, Takafumi Kamimura and Kazuhiko Matsumoto, Jpn. J. Appl. Phys., 44, (2005) 1611-1614.

Field-Emission Characteristics from Carbon Nanotube Single Tip Grown on Si Cone Tomomi Yoshimoto, Tatsuo Iwata, Kazuhiko Matsumoto, Jpn. J. Appl. Phys., 44, (2005) 6739-6741.

n-type Doping for Single Walled Carbon Nanotube by Oxygen Ion Implantation with Ultra-low Energy Ion Beam of 25eV, Takafumi Kamimura, Kazuhiro Yamamoto, Takushi Kawai, and Kazuhiko Matsumoto, Jpn. J. Appl. Phys., 44, (2005) 8237-8239

Patents

Production Method of Low-Dimensional Quantum Structures of a Nano-Size and Their Integrated Circuits, K.Maehashi, Y.Fujiwara, K.Inoue, K.Matsumoto, Y.Ohno: PCT/JP2005/015776

Sensor Units, Reaction-Cell Units, and Analyzing Equipments, K.Matsumoto, A.Kojima, S.Nagao, H.Kato, Y.Ifuku, H.Mitani, Y.Saito: PCT/JP2005/15983

Production Method of n-Type Transistor, n-Type Transistor Sensor, n-Type Transistor Channel, and n-Type Semiconducting Nanotube-Structures, K.Matsumoto, A.Kojima, S.Nagao: PCT/JP2006/302349

International Conferences

Aptamer-modified carbon nanotube field-effect transistors for high-sensitive detection of IgE. *Taiji Katsura, Kenzo Maehashi, Kazuhiko Matsumoto, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka Japan, Feb. 8-9, 2006.

Single-Walled Carbon Nanotubes Grown by Laser-Irradiated Chemical Vapor Deposition, *Yoshihiro Asai, Yasuyuki Fujiwara, Kenzo Maehashi, Yasuhide Ohno, Koichi Inoue, Kazuhiko Matsumoto, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka Japan, Feb. 8-9, 2006.

Electrochemical detection of biomolecules with electrodes modified by single-walled carbon nanotubes, *Jun Okuno, Kenzo Maehashi, Kazuhiko Matsumoto¹, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka Japan, Feb. 8-9, 2006.

Formation and Electrical Characteristics of Carbon Nanotube Field-Effect Transistors with SiN Passivation Films, *Kohei Nishiguchi, Kenzo Maehashi, Daisuke Kaminishi, Yasuhide Ohno, Koichi Inoue, Kazuhiko Matsumoto, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka Japan, Feb. 8-9, 2006.

High-Sensitive Label-Free Biosensors Based on Single-Walled Carbon Nanotubes (invited), *Kenzo Maehashi, and Kazuhiko Matsumoto: SPIE Int. Photonics West, San Jose, USA, Jan. 21-26, 2006.

Precise control of carbon nanotube growth by current monitoring (invited), *M.Maeda, T.Kamimura, C.Hyon, K.Murata, K.Matsumoto: SPIE Int. Photonics West, San Jose, USA, Jan. 21-26, 2006.

Electrical observation of 1D sub-band structure of carbon nanotube in Schottky barrier transistor (invited) *T.Kamimura, K.Matsumoto: SPIE Int. Photonics West, San Jose, USA, Jan. 21-26, 2006.

Island Size Control of carbon Nanotube Single Electron Transistor operating at Room Temperature by AFM Electrical Manipulation (invited) *C.Hyon, T.Kamimura, M.Maeda, K.Matsumoto: SPIE Int. Photonics West, San Jose, USA, Jan. 21-26, 2006.

Carbon Nanotube Devices and Applications (invited), Kazuhiko Matsumoto, International COE Workshop on Nano Processes and Devices, and Their Applications, Nagoya-University, Japan, Dec. 15, 2005.

Magnetoresistance in single-walled carbon nanotubes with different ferromagnetic electrodes; *Yasuhide Ohno, Kazuki Narumi, Kenzo Maehashi, Koichi Inoue, and Kazuhiko Matsumoto, Second Joint International Conference on New Phenomena in Mesoscopic Systems and Surfaces and Interfaces of Mesoscopic Devices, Hawaii, USA, Nov. 27-Dec. 2, 2005.

Carbon Nanotube Nanodevices Fabricated by Ion Beam Lithography, *Hirokazu Ozaki, Kenzo Maehashi, Yasuhide Ohno, Koichi Inoue, Kazuhiko Matsumoto, Shu Seki and Seiichi Tagawa: 4th 21st Century COE; Towards Creating New Industries Based on Inter-Nanoscience, International Symposium, Shiga, Japan, Nov. 18-19, 2005.

Magnetoresistance in Ferromagnetically Contacted Single-Walled Carbon Nanotubes. *Kazuki Narumi, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, and Kazuhiko Matsumoto: 4th 21st Century COE; Towards Creating New Industries Based on Inter-Nanoscience; International Symposium, Shiga, Japan, Nov. 18-19, 2005.

Carbon nanotube field-effect transistors for ultrasensitive real-time detection of DNA hybridization. *Kenzo Maehashi The 1st CNU-SANKEN Joint Symposium on Advanced Materials Science, Chungnam, Korea, Nov. 1-2, 2005.

Air-Stable p-Type and n-Type Carbon Nanotube Field-Effect Transistors with Top-Gate Structures on SiNx Passivation Films Formed by Catalytic Chemical Vapor Deposition. *Daisuke Kaminishi, Hirokazu Ozaki, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, Kazuhiko Matsumoto, Yasuhiro Seri, Atsushi Masuda, Hideki Matsumura and T. Niki 2005 International Conference on Solid State Device and Materials (SSDM2005), Kobe, Japan, Sept. 13-15, 2005.

Direct Ultrasensitive DNA Sensors Based on Carbon Nanotube Field-Effect Transistors, *Kenzo Maehashi, Kazuhiko Matsumoto, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya 2005 International Conference on Solid State Device and Materials (SSDM2005), Kobe, Japan, Sept. 13-15, 2005.

Fermi Level Modulation of n-type Doped Single Walled Carbon Nanotube using Buried Local-Gate FET Structure by Oxygen Ion Implantation with Ultra-low Energy Ion

Beam of 25eV Takafumi Kamimura, Kazuhiro Yamamoto, and Kazuhiko Matsumoto
The 2005 International Conference on Solid State Devices and Materials (SSDM), Kobe, Japan, Sept. 13-15, 2005.

Precise Control of Island Size for Carbon Nanotube Single Electron Transistor operating at Room Temperature by AFM Electrical Manipulation, C. K. Hyon, T. Kamimura, M. Maeda, K. Matsumoto, The 2005 International Conference on Solid State Devices and Materials (SSDM), Kobe, Japan, Sept. 13-15, 2005.

One by One Control of Number of Carbon Nanotube Growth by Current Monitoring, M. Maeda, T. Kamimura, C. K. Hyon, K. Murata, K. Matsumoto, The 2005 International Conference on Solid State Devices and Materials (SSDM), Kobe, Japan, Sept 13-15, 2005.

Laser-Irradiated Chemical Vapor Deposition for Position-Controlled Growth of Single-Walled Carbon Nanotubes, *Y. Fujiwara, K. Maehashi, Y. Ohno, K. Inoue and K. Matsumoto 6th International Conference on the Science and Application of Nanotubes, Gothenburg, Sweden, June 26 - July 1, 2005

Ultrasensitive Real-time DNA Sensors Based on Carbon Nanotube Field-Effect Transistors Modified by Peptide Nucleic Acid, *Kenzo Maehashi, Kazuhiko Matsumoto, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya 6th International Conference on the Science and Application of Nanotubes Gothenburg, Sweden, June 26 - July 1, 2005.

Air-Stable Carbon Nanotube Field-Effect Transistors with Top-Gate Structures on SiNx Passivation Films Formed by Catalytic Chemical Vapor Deposition, *Daisuke Kaminishi, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, Kazuhiko Matsumoto, Yasuhiro Seri, Atsushi Masuda, Hideki Matsumura and Toshikazu Niki 47th TMS 2005 Electronic Materials Conference (EMC2005), University of California, Santa Barbara, USA, June 22-24, 2005.

Staircase Characteristics of Oxygen-Free Carbon Nanotube Field Effect Transistors Desorbed by Electrical Heating, *Takafumi Kamimura, Masatoshi Maeda, Chan Kyeong Hyon and Kazuhiko Matsumoto, 47th TMS 2005 Electronic Materials Conference (EMC2005), University of California, Santa Barbara, USA, June 22-24, 2005.

Electrical Observation of One Dimensional Sub-band Structure of Carbon Nanotube in Schottky Barrier Transistors, T. Kamimura, M. Maeda, Y. Nagamune, T. Nakanishi, and K. Matsumoto, Device Research Conference (DRC) Late News University of California, Santa Barbara, USA, Jun 22-24, 2005.

Staircase Characteristics of Carbon Nanotube Field Effect Transistors Desorbed Oxygen by Electrical Heating T. Kamimura, M. Maeda, and K. Matsumoto The Electronic Materials Conference (EMC), University of California, Santa Barbara June 22-24, 2005.

Carbon Nanotube Nanodevices and Biosensors, *Kazuhiko Matsumoto, Kenzo Maehashi, Yasuhide Ohno, and Koichi Inoue, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Shiga, Japan, March 9-10, 2005.

Air-Stable n-Type Carbon Nanotube Field-Effect Transistors Formed with Si₃N₄ Passivation Films on Carbon Nanotube Channel, *Daisuke Kaminishi, Hirokazu Ozaki, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue, Kazuhiko Matsumoto, Yasuhiro Seri, Atsushi Masuda, and Hideki Matsumura, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Shiga, Japan, March 9-10, 2005.

Single-Walled Carbon Nanotubes Implanted with Ultra-Low-Energy Oxygen, *Yasuhide Ohno, Koichi Inoue, Takafumi Kamimura, Kenzo Maehashi, Kazuhiko Yamamoto and Kazuhiko Matsumoto, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Shiga, Japan, March 9-10, 2005.

Direct Ultrasensitive Electrical Detection of DNA Hybridization Using Carbon Nanotube Field-Effect Transistors, *Kenzo Maehashi, Kazuhiko Matsumoto, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Shiga, Japan, March 9-10, 2005.

Contributions to International Conference and Journals

- | | |
|--------------|--|
| K. Matsumoto | 2006 Advanced Heterostructure Workshop (co-chairperson) |
| K. Matsumoto | The 3rd International Conference on Quantum Sensing:
Evolution and Revolution from Past to Future at the SPIE
Optoelectronics (Organizing committee) |
| K. Matsumoto | 2005 International Conference on Solid State Device & Materials
(Program committee) |

Publications in Domestic Meetings

The Japan Society of Applied Physics	22 papers
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Academic Degrees

Doctor Degree of Engineering

T. Kamimura	Control of Transport Properties of Single-Walled Carbon Nanotube Field Effect Transistors
-------------	--

Master Degree of Engineering

H. Ozaki	Fabrication of Carbon Nanotube Single-Electron Devices Operating at Room Temperatures
----------	--

Master Degree of Engineering

D. Kaminishi Development of Carbon Nanotube Field Effect Transistors of High Performance

Master Degree of Engineering

K. Narumi Study on Carbon Nanotube Spin Bulbs

Master Degree of Engineering

Y. Fujiwara Formation and Characterization of Single-Walled Carbon Nanotubes by Laser-Irradiated Chemical Vapor Deposition

Other Research Fund

K.Matsumoto	Japan Science and Technology Agency	Carbon nanotube single electron electron single spin measurement systems	¥180,000,000
K.Matsumoto	New Energy & Industrial Technology Development Organization	Development of CNT High Sensitive Biosensor for Personal QOL System	¥19,000,000
K.Matsumoto	Schlumberger K.K	Carbon Nanotube Sensor	¥1,000,000

Department of Condensed Matter Physics

Professor:	Hiroshi KATAYAMA-YOSHIDA
Associate Professor:	Yoshitada MORIKAWA
Guest Professors:	Akira YANASE, Mitsuhiro MOTOKAWA
Post Doctoral Fellows:	Van An DINH, Hiroyuki NAKAYAMA, Ikutaro HAMADA, Susumu YANAGISAWA, Kyuhoo LEE, Kunihiko YAMAUCHI
Research Student:	Jon Bergmann MARONSSON
Graduate Students:	Naoki MITSUDA, Hiroki FUNASHIMA, Kazuhito MATSUKAWA, Hidetoshi KIZAKI, Masayuki TOYODA, Tetsuya FUKUSHIMA Akio OGURA, Takayuki NOGUCHI, Kousuke TAKEUCHI, Akihiro NAGOYA, Masaki HIRAMATSU, Haruhiko DEKURA, Hitoshi MINAI
Under Graduate Students:	Jun ISHISADA, Yosuke NAKANO, Kunihiko HARADA
Support Staff:	Mika ASADA

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 Programs

***Ab initio* Molecular Dynamic Simulation under the Electronic Excitation and Materials Design by Electronic Excitation**

We have developed new simulation method for the application of the electronic excitation-induced atomic migration, and applied for the materials design to use the atomic migration through the meta-stable atomic position. We have designed new fabrication process from graphite to diamond at the normal condition by using the core electron excitations. We have simulated the enhancement of the atomic diffusion of boron (B), hydrogen (H), and oxygen (O) in silicon under the electronic excitation.

Materials Design for Semiconductor Spintronics.

Based upon *ab initio* electronic structure calculation, we have proposed the materials design to control the spin interaction for II-VI and III-V compound semiconductors. We have designed the transparent half-metallic ferromagnets for GaN-, AlN-, ZnO-, ZnS-

based diluted magnetic semiconductors. We also design the p-type and n-type carrier-concentration dependence of Curie temperature (T_c) and 3d transition atom dependence of T_c in above diluted ferromagnetic semiconductors. We propose materials design of ferromagnetic diamond without any transition metal elements based on first principles calculations. The electronic structure and the magnetic properties of impurities-doped diamond are calculated by using the Korringa-Kohn-Rostoker method within the local spin density approximation with taking into account disorder using coherent potential approximation. It is found that H atoms which are doped into tetrahedral interstitial sites show finite local magnetic moments. Moreover, the impurities-doped diamond show ferromagnetism with half-metallic density of states. We have determined the magnetic ground states of non-3d transition metal impurity doped CaO, BaO and SrO. We have proposed a new class of high- T_c diluted magnetic semiconductors, which is transparent for our visible light. Based upon the deep impurity band engineering by controlling the correlation energy and impurity band width, we can stabilize the half-metallic ferromagnetism without magnetic impurities such as 3d-transition metal or rare-earth metal impurities.

We show that spinodal decomposition phase in dilute magnetic semiconductors (DMS) offers the possibility to have high Curie temperatures (T_C) even if the magnetic exchange interaction is short ranged. The spinodal decomposition is simulated by applying the Monte Carlo method to the Ising model with realistic (*ab initio*) chemical pair interactions between magnetic impurities in DMS. Curie temperatures are estimated by the random phase approximation with taking disorder into account. It is found that the spinodal decomposition phase inherently occurs in DMS due to strong attractive interactions between impurities. This phase decomposition supports magnetic network over the dimension of the crystal resulting in a high- T_C phase.

The electronic structures and the magnetic properties of dilute magnetic semiconductors (DMSs) based on transparent semiconducting oxide CuAlO_2 are calculated by using the Korringa-Kohn-Rostoker method combined with the coherent potential approximation (KKR-CPA) within the local density approximation. We see from the results that we can expect to obtain the half-metallic and high-spin ferromagnetic state is expected to be stable in Mn-, Fe-, Co- and Ni-doped CuAlO_2 .

Materials Design and Valence Control of Wide Band-gap Semiconductors.

Based upon *ab initio* electronic structure calculation, we have proposed codoping method for the fabrication of the low-resistive p-type CuAlO_2 , and n-type diamond. Our predictions of co-doping for the valence control are confirmed by the experiment. We have calculated the formation energy of P, N, and B in diamond, and oxygen-interstitial, Cu-vacancy, Al-vacancy, Be-acceptor, Mg-acceptor in CuAlO_2 . We also proposed the possibility of high efficient thermoelectric material ($ZT > 3$) and transparent superconductivity upon slightly p-type or heavily p-type doped CuAlO_2 .

Design of High- T_c Nano-superstructure for Spintronics by Spinodal Decomposition

We show that spinodal decomposition phase in dilute magnetic semiconductors (DMS) offers the possibility to have high Curie temperatures (T_C) even if the magnetic exchange interaction is short ranged. The spinodal decomposition is simulated by applying the Monte Carlo method to the Ising model with realistic (*ab initio*) chemical pair interactions between magnetic impurities in DMS. Curie temperatures are

estimated by the random phase approximation with taking disorder into account. It is found that the spinodal decomposition phase inherently occurs in DMS due to strong attractive interactions between impurities. This phase decomposition supports magnetic network over the dimension of the crystal resulting in a high-TC phase.

We show that spinodal decomposition phase in dilute magnetic semiconductors (DMS) offers the possibility to have high Curie temperatures (TC) even if the magnetic exchange interaction is short ranged. The spinodal decomposition is simulated by applying the Monte Carlo method to the Ising model with realistic (*ab initio*) chemical pair interactions between magnetic impurities in DMS. Curie temperatures are estimated by the random phase approximation with taking disorder into account. It is found that the spinodal decomposition phase inherently occurs in DMS due to strong attractive interactions between impurities. This phase decomposition supports magnetic network over the dimension of the crystal resulting in a high-TC phase.

Magnetic Anisotropy Energy of L1₀-type alloy

The electronic bandstructure and Fermi surfaces for ferromagnetic L1₀-FePd have been calculated. The resulted magnetic anisotropy energy shows good agreement with the experimental results.

Electronic Structures of Newly Reported Superconductors

Electronic band-structures have been calculated for new superconductors Y₂C₃ and KOs₂O₆. From the result, in Y₂C₃, C-p electrons should play a significant role in its superconductivity.

Design of High-efficient Thermoelectric Materials

Based upon *ab initio* electronic structure calculation, we have developed the design method for high-efficient thermoelectric materials and applied to explain the existing and available experimental data for PbTe and Bi₂Te₃ compounds. We obtained good agreement between the calculation and experiment. We have design high-efficient thermoelectric power for p-type CuAlO₂.

Materials Design for the High-efficient Silicon Solar Cells.

We have proposed a mechanism of CN diffusion and termination of defect states in Si by using *ab initio* molecular dynamics simulations. In this mechanism, CN diffuses in the Si network by changing the bond orders of CN bond between single and double bonds giving rather small diffusion barriers. This makes CN diffusion to defect sites very efficient and is important for defect states termination by CN treatment.

Pentacene and Metal Surface Interaction

The interaction between pentacene and metal surfaces has been studied by means of density-functional theoretical calculations within a generalized gradient approximation GGA. We demonstrate that the most significant factor determining the interface electronic structure is the distance between the molecule and the substrate. We showed LDA and GGA approximations give rather different results and we are now improving these approximations by introducing new energy functionals which can reproduce dispersion interaction between metal and organic molecules quite accurately.

Atomic Geometries and the Electronic Properties of Alq₃/Al Interfaces

We have studied the atomic geometries and the electronic properties of the Alq₃/Al interface by using density functional theoretical calculations. Experimentally, an interface gap state is observed and this is thought to be a result of chemical reactions at the interface. Furthermore, the large interface dipole formation of -1.4 eV was observed and this is also thought to be a result of chemical interaction. By using first-principles molecular dynamics simulations, we clarified the origin of the interface state and also the origin of the interface dipole formation. We showed that there are several meta-stable adsorption states of Alq₃ molecules on Al surfaces and these states give different interface states. Due to the co-existence of these states, the interface state appears. We also showed that the interface dipole mainly comes from the alignment of molecular permanent dipole moment. These results are quite important in designing new interface materials.

Chemical Reactions between Alq₃ and Al Atoms

In the actual production process of organic electroluminescent (EL) devices, electrode metals are deposited onto organic EL materials such as Alq₃. In order to clarify the chemical reactions at the metal-organic interfaces, we have examined the deposition process of Al onto Alq₃ by using density functional theoretical simulations. We found that the first Al interacts strongly with Alq₃ molecule while the second one interacts with Alq₃-Al complex quite weakly. We also showed that by increasing deposited Al atoms, Al clusters are formed and interface states are clarified.

First-principles molecular dynamics simulations of chemical reactions at electrode surfaces.

Fuel cells are clean and efficient energy converters and are attracting much attention recently. It is very important to replace Pt electrodes by cheap materials to reduce the costs of fuel cells. In our project, we are simulating electrode reactions at Pt surfaces in order to clarify the important factors determining the reactivity of electrode catalysis and to design new efficient electrode materials. In this year, we carried out hydrogen evolution reactions at Pt surfaces.

First-principles molecular dynamics simulations of chemical reactions at TiO₂ surfaces

TiO₂ is famous for its photo-catalytic activities and is also used as substrates of various catalysts. It is very important to clarify the reactivity of TiO₂ surfaces. In this project, we clarified Hydrogen adsorption, diffusion and desorption processes on the TiO₂(110) surfaces. Our results can well account for seemingly contradicting experimental results and give insights for catalytic reactivity of oxide surfaces.

First-principles molecular dynamics simulations of N solution into Ga-Na liquid alloys.

GaN is very important material for generating the blue laser. It is difficult to grow GaN crystal from liquid phase. Very high pressure of 15,000 atm and high temperature of 1500 degrees are necessary to dissolve N gas into liquid Ga. However, N can be dissolved into Ga-Na liquid alloys much more easily, at 20 atm and 800 degrees. It is very mysterious that pure Ga and pure Na cannot dissolve N but mixed

Ga and Na alloys can dissolve N very much. By using first-principles molecular dynamics techniques, we clarified the mechanism of N solution into Ga-Na liquid alloys. We clarified the cluster structure of N-Ga complexes in the liquid Na and the stability of N-Ga cluster can be explained from the electronic structure calculations. This new finding can be used to design new fluxes for other wide-gap semiconductor crystal growth.

Publications

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International Symposium, Osaka, Japan, Jan 30-Feb 1, 2006

Materials Design for Moltronics, *Y. Morikawa, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan 30-Feb 1, 2006

High Curie Temperature Spinodal Decomposition Phase in Dilute Magnetic Semiconductors, *K. Sato, T. Fukushima, H. Katayama-Yoshida and P. H. Dederichs (Oral), 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

Controlling of Impurity Diffusion in Silicon, *K. Shirai and H. Katayama-Yoshida, 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

High-Pressure Control of Boron Crystals, *K. Shirai, H. Dekura and H. Katayama-Yoshida, 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

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Self-interaction-corrected Calculations of Dilute Magnetic Semiconductors, *M. Toyoda, H. Akai, K. Sato and H. Katayama-Yoshida, 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

Computational Nano-materials Design for Semiconductor Nano-Spintronics and EU-Japan Research Training Network, *H. Katayama-Yoshida, 1st Symposium on Nanoscience and Nanotechnology between Sanken and CNRS, Paris, France, Feb. 12-13, 2006

First-principles Calculations of Exchange Interactions in CuAlO₂ Based Dilute Magnetic Semiconductors with Carrier Doping, *H. Kizaki, K. Sato and H. Katayama-Yoshida, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006

Spinodal Decomposition under Layer by Layer Growth Condition and High Curie Temperature Quasi-One-Dimensional Nano-structure in Dilute Magnetic Semiconductor, *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006

Contributions to International Conferences and Journals

H. Katayama-Yoshida	23 rd International Conference on Defects in Semiconductors : ICDS23 (Conference Chair)
H. Katayama-Yoshida	The third international school and conference on spintronics and quantum information technology: Spintech III (Conference Chair)
H. Katayama-Yoshida	4 th International Conference on Physics and Application of Spin-related Phenomena in Semiconductors: PASPS-VI (International Advisory Committee and Program Committee)
H. Katayama-Yoshida	International Conference on Magnetism: ICM2006 (Organizing Committee)

Publications in Domestic Meetings

The Physical Society of Japan	9papers
The Japan Society of Applied Physics	11papers

Academic Degrees

Doctor Degree of Science

H. Funashima	Thermoelectric properties study of semiconductors with First Principles Calculation
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Sponsorship

Grant-in-Aid for Scientific Research on the Priority Area

Y. Morikawa	Development and releasing of quantum simulator for ¥1,400,000 submicron scale systems
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Grant-in-Aid for Scientific Research on the Priority Area

Y. Morikawa	Development of efficient parallel quantum dynamics ¥9,400,000 simulator
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Grant-in-Aid for Scientific Research on the Priority Area (1)

Y. Morikawa	Theory of nano-scale linked molecules	¥2,900,000
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Grant-in-Aid for Creative Scientific Research (K. Seki)

Y. Morikawa	Elucidation and Control of Interfaces Related to Organic Electronic Devices
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Grant-in-Aid for Scientific Research on the Priority Area (M. Shirai)

H. Katayama-Yoshida	Design for Opto-spintronics and Spin Prove
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Grant-in-Aid for Scientific Research on the Priority Area (K. Sato)

H. Katayama-Yoshida Development and application of computational nano-materials design engine

Entrusted Research

JSPS Core-to-Core Program –Integrated Action Initiative-

H. Katayama-Yoshida Computational Nano-Materials Design ¥18,000,000

Ministry of Education, Culture, Sports, Science and Technology

Grant-in-Aid for the Creation of Innovations through Business-Academic-Public Sector Cooperation

H. Katayama-Yoshida Research on selective and low-temperature impurity diffusion in semiconductor by infra-red laser excitation ¥12,350,000

Japan Science and Technology Corporation

Y. Morikawa Core Research for Evolutional Science and Technology (Y. Asai) ¥10,000,000
Contact effects and transport properties of single molecules.

Japan Science and Technology Corporation

Y. Morikawa Core Research for Evolutional Science and Technology (T. Ikeshoji) ¥7,900,000
Electrode Chemistry at Interfaces Between Two Phases

Japan Science and Technology Corporation

H. Katayama-Yoshida Core Research for Evolutional Science and Technology (H. Kobayashi)
Silicon Thin Film Solar Cells with New Chemical Bonds

New Energy and Industrial Technology Development Organization (NEDO)

H. Katayama-Yoshida Development of Method for Nano-materials Simulation (H. Akai)

Cooperative Research

H. Katayama-Yoshida	Japan Science and Technology Corporation	Case study on advanced measurements and analysis	¥1,960,000
H. Katayama-Yoshida	Institute for Materials Research, Tohoku Univ.	Design and fabrication of transparent high-Tc spintronics materials	¥2,000,000
H. Katayama-Yoshida	SPRING8	Mechanism of New Materials Fabrication Using Electronic Excitation	
H. Katayama-Yoshida	International Institute of Advanced Study	New functionality of electronic systems	
H. Katayama-Yoshida	Jülich Institute (Germany)	Computational Materials and Devices Design for Nanospintronics	
Y. Morikawa	School of Science, the University of Tokyo	Catalytic reactions on metal oxide surfaces	
Y. Morikawa	National Institute of Advanced Industrial Science and Technology (AIST)	Simulation on Metal-Organic Interfaces and Electrochemical Reactions	
Y. Morikawa	Institute of Materials Science, Univ. of Tsukuba	Reaction processes of formate on Cu catalysis	
Y. Morikawa	The Institute for Solid State Physics, The Univ. of Tokyo	Atomic geometries, electronic properties and chemical reactions at water/transition-metal interfaces	

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, Structural Ceramic Materials 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 atomic structures and crystallization behavior in metallic glasses
- Fabrication and characterization of L1₀-type hard magnetic nanoparticles
- Atomistic structures of amorphous covalent materials
- Development of continuous casting technique for producing lotus-type porous metals
- Elucidation of vibration-damping, superelasticity and fatigue behaviors of lotus-type porous metals and intermetallic compounds
- Fabrication of nano-sized hollow sphere metals
- Construction of function harmonized superlattices, ferromagnetic oxide heterostructures with for highly sensitive spin devices for external fields
- 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
- Development of Multi-functional ceramic and polymer nanocomposites by nano- and interface control and their application.
- Synthesis, analysis and performance enhancement of novel nanotube materials.
- Creation of novel phases of solids via photoinduced phase transitions
- Photoinduced structural instability on semiconductor surfaces
- Ultra fast carrier dynamics on semiconductor surfaces

Department of Structural Characterization and Design

Professor: Yoshihiko HIROTSU
Associate Professor: Manabu ISHIMARU
Research Associates: Kazuhisa SATO, Akihiko HIRATA
Research Fellows: In-Tae BAE, Hiroshi NAGANUMA
JSPS Postdoctoral Fellow: Andras KOVACS
Research Technical Expert: Atsuo KOREEDA
Research Students: Jong Han WON, Han Woo RYU, Keisuke OMAE, Takuro MORINO, Satoru KUBOYA, Hayato HASUI
Support 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 Programs

Local atomic structures and crystallization behaviours in metallic glasses

We have examined local atomic structures and crystallization behaviours in metallic glasses by means of transmission electron microscopy. The following results were obtained this year. (1) We investigated a relationship between a crystallization process and a glass forming ability in Fe-based metallic glasses. In a high glass-former, it was found that a complex crystalline phase is directly produced from the glass matrix with a large structural change. (2) A novel nanobeam diffraction analysis was performed for various Zr-based metallic glasses. On the basis of the results, we discussed a correlation between the local atomic structures and the glass forming ability. (3) Local atomic arrangements of a Pd-based metallic glass were observed by using an aberration-corrected high-resolution electron microscope. A determination of optimum defocus conditions yielded a clear imaging of the medium range ordered regions embedded in the glass matrix.

Fabrication and Characterization of L1₀-type Hard Magnetic Nanoparticles

We have been developing a new fabrication method of thin films with oriented L1₀ hard magnetic nanoparticles. The following results were obtained in this year: (1) Disappearance of long-range atomic order in 10-nm-sized FePd nanoparticles has been studied by electron diffraction. The observed order-disorder transformation temperature of 982K for FePd nanoparticles was about 80K lower than that of the bulk alloy.

Nanobeam electron diffraction revealed the existence of short-range order in the nanoparticles even at the transformation temperature. (2) Perpendicular magnetic anisotropy as well as low temperature atomic ordering have been achieved by small amount of Cu addition into FePd nanoparticles. It was found that perpendicular magnetic anisotropy of the $L1_0$ -FePdCu nanoparticles is sensitive to the alloy composition. (3) 10-nm-sized $L1_0$ -FePtCu nanoparticles with orientation and high-density dispersion were fabricated by rf-magnetron sputtering under the lower substrate temperature as low as 563K. Substrate temperature dependence of structure and morphology of the FePtCu nanoparticles has been studied by TEM and electron diffraction. Atomic ordering was largely enhanced at the substrate temperature of 613K.

Local Structure Analysis of Amorphous Materials

We analyzed atomistic structures of functional amorphous materials by transmission electron microscopy and computer simulations. The following results were obtained. (1) Ion-beam-induced amorphous structures of SiC were examined as a function of irradiation temperatures. From radial distribution function analyses, it was found that the amount of Si-Si atomic pairs increases rapidly than that of C-C atomic pairs with the progress of chemical disordering. The difference of the formation speed between the homonuclear bonds is attributed to the significant volume swelling under radiation environments. (2) Microstructures of high-dose Fe ion implanted Si were examined by high-resolution electron microscopy and microbeam diffraction techniques. A layered structure consisting of amorphous Fe-Si and Si was obtained. It was found that the amorphous structures of Fe-Si are similar to those of crystalline Fe-Si.

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(July 3-7, 2005).

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Structure Analysis of Ion-Beam Synthesized Amorphous Fe-Si Layers using Transmission Electron Microscopy, *M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez, and K. E. Sickafus, 13th Int'l Conf. Radiation Effects in Insulators, Santa Fe, USA (Aug. 28-Sept. 2, 2005).

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Contributions to International Conferences and Journals

Y. Hirotsu	5 th International Bulk Metallic Glasses Conference (Co-Chair)
Y. Hirotsu	16 th International Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Advisory Committee)
Y. Hirotsu	The IUMRS International Conference in Asia 2006 (Session Organizer)
Y. Hirotsu	6 th Japan-Polish Joint Seminar on Materials Analysis (Organizing Committee)
Y. Hirotsu	International Conference on Magnetism 2006 (Organizing Committee)

Publications in Domestic Meetings

The Japan Institute of Metals	9 papers
The Japan Society of Applied Physics	3 papers
The Magnetic Society of Japan	1 papers
Others	10 papers

Academic Degrees

Doctor Degree of Engineering

Kazuhisa Sato	Electron structure analyses and magnetic property measurements of L1 ₀ -type ordered alloy nanoparticles
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Master Degree of Engineering

Keisuke Omae	Formation process of β -FeSi ₂ /Si heterostructure in high-dose Fe ion implanted Si
Takuro Morino	Electron diffraction analysis of local atomic structures in Zr-based metallic glasses

Sponsorship

Grant-in-Aid for Scientific Research on Priority Area (2)

Y. Hirotsu	In situ observation of atomistic structures in metallic liquid and metallic glass	¥20,300,000
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Grant-in-Aid for Scientific Research (S)

Y. Hirotsu	Fabrication and characterization of hard magnetic alloy nanoparticles produced by vapor quenching	¥22,600,000
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Grant-in-Aid for Scientific Research (C)

M. Ishimaru	Amorphous structures of phase-change recording materials and their rapid crystallization mechanisms	¥1,600,000
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Grant-in-Aid for Encouragement of Young Scientists (B)

K. Sato	Quantitative analyses of structure and magnetic properties of L1 ₀ -type FePt and FePd nanoparticles by transmission electron microscopy	¥2,900,000
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Entrusted Research

Y. Hirotsu	NEDO (Advanced Materials Technology Utilizing Glassy Metals for Commercial Uses)	Nano-structure Analysis for the Evaluation of Mechanical Properties in Glassy Metals	¥4,200,000
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Department of Metallic Materials Process

Professor:	Hideo NAKAJIMA
Associate Professor:	Shinsuke SUZUKI
Research Associates:	Masakazu TANE, Ryusuke NAKAMURA
Research Technical Expert:	Yoshitada NAKAI
Graduate Students:	Toshihiko KUJIME, Je-Sung PARK, Takuya IDE, Hirofumi ONISHI, Kelly ALVAREZ, Hironori SEKI, Hidekazu SUENO, Masayuki SUGIYAMA, Daisuke TOKOZAKURA, Leimei LIN
Supporting Staff:	Miki ASANO

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 developed by this department are unique materials which exhibit extraordinary superior mechanical strength. The materials are fabricated by unidirectional solidification of the melts under pressurized gases. Main issues are to investigate properties of lotus-type porous metals and to develop the engineering applications. In this year, we have established the fabrication method for porous metals using continuous casting technique, and fabricated porous intermetallic compounds, and aluminium.

Current Research Programs

1. Fabrication of Lotus-type Porous Metals and Alloys

In our research group, porous metals with cylindrical pores elongated in one direction have been fabricated by unidirectional solidification under pressurized gas atmosphere utilizing the solubility gaps of gas atoms in metals at melting points. Lotus-type porous metals are superior in mechanical strength to conventional sphere-type porous metals, since the stress concentration around pores does not occur by the stress parallel to the pore growth direction. In this year, we have fabricated lotus-type porous TiAl intermetallic compounds, and Ni-free stainless steel.

Furthermore, we developed a new “Lotus continuous casting (LCC) technique”, which enables to fabricate long lotus-type porous plates or rods. Using this technique, we successfully fabricated the lotus copper, the pore size of which can be controlled by the solidification velocity. This is a promising technique for low cost and mass-production for commercial application of the lotus metals and provides various products for applications such as sport utility, airplane device, heat sink and biomaterials, etc.

2. Fabrication of Lotus-type Porous TiAl

Ti₄₈Al₅₂ alloy was melted and unidirectionally solidified by using a continuous zone melting method in pressurized hydrogen atmospheres. Observation via an optical microscope and phase identification via XRD clarified that the unidirectionally solidified TiAl consists of cylindrical pores aligned in the solidification direction and a matrix of TiAl intermetallic compounds, which indicate that lotus-type porous TiAl intermetallic compound can be fabricated by using the continuous zone melting method.

3. Fabrication of Lotus-type Porous Ni-free Stainless Steel

Lotus-type porous nickel-free stainless steel was fabricated using “continuous zone melting technique”. After applying a high temperature nitriding treatment, the fabricated lotus-type porous nickel-free stainless steel absorbed large amount of nitrogen compared with non-porous alloy of the same composition since the surface area of the lotus sample exposed to the gas is larger than that in the non-porous samples. In the lotus-type porous Fe-25wt.%Cr and Fe-23wt.%Cr-2wt.%Mo alloys, the nitrogen concentration achieved after the nitriding was approximately 1.2 wt.% and γ -phase with non-magnetism was observed.

4. Formation of Hollow Oxide Nanoparticles through Oxidation of Metal Nanoparticles

Hollow nanoparticles have attracted growing interest as a new functional material, because they have a potential to be used as drug delivery vehicle. We have started to study the formation processes of hollow metallic nanoparticles utilizing interdiffusion. In particular, hollow phenomenon related to oxidation has been investigated using transmission electron microscopy. Formation of hollow ZnO nanoparticles was observed after oxidation of Zn nanoparticles. The nano-hole formed inside ZnO seems to result from generation and clustering of vacancies in the oxidation process of Zn nanoparticles. A similar phenomenon was also confirmed after the oxidation of Cu nanoparticles.

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Anisotropic Electrical Conductivity of Lotus-type Porous Nickel, M. Tane, S.K. Hyun, and H. Nakajima : J. Appl. Phys., 97 [10] (2005) 103701

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Review papers

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Fabrication of Lotus-Type Porous Silicon, T. Nakahata, H. Nakajima: Materia Japan, 44 [5] (2005) 389-394.

Book

Medical devices friendly to human bodies, edited by H.Nakajima, Kubapro(2005) 1-16.

Patents

Production Method for Porous Metal Body, H. Nakajima, Ukraine, No72263

Cooling Device, H. Nakajima, Mitsubishi Electric Corporation, JP3669569

Medical Device or Parts Applicable for Sonographic Diagnosis, H. Nakajima, Asahi Intecc Co.,LTD., JP3735019

Production Method for Porous Metal Body, H. Nakajima, European Patent, No.1231287 (UK, France, Germany, Netherlands, Italy, Switzerland)

Connecting Structure between Semiconductor Device Electrodes and Bonding Wire, H. Nakajima, Tatsuta Electric Wire and Cable Co.,LTD., JP3765751

Method of Manufacturing Gas Turbine Part using Porous Metal, H. Nakajima, Kawasaki Heavy Industries, LTD., USA, No10/775144

Method of Manufacturing Gas Turbine Part using Porous Metal, H. Nakajima, Kawasaki Heavy Industries, LTD., European Patent (U.K., Germany, France)

Machine Tool, H. Nakajima, Mori Seiki Co., LTD, PCT Application, PCT/JP2004/000632, USA, P.R.China, Korea, Canada, Russia, Japan, EP (Germany, France, U.K., Switzerland)

Heat sink, H. Nakajima, Mitsubishi Electric Corporation, PCT Application, PCT/JP2005/014731

Controlling Technique for Pore-opening in Porous Materials, H. Nakajima, S.-K. Hyun, Kawasaki Heavy Industries, LTD., PCT Application, PCT/JP2006/303167a

International Conferences

Casting and Mechanical Properties of Lotus-type Porous Hastelloy X, *K.Taguchi, M. Sato, A. Mizuda, Y. Matsuzaki, S.K. Hyun, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

Fabrication of Lotus-type Porous Ni₃Al by Unidirectional Solidification, *T. Ide, M. Tane, S.K. Hyun, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

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International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

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Measurement of Pore Length of Lotus-type Porous Nickel, *H. Onishi, S.K. Hyun, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

Effect of Applied-Stress Direction on Compressive Properties of Lotus-type Porous Stainless Steel, *T. Ide, T. Ikeda, M. Tane, S.K. Hyun, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

Effect of Dissolved Hydrogen on Corrosion Behavior of Lotus-type Porous Stainless Steel, *M. Fuseya, T. Nakahata, S.K. Hyun, S. Fujimoto, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

Tensile Properties of Lotus-type Porous Copper: Effect of Specimen Dimensions, *H. Sueno, M. Tane, J.S. Park, S.K. Hyun, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

Electrical Conductivity of Lotus-type Porous Nickel: Measurements and Effective-Mean-Field Theory, *M. Tane, S.K. Hyun, and H. Nakajima, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto, Japan, Sept. 21-23, 2005.

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Relationship between Specimen Size and Compressive Yield Strength of Lotus-type Porous Copper, *J.-S. Park, H. Sueno, S.-K. Hyun, M. Tane, H. Nakajima, Y.-S. Um, B.-Y. Hur, and F. Ono, 4th International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005), Kyoto International Conference Hall, Kyoto,

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Contributions to International Conferences and Journals

H. Nakajima	Materials Letters (Principal Editor)
H. Nakajima	Scripta Materialia (Guest Editor)
H. Nakajima	Fourth International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005) (Organizing Committee Chairman)
H. Nakajima	High Temperature Materials and Process (Editorial Board)
H. Nakajima	Diffusion and Defect Data (Editorial Advisory Board)
H. Nakajima	Materials Science Foundations (Editorial Advisory Board)
H. Nakajima	Pacific Rim International Conference on Materials (Organizing Committee Member)
H. Nakajima	International Symposium on Structural and Functional Materials Design (Organizing Committee Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	THEMEC'2006 Symposium on Metallic Foams (Organizing Committee Member)
H. Nakajima	International Conference on Diffusion in Materials (Organizing Committee Member)
H. Nakajima	The 7 th International Symposium on Eco-Materials Processing and Design (International Advisory Committee Member)
H. Nakajima	IUMRS International Conference in Asia2006 (International Advisory Committee Member)
H. Nakajima	2 nd International Conference on Diffusion in Solids and Liquids (International Advisory Committee Member)
H. Nakajima	5 th International Conference on Porous Metals and Metallic Foams (International Advisory Board Member)
H. Nakajima	International Workshop on Designing of Interfacial Structures in Advanced Materials and their Joints (Organizing Committee Member)
H. Nakajima	The 8 th International Symposium on Eco-Materials Processing and Design (ISEPD2007) (International Advisory Committee Member)

Publications in Domestic Meetings

The Japan Institute of Metals	25 Papers
The Iron and Steel Institute of Japan	6 Papers
High Temperature Society of Japan	2 Papers
Light Metals Society of Japan	1 Paper

Japan Electronic Materials Society
Japan Society of Thermophysical Properties

1 Paper
4 Papers

Academic Degrees

Master Degree of Engineering

H. Sueno	Relationship between Specimen Size and Tensile Properties of Lotus-type Porous Copper
M. Sugiyama	Fabrication and Compressive Properties of Lotus-type Porous Nitinol

Sponsorship

Grant-in-Aid for Scientific Research on Exploratory Research

H. Nakajima	Biomaterials	¥3,880,000
H. Nakajima	Fabrication of Novel Nano-hollow Sphere Metals and Metallic Nano-tube and Elucidation of Physical Properties	¥42,120,000
S.K. Hyun	Fabrication and Mechanical Properties of Lotus-type Porous Intermetallics	¥800,000

Entrusted Research

H. Nakajima	Engineering Research Association for Supersonic Transport Propulsion System : Development of Innovative Multifunctional Foundry Process	¥27,772,000
H. Nakajima	Development of High Performance Machinery Processing System	¥13,915,000

Other Research Funds

H. Nakajima	New Energy and Industrial Technology Development Organization: Investigation Research of Standard Test Method for Property Estimation of Lotus-type Porous Metals	¥15,000,000
H. Nakajima	The Iron and Steel Institute of Japan Database of porous metals	¥1,200,000
H. Nakajima	Commemorative Organization for the Japan World Exposition '70	¥3,000,000
H. Nakajima	The Japan Institute of Metals Grant-in-Aid for International Conference on Porous and Foamed Metals	¥3,500,000
H. Nakajima	Grant-in-Aid from The Japan Institute of Light Metals	¥250,000

H. Nakajima	Japan Science and Technology Agency Development Project for Creative Seeds	¥200,000,000
H. Nakajima	Tanigawa Heat Technical Foundation Development of Porous Metal Support for Emission Catalyst	¥1,300,000
H. Nakajima	Mitsubishi Electric Co. Ltd. Development of Heat Sinks	¥440,000
H. Nakajima	Murayama Co.,LTD. Development of Hydrostatic Bearing	¥1,000,000
M. Tane	Iketani Science and Technology Foundation Shape Memory and Super Elastic Behaviors of Lotus-type Porous NiTi Alloys	¥1,300,000

Department of Atomic Scale Science

Professor:	Tomoji KAWAI
Associate Professor:	Hidekazu TANAKA
Visitor Associate Prof:	Hea-Yeon LEE
Research Associates:	Hiroyuki TANAKA, Takeshi YANAGIDA
Post Doctoral Fellows:	Issei SATOH, Munetoshi SEKI, Kota Sreenivasa Rao,
Visitor Researchers:	Kaoru OJIMA, Keiichi ADACHI, Toshihito OHTAKE, Naoki SUZUKI, Bong-Kuk Lee, Hiroshi Matsuura, Takeshi UNO, Masaki KANAI, Eriko MIKAMO, Naoki KAWAZOE, Toshihiko MATSUURA, Yusuke YOSHIDA, Hitomi YAMAGUCHI, Hee-Jin LIM, Satoru MIZUGUCHI, Takashi KAWABE, Toshio KAWAHARA, Mattias ANDERSSON, Shinichi TANAKA
Technical Assistants:	Chiemi TAKAMORI, Yoshimi KANZAKI
Graduate Students:	Koji SUZUKI, Masafumi NAKAMURA, Yoichi OHTSUKA, Masatoshi OHNISHI, Itsuki YAMAMOTO, Fumihiko YAMADA, Song-Eun LEE, Yoshihiko YANAGISAWA, Suguru NAKAZATO, Yoshihiro NOJIMA, Takuya TAKAHASHI, Mizue ISHIKAWA, Takumi KOBAYASHI, Kazumichi YOKOTA, Norihiko KUBO
Under Graduate Students:	Yasuto ITOGA, Kazuki NAGASHIMA, Hideyuki KAWAGUCHI, Yasunori TANAKA
Support Staffs:	Noriko FUJIBAYASHI, Yumi NAGAI

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 Programs and Achievements

Function harmonised superlattices.

- New ferromagnetic oxide, ($\text{Mn}_x\text{Fe}_{3-x}\text{O}_4$) was designed and prepared to construct highly sensitive spin devices for external fields (magnetic & electric field) at room temperature.
- At the thickness around 40nm, the $\text{La}_{0.8}\text{Ba}_{0.2}\text{MnO}_3$ thin films possessed high TCR value and low noise amplitude at room temperature, showing higher potential as an uncooled bolometer than the ordinary VO_x-based IR sensor.
- The ultimate nano-lithography for various kinds of transition metal oxide films has achieved down to 30nm using atomic force microscopy.

Nano-science by using of Scanning Probe Microscopes.

- By using scanning tunneling microscopy (STM), we obtained submolecular-resolution STM images of a single molecule of DNA labeled with a fluorophore, such as FITC, RITC, HEX, etc., which can be a good molecular marker even in STM.
- By using STM/STS measurements, a characteristic peak in dI/dV spectra of Guanine molecule has been detected.
- Using the atomic force microscopy (AFM), we found the valuable information to identify the solution for the rate-limiting step of small-scale protein synthesis system by analyzing the reaction process.
- Using the base recognition function of the immobilized ribosome, the base sequencing process of mRNA was detectable with the optical technique, which did not need any special purification.

Development of NanoBiosensor

- Developing ultra-sensitive biosensor/devices utilizing highly-specific bindings on nano-sized electrode arrays.
- Development of novel bio-sensor was achieved by coordinating functional groups on the surface of lipid-bilayer.

Development of bio-molecular device constructed from DNA.

- DNA nano-patterning by a nanoimprint lithography (NIL) and novel patterning technique toward DNA electronic nano devices were developed.
- One dimensional gold particle array has been formed using DNA template.
- Nano-scale gold electrodes have been fabricated by using nanotransfer printing lithography.
- Direct detection of the known SNPs (single nucleic polymorphism) of Cytochrome P450 2C9 (CYP2C9), which is a polymorphic enzyme responsible for the metabolism of a large number of clinically important drugs in the Cytochrome P450 superfamily, using a PNA-modified IS-FET biosensor.

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Patents

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DNA chip and Biosensor using DNA chip, Tomoji Kawai, Hea-Yeon Lee, J.W.Park, J.M.Kim, H.S.Jung, JP2003-403398

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Ferromagnetic conductor and its process, and magnetoresistance devices, field effect transistors, Hidekazu Tanaka, Mizue Ishikawa, Tomoji Kawai, JP2005-050216

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Magnetoresistive device and inversion method of magnetization, Hidekazu Tanaka, Teruo Kanki, Tomoji Kawai, JP2005-101328

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Method and apparatus to determine sequence of nucleic acid. Hiroyuki Tanaka, Tomoji Kawai, JP2005-214806.

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Nano-Structured Biosensors Toward Single Molecular Detection Discussion (Invited), *T. Kawai: ESF Research Conferences, Spain, June 18-23, 2005.

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M. Taniguchi, T. Kawai: The 8th International Conference on Atomically Controlled Surfaces, Interfaces & Nanostructures / 13th International Congress on Thin Films, Stockholm International Fairs, Stockholm, Sweden, June 19-23, 2005.

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Conduction through Cytochrome c Molecules, *T. Matsumoto, M. Kataoka, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

Kinetic and Thermodynamic Control by Chemical Bond Rearrangement on a Si(001) Surface, C. Hamai, *A. Takagi, M. Taniguchi, T. Matsumoto, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

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Tanaka, T. Matsumoto, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

Nanopatterning of Transition Metal Oxides by the Voltage-Biased Tip of an Atomic Force Microscope, *L. Pellegrino, E. Bellingeri, I. Pallecchi, G. Canu, A.S. Siri, D. Marré M. Hirooka, Y. Yanagisawa, M. Ishikawa, Hide. Tanaka, T. Matsumoto, A. Takagi, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

Observation of Various Porphynoids Adsorbed on a Substrate by Using AFM/STM, *A. Takagi, N. Aratani, T. Matsumoto, A. Osuka, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

Potential Mapping of Top-contacted Junctions: Molecules and Nanotransfer Printing Electrode, *K. Ojima, K. Nakamatsu, Y. Otsuka, T. Matsumoto, S. Matsui, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

Structure and Electrical Property of DNA Molecules Immobilized on Patterned Hydrophobic / Hydrophilic Surface, *Y. Otsuka, K. Ojima, T. Matsumoto, H. Tabata, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

Surface Potential and Capacitance Measurement of Molecules on Insulating Substrate, *F. Yamada, A. Takagi, T. Matsumoto, Hide. Tanaka, T. Kawai: 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, July 3-8, 2005.

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Architecture Electronic-BioSensor Integrated with Nanofabrication (Invited), *H.Y. Lee, T. Kawai: Summer Seminar of Biochemical Engineering Society, Kyoto, Japan, July 8-9, 2005.

Construction of Metal Oxide Nano-Heterostructures Using Laser-MBE and AFM Nanolithography Toward Room Temperature Spintronics. (Invited), *Hide. Tanaka, T. Kawai, International Conference on Composites/nano Engineering (ICCE - 12), Tenerife, Spain, August 2-4, 2005.

Surface Potential and Capacitance Image of Molecules on Insulating Substrates, *T. Matsumoto, F. Yamada, T. Kawai: 8th International Conference on Non-Contact Atomic Force Microscopy, Bad Essen, Germany, August 15-18, 2005.

Enhancement of Integrated Electric Gene Chip Utilizing Nano-Well Array Geometry (Invited), *H.Y.Lee, B.K.Lee, and T. Kawai, Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, August 28-31, 2005.

Conductivity Measurement of Single/Small Number of DNA (Invited), *T. Matsumoto: Nanoelectronics and Dynamics of DNA, Hawaii, U.S.A., August 28-31, 2005.

DNA Nanotechnology in Kawai Laboratory (Invited), *T. Kawai: Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, August 28-31, 2005.

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High Resolution STM Imaging of DNA and Supramolecules (Invited), Hiro. Tanaka, T. Kawai: Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, August 28-31, 2005.

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Tunneling Spectroscopic Study for the Single Molecule of The Fluorescein Derivatives Attached Deoxyribonucleic Acid (Invited), T. Kawahara, Hiro. Tanaka, T. Kawai: Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, August 28-31, 2005.

Conduction in Single/Small Number of Molecules Including DNA and Cytochrome c (Invited), *T. Matsumoto, T. Kawai: The 54th Fujihara Seminar, Tomakomai, Japan, August 31- September.4, 2005.

Visualization of Nano-Scale Magnetic Structures of Magnetoresistive (La,Ba)MnO₃ and Granular Fe/ Al₂O₃ by Frequency-Modulation Magnetic Force Microscopy (Invited), *T. Matsumoto, T. Kawai : 6th Pacific Rim Conference on Ceramic and Glass Technology, Maui, Hawaii, U.S.A., September 11-16, 2005.

Electrical Properties of Ferromagnetic Oxide Nano-Channels Prepared by Atomic Force Microscopy, *Y. Yanagisawa, L. Pellegrino, Hide. Tanaka, M. Hirooka, T. Kawai: 12th international Workshop on Oxide Electronics, Boston, U.S.A., October 2-5, 2005.

Fabrication of Mn-doped Fe₃O₄ Nano-Channel Structures by AFM Lithography and Applications to Nano FET Devices, *L. Pellegrino, Y. Yanagisawa, M. Ishikawa, T. Yanagida, T. Matsumoto, Hide. Tanaka, T. Kawai: 12th International Workshop on Oxide Electronics, Boston, U.S.A., October 2-5, 2005.

Nano Technology and the Global Best Practices of Its Development, Tomoji Kawai, World Knowledge Forum 2005, Korea, October 10-12, 2005

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Conduction Through Cytochrome c Molecules, *T. Matsumoto, M. Kataoka, T. Kawai: AVS 52nd International Symposium and Exhibition, Boston MA, U.S.A., October 30-November 4, 2005.

Potential Difference Mapping of Molecules and Particles on Insulating Substrate, *F. Yamada, T. Matsumoto, H. Tanaka, T. Kawai: AVS 52nd International Symposium and Exhibition, Boston MA, U.S.A., October 30- November 4, 2005.

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Electrical Detection of Chemical Reactions on Nano-Space, *K. Yokota, M. Taniguchi, T. Kawai: International Symposium on Surface Science and Nanotechnology, Omiya, Japan, November 14-17, 2005.

Fabrication of DNA Nanofibers by Electrospinning, *T. Takahashi, M. Taniguchi, T. Kawai: International Symposium on Surface Science and Nanotechnology, Omiya, Japan, November 14-17, 2005.

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Surface Potential and Capacitance Measurement of Molecules on Insulating Substrates Molecular Electronics, *F. Yamada, A. Takagi, T. Matsumoto, T. Kawai: International Symposium on Surface Science and Nanotechnology, Saitama, Japan, November 14-17, 2005.

Electrochemical Detection and Kinetic Study of Amyloid Fibril Formation, *B.K.Lee, H.Y. Lee, T. Kawai: 4th 21st Century COE International Symposium, Toba, Japan, November 18-19, 2005.

Patterning Solid-supported Membranes Using PEG Polymers Within Microfluidic Channels, *S.E. Lee, B.K. Lee, H.Y. Lee T. Kawai, P.N. Kim, K.Y. Suh: 4th 21st Century COE International Symposium, Toba, Japan, November 18-19, 2005.

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Fabrication of Oxide Nano-structure Using Atomic Force Microscopy and Its Electrical Properties.*Y. Yanagisawa, L. Pellegrino, Hide. Tanaka, M. Hirooka, T. Kawai: 4th 21st Century COE International Symposium, Toba, Japan, November 18-19, 2005.

In Preparation for Realization of Field Effect Transistor Being Able to Control of Ferromagnetism at Room Temperature on The Pb(Zr,Ti)O₃/(La,Ba)MnO₃ Heterostructure. *M. Ohnishi, T. Kanki, Hide. Tanaka, T. Kawai: 4th 21st Century COE International Symposium, Toba, Japan, November 18-19, 2005.

The Electrical/magnetic Property and the Electronic Structure of Highly Conductive Mn_xFe_{3-x}O₄ Thin Films With Spin Polarization at Room Temperature. *M. Ishikawa, Hide. Tanaka, T. Kawai, E. Ikenaga, A. Takeuchi, M. Awaji, K. Kobayashi, Y. Saito, K. Takeda: 4th 21st Century COE International Symposium, Toba, Japan, November 18-19, 2005.

Ambipolar Organic Field-Effect Transistors Using Gate Insulator Hysteresis, *M. Taniguchi, E. Mizuno, T. Kawai: 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” Fourth International Symposium 2006, Toba, Japan, November 18-19, 2005.

Approach to Electrical Conductance Spectroscopy of Chemical Reaction on Nano-Space, *K.Yokota, M.Taniguchi, T.Kawai: 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” Fourth International Symposium 2006, Toba, Japan, November 18-19, 2005.

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Electrochemical Detection and Kinetic Study of Amyloid Fibril Formation, *Bong-Kuk Lee, Hea-Yeon Lee, T. Kawai: 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Toba, Japan, November 18-19, 2005.

Lipid Membranes Patterning Using PEG Polymers Onto Substrates Within Microfluidic Channels, *SangEun Lee, BongKuk Lee, HeaYeon Lee, T. Kawai, Pilnam Kim, Kahp Y. Suh: 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Toba, Japan, November 18-19, 2005.

Fabrication of Mn-Doped Fe₃O₄ Nanochannel Structures and Application to Nano FET Devices by AFM Lithography. *Hide. Tanaka, L. Pellegrino, Y. Yanagisawa, M. Ishikawa, T. Matsumoto, T. Kawai: 2005 MRS (Materials Research Society) Fall Meeting, Boston, U.S.A., November 28 - December 2, 2005.

Investigation on Ferromagnetism in La_{1-x}Ce_xMnO₃ Thin Films Using Soft x-ray Absorption Magnetic Circular Dichroism. *T. Yanagida, Hide. Tanaka, T. Kawai, Y. Saitoh, Y. Takeda, A. Fujimori: 2005 MRS (Materials Research Society) Fall Meeting, Boston, U.S.A., November 28 - December 2, 2005.

Magnetic and Electrical Properties of Room-Temperature Spin-Polarized Mn-Doped Fe₃O₄ Ultrathin Films Grown on Various Insulating Substrates. *I. Satoh, M. Ishikawa, L. Pellegrino, Hide.Tanaka, T. Kawai: 2005 MRS (Materials Research Society) Fall Meeting, Boston, U.S.A., November 28 - December 2, 2005.

Preparation of Highly Conductive Mn-Doped Fe₃O₄ Thin Films with Spin Polarization at Room Temperature Using Pulsed Laser Deposition Technique. *Hide. Tanaka, M. Ishikawa, T. Kawai: 2005 MRS (Materials Research Society) Fall Meeting, Boston, U.S.A., November 28 - December 2, 2005.

Structural, Magnetic Properties and x-ray Absorption Apectroscopy of Nd_{1-x}Ce_xMnO₃ Thin Films. *T. Yanagida, Hide. Tanaka, T. Kawai, Y. Saitoh, Y. Takeda, A. Fujimori: 2005 MRS (Materials Research Society) Fall Meeting, Boston, U.S.A., November 28 - December 2, 2005.

Molecular Electronic Using Biological Materials (Invited), *T. Matsumoto, T. Kawai, International Symposium on Molecular Scale Electronics (In Conjunctlon with 6th Molecular Scale Electronics Workshop in Japan), Tsukuba, Japan, December 5-6, 2005.

Contributions to International Conferences and Journals

Tomoji Kawai	Nanotech (Chairman)
Tomoji Kawai	Surface Science (Editorial Board)
Hidekazu Tanaka	Japan Society of Applied Physics, Program Editor, Joint Seession E "Spin electronics/Nano-Magnetics"

Hidekazu Tanaka	Japan Society of Applied Physics, Program Editor, session "8.1 Field of magnetic material and Devices"
Hiroyuki Tanaka	Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, August 28-31, 2005. Organizing member
Toshio Kawahara	Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, August 28-31, 2005. Organizing member

Publications in Domestic Meetings

The Physical Society of Japan	3 papers
The Japan Society of Applied Physics	29 papers
The Chemical Society of Japan	1 papers
The Molecular Biology Society of Japan	1 papers
The Surface Science Society of Japan	2 papers
Others	27 papers

Academic Degrees

Master Degree of Science

Y. Nojima	Fabrication of photo-switching molecular device and detection of photochemical isomerization
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Master Degree of Engineering Science

T. Takahashi	Development of stretch-and-positioning method for DNA and electrical conductivity of DNA
M. Ishikawa	Preparation of highly conductive $\text{Mn}_x\text{Fe}_{3-x}\text{O}_4$ thin films with spin polarization at room temperature and their electronic structure

Doctor Degree of Engineering Science

C. Takato	Studies on DNA-templated Porphyrin Arrays and Their Molecular-scale Electrical Properties
Y. Otsuka	Study on Charge Transport Properties through DNA by Nanoscale Electrical Measurements

Sponsorship

21st Century Center of Excellence

T. Kawai	Toward Creating New Industries Based on Inter- Nanoscience	¥309,100,000
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Grant-in-Aid for Scientific Research (B)

Hide. Tanaka	Construction of room temperature spin electronics devices by strongly correlated oxide nano-structure	¥4,200,000
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Grant-in-Aid for Scientific Research (A)

Hide. Tanaka	Creation of opt-magnetic materials by programmed self-assembly using DNA molecules and nano-particles	¥7,700,000
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Fund for JSPS Research fellowships for Young Scientist

T. Yanagida	Fabrication of functional harmonic artificial lattice by controlling surface structures towards realization of biomimic sensors	¥1,100,000
I. Satoh	Construction of room temperature spin electronics devices by strongly correlated oxide nano-structure	¥1,200,000
M. Seki	Creation of Room Temperature Photomagnetic Materials and Elucidation of Photoinduced Magnetization	¥900,000
M. Ohnishi	Construction of room temperature spin electronics devices by strongly correlated ferromagnetic oxide	¥900,000
Y. Otsuka	Controlling the structure and sequences of DNA and the elucidation of the charge transport phenomenon in nanoscale	¥900,000
F. Yamada	Arrangement of nano-magnet using programmed self-organization system and investigation of novel magnetic properties	¥900,000

Entrusted Research

T. Kawai	NEDO: Focus 21 Advanced nanobio device project	〔TORAY〕 Research and Development of High Through Put Protein Chip: Analysis of Protein Synthesis Mechanism	¥7,560,000
		〔Matsushita Electric Industrial Co., Ltd.〕 Research and Development of Immobilization Method of Biomolecules	¥7,350,000
		〔Shimadu Co.〕 Development of the System for Single-Molecule DNA Analysis	¥11,550,000

Other Research Funds

Tomoji Kawai	Core Research for Evolutional Science and Technology (CREST), Japan Science and Technology Agency	Creation of bio-mimetic intellectual material based on programmed self-assembly	¥143,860,000
Tomoji Kawai	Nanotechnology Researchers	Nanotechnology Process Foundry	¥9,700,000

Network Center of
Japan

Hidekazu Tanaka	Japan Science and Technology Agency	【Development of Systems and Technology for Advanced Measurement and Analysis】 Development of Hard X-ray Photoemission electron microscope and thier application to strogly correlated nano- film/nano-heterostruture	¥5,000,000
Hidekazu Tanaka	Japan Science and Technology Agency	【 Assist Program of seeds research】 Construction of electric field assited Magnetic Random Access Memory devices by oxide heteoro-strucutre	¥2,000,000
Hiroyuki Tanaka and Kiyohiko Kawai	21st Century COE Jung Scientists Joint research program	Synthesis and evaluation of the nanocomplex of DNA and porphyrin	¥2,000,000

Department of Functional Ceramic Materials

Professor:	Hikaru KOBAYASHI
Associate Professor:	Masao TAKAHASHI
Research Associates:	Kohji NOBUGAI, Osamu MAIDA
Visiting Professors:	Hitoo IWASA, Sumio TERAOKA, Taisei YAMAMOTO
Research Technical Expert:	Masami Shoji
Researchers:	ASUHA, Liu Yueh-Ling, Takemitsu MIURA
Graduate Students:	Im Sung-Soon, Yukio ISHIKAWA, Katunori KOBAYASHI, Kenichi FUKAYAMA, Kensaku HATTORI, Hideki OOE, Hiroaki NARITA
Undergraduates:	Kentarou IMAMURA
Support Staffs:	Yumiko SUZUKI, 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 structure. 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 Programs

Low temperature fabrication of thick SiO₂/Si structure 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 because of the imperfect bond formation and the presence of impurities, 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 oxygen atoms with high oxidizing activity. The SiO₂/Si structure fabricated by use of the two-step nitric acid oxidation method possesses much superior electrical characteristics to those formed by CVD methods. The leakage current density of the SiO₂ layers formed by the two-step nitric acid oxidation method is as low as that for thermal oxide layers formed above 800 °C in spite of the low temperature oxidation at ~ 120 °C. SiO₂ 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, SiO₂ 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 SiO₂ layers can be formed at low temperature of ~ 120 °C by use of the two-step nitric acid oxidation method.

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 0.2 % 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.

In this academic year, we have proved that the developed semiconductor cleaning solutions can remove various kinds of metal impurities such as Cu, Ni, Fe, Co, Mn, Zn, Ca, and Na from SiO₂ and Si surfaces. The mechanism of the Cu removal has been clarified.

Publications

Original Papers

Formation and electrical characteristics of silicon dioxide layers by use of nitric acid oxidation method, S. Imai, M. Takahashi, K. Matsuba, Asuha, Y. Ishikawa, and H. Kobayashi, *Acta. Phys. Slov.* 55(3) (2005) 305-313.

Deoxidation of gallium arsenide surface via silicon overlayer: a study on the evolution of the interface state density, J. Ivanco, T. Kubota, and H. Kobayashi, *J. Appl. Phys.* 97 (2005) 073712.

Electronic properties of very thin native SiO₂/a-Si-H interfaces and their comparison with those prepared by both dielectric barrier discharge oxidation at atmospheric pressure and by chemical oxidation, M. Kral, A. Bucek, H. Gleskova, M. Cernak, H. Kobayashi, J. Rusnak, M. Zahoran, R. Brunner, and E. Pincik, Act. Phys. Slov. 55(4) (2005) 373-378.

Patents

Thin film transistors and their fabrication method, display apparatus, and method of improving oxide characteristics, H. Kobayashi, S. Imai, and K. Inoguchi, Tokugan 2005-139326..

Solar cells and their fabrication method, H. Kobayashi and M. Takahashi, Tokugan 2005-139326.

Method of producing semiconductor treatment liquid, its production apparatus, and production system, H. Kobayashi, M. Takahashi, and K. Seki, Tokugan 2005-116223

Method of the formation of oxide layers on semiconductors, method of regeneration of high purity nitric acid, and regeneration apparatus, H. Kobayashi, S. Oota, S. Shimizu, and T. Nozaki, Tokugan 2005-313429

Method of improving crystal characteristics for semiconductor devices, H. Kobayashi, S. Hasegawa, and M. Matsumoto, Tokugan 2005-255418

International Conferences

Detection and elimination of semiconductor interface states and improvement of solar cell characteristics, (Invited) *H. Kobayashi, J. Ivanco, O. Maida, and M. Takahashi, Solar Renewable Energy News – Research and Applications 2005 International Conference, Florence, Italy, 4. 2-8, 2005.

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Contributions to International Journals

H. Kobayashi Applied Surface Science, Editor

Publications in Domestic Meetings

The Physical Society of Japan	3 papers
The Japan Society of Applied Physics	6 papers
Symposium on Chemical Kinetics and Dynamics	3 papers
Surface Science Society of Japan	1 paper

Academic Degrees

Master Degree of Science

K. Kobayashi	Fabrication of amorphous silicon solar cells with light trapping structure and measurements of characteristics
K. Fukayama	Fabrication of Hf-containing high dielectric thin layer/Si structure and its interface and thin film characteristics
K. Hattori	Low temperature formation of SiO ₂ /Si structure by use of nitric acid method
H. Ooe	Si defect control by addition of Si in Al electrodes and improvement of energy conversion efficiency of solar cells

Doctor Degree of Science

Y.-L. Liu	Reaction of cyanide ions with metals on silicon surfaces and its application to semiconductor device cleaning
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Sponsorship

Entrusted Research

H. Kobayashi	Japan Science and Technology Organization	Development of Semiconductor Cleaning Solutions with Defect Passivation Effect	¥59,800,000
H. Kobayashi	Japan Science and Technology Organization	Development of Extremely Low Power System Display by Use of Limit Gate Structure	¥53,586,000
H. Kobayashi	Japan Science and Technology Organization	Silicon Thin Film Solar Cells with New Chemical Bonds	¥2,600,000
M. Takahashi	Japan Science and Technology Organization	Suppression of Charge Carrier Recombination in Polycrystalline Si by cyanide treatment	¥845,000
H. Kobayashi	Kansai Bureau of Economy, Trade and Industry	Practical Study of Low Temperature Silicon Oxidation Apparatus by Use of Nitric Acid Oxidation Method	¥4,434,000

Other Research Funds

H. Kobayashi	Core Research for Evolutional Science and Technology	Silicon Thin Film Solar Cells with New Chemical Bonds	¥21,625,000
M. Takahashi	Core Research for Evolutional Science and Technology	Suppression of Charge Carrier Recombination in Polycrystalline Si by Cyanide Treatment	¥6,500,000

Department of Structural Ceramic Materials

Associate Professor:	Tohru SEKINO
Research Associates:	Takafumi KUSUNOSE, Tadachika NAKAYAMA
Research Technical Experts:	Satoshi SEINO, Seung-Ho KIM
Graduate Students:	Ari HIRVONEN, Kazunori TANAKA, Iwao UENO, Yoshitaka SAIJO, Tomonori SHIBATA, Tsukuru MIZUGUCHI, Shin-ya ITANO, Nobuaki SAKAYANAGI
Research Students:	Yoshinobu SUZUKI, Asuka HAYASHI
Support Staff:	Rie SUEHIRO

Outlines

Ceramic material is now strongly required to have a multi-functionality to meet the future demands to be solved in the 21st century. The "nanocomposite technology" realizes the dominant improvement of mechanical properties of ceramics by controlling nano- and atomic-scale structure of the polycrystalline ceramics. Based on this concept, this department has been focusing mainly on the basic researches for developing high-performance ceramic-based materials with multiple functionalities over the decade. Special emphasis is placed on the understanding of the relation between the nanostructures and various performances. Systematic researches have revealed that the mechanical properties of these nanocomposite ceramics are remarkably enhanced even at high temperatures. In addition excellent functional properties, such as machinability, superplasticity, electric/magnetic properties and so on, are also found to be consistent with the improved mechanical property. Recent studies suggest that the nanocomposite concept is also applicable to metal and organic materials. Thus the target of these researches is to develop new class of hyper-functionalized materials, which ranges ceramic, metal and organic materials.

Current Research Programs

Design of Nanocomposite Concept and Development of High Performance Ceramic-based Nanocomposites.

To develop high performance ceramic-based materials we focused on the microstructural control of ceramics in nanometer-scale. It realizes "Nanocomposite" in which nanometer-sized second phase exists within several oxide and nonoxide ceramics. These composite materials exhibit superior mechanical properties, i.e., high fracture strength, toughness, creep resistance, thermal shock resistance and so on, not only at room temperature but also at elevated temperature. Development of new ceramic nanocomposites possessing superplasticity, machinability are also achieved by synthesizing nanostructured and nanocomposite powders, and/or by using conventional sintering method, novel in-situ sintering, reaction sintering and spark plasma sintering methods. In this study preparation process, micro/nano/interface structure, and properties relation have been investigated. Roles of nanostructures on properties enhancements are also studied in detail.

Design of 3-Dimensional Continuous Nano-network Structure in Ceramics and their Hyper-functionalization.

Nano-scale continuous 3D network structures have been realized among ceramic materials by using grain boundaries and/or by dispersing 1D-structured nanotube such as carbon nanotubes. These 3D network was used for the conductive pathway of electric current that realized conductive structural ceramics. Various compounds were formed as the grain-boundaries of AlN, ZrO₂ and so on, and also CNT was uniformly dispersed and composed with ceramics. Novel fabrication techniques have therefore been developed to achieve uniform 3D networks among ceramic matrix. As the results, these materials exhibited multi-functions such as both high mechanical performance and excellent electrical properties such as electro-discharge machining capability like metals, that would open new window for ceramic materials.

Fabrication and Properties of Ceramic/Metal Nanocomposites.

Dispersing metallic second phase particles into ceramics is suitable to improve mechanical properties of ceramics. Furthermore wide variety of advantages for addition of new function such as magnetic, electric and optical properties can be considered due to the size effect of nano-sized metal dispersion. Conventional powder metallurgical method and solution chemical process like sol-gel, co-precipitation method have been used to prepare the composite powder for ceramic/metal nanocomposites such as Al₂O₃/W, Mo, Ni, Cu, Co, Fe, ZrO₂/Ni, Mo, MgO/Fe, Co, Ni, and also for ceramic/intermetallic compound such as ZrO₂/NiTi etc. They are sintered in a reductive atmosphere that gives homogeneous dispersion of metallic particles within the ceramic matrices. Fracture strength, toughness, and/or hardness are enhanced due to the microstructural refinement by nano-dispersion and their plasticity. For transition metal dispersed oxides ceramic composites, ferromagnetism is also compatible with its excellent mechanical properties. In addition, good magnetic response for the applied stress was found in these ceramic/ferromagnetic-metal nanocomposites, showing the possibility of remote-sensing of fracture/deformation of ceramic materials.

Design and Development of Novel Environmental Barrier Nanocomposite-Coatings.

New type of ceramic-based nanocomposites have been developed to achieve novel environmental barrier coatings such as thermal and/or corrosion/erosion barrier ceramic coating system. Cordierite and monazite were dispersed as the nanodispersion into zirconia ceramic, and micro/nano-structures, mechanical properties have been investigated in detail. The nanocomposite system has been spray coated onto metal substrate and performances have been investigated. In addition, novel low-temperature processing and oxide/monoxide nanocomposite have been developed to realize new class of environmental barrier coating systems, and it was confirmed that the coating system has high potential as the new coating system for protecting metal materials.

Development of Functional Ceramic-based Nanocomposites and Their Properties Improvement.

Nanocomposite technology is also applicable to the functional ceramics such as semiconductor, ferroelectric, piezoelectric, varistor and ion-conducting materials. Incorporation of small amount of ceramic or metallic nanoparticles into BaTiO₃, ZnO, c-ZrO₂ can significantly improve their mechanical strength, hardness and toughness which are very important to realize high reliable electric devices operating in a severe environmental condition. In addition, electric properties can also be enhanced by dispersing nanoparticles. Relationships between nano- and interface-structure, mechanical properties and electric properties have been investigated in detail. Also nano-grain and nano-pores structures have been controlled for novel oxide thermoelectric materials, and resultant enhancement of thermoelectric performance at high temperatures has been achieved for oxide ceramic thermoelectric materials.

Design and Development of Novel Ceramic-Nanocomposites with Pseudoplastic Deformation Properties.

Dispersing soft materials into hard ceramic is generally thought to decrease its mechanical properties. However, we discovered that nanocompositing of soft materials with several kinds of ceramics can be improve their mechanical properties. For example addition of hexagonal boron nitride into silicon nitride ceramic can enhance its fracture strength not only at room temperature but also at very high temperature up to 1500°C. In addition, this nanocomposite exhibits superior thermal shock resistance and machinability because of the characteristic pseudoplasticity of the nanocomposites like metallic materials. This is due to the micro-fractures of materials within and around the soft nano-dispersion. These results indicate that ceramic/h-BN nanocomposites can be directly applicable to the high temperature structural materials. In this research optimization of preparation processes, properties and microstructures have been studied for several combination of composites.

Development of High Performance Organic/Inorganic Nano-Hybridization Technology.

To overcome the disadvantage of low mechanical properties of polymer (organic) materials, nano-sized ceramic particles have been incorporated. It is well known that chemical bonding as well as physical properties of ceramic and polymer is quite different, thus the optimization of preparation process is important. In this study, fabrication processes, microstructure, physical and mechanical properties of the polymer/ceramic composites have been investigated. By optimization of the fabrication process and controlling the nano-sized second phase dispersion, thermal stability and mechanical properties such as adhesion resistance, flexural strength, toughness and hardness can be enhanced which exhibits the great advantage of nano-dispersion. Moreover, the nanocomposite technology has been attempted to the novel elastomer/inorganic system to develop novel nano-hybrid pressure sensor materials, and the relationship between sensing performance, nano- and interface structures have been clarified. These materials have thus been practically applied as many sensor devices.

Development and Multi-functionalization of Low-dimensional Nanotube Materials.

Recently, we succeeded to synthesize Titania (TiO₂) Nanotube by using low-temperature solution chemical processing. It has approximately 10 nm in outer-diameter and more than 200 nm in length, and has open-end structure. This new-type of material

has attracted much attention because of its low-dimensional nanotube structure of oxide semiconductor and resultant high surface area, and we have clarified it has excellent photocatalytic properties and high capability as electrode of solar cell and ion battery. Also, various cations has been successfully been doped into the nanotubes, and the electrical conductivity was increased with the addition of small amount of dopants. Thermal stability was also enhanced by the doping. In this study multi-functionalization, nano-compositing and performance enhancement as well as structure analysis and mechanisms evaluation have been intensively carried out for the novel oxide nanotubes as well as for the carbon nanotubes to realize new class of materials which will be utilized for environmental/energy systems.

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Application of HVOF Techniques for Spraying of Ceramic Coatings (Invited), *E. Turunen¹, A. Hirvonen, T. Varis, T. Falt, S. P. Hannula, T. Sekino, and K. Niihara, International Symposium on Eco-Materials Processing & Design, Holiday Inn Crowne Plaza Hotel, Chengdu, China, Jan. 8-11, 2006.

Novel Nano-Processing Using the Atmospheric Plasma Technology, *T. Nakayama, S. Shinoda, T. Yokoo, W. Jiang, T. Suzuki, H. Suematsu, S. Seino, T. Kusunose, T. Sekino, and K. Niihara, International Symposium on Eco-Materials Processing & Design, Holiday Inn Crowne Plaza Hotel, Chengdu, China, Jan. 8-11, 2006.

Fabrication of Electrically Conductive AlN by Composition Control of Grain Boundary Phase, *T. Kusunose, T. Nakayama, K. Niihara, and T. Sekino, International Symposium on Eco-Materials Processing & Design, Holiday Inn Crowne Plaza Hotel, Chengdu, China, Jan. 8-11, 2006.

Mechanical and Thermal Properties of 3YSZ/LaPO₄ Nanocomposites, *S. H. Kim, T. Sekino, T. Kusunose and A. T. Hirvonen, International Symposium on Eco-Materials Processing & Design, Holiday Inn Crowne Plaza Hotel, Chengdu, China, Jan. 8-11, 2006.

Mechanical and Electrical Properties of Tetragonal Zirconia-Based Composite Materials Containing Nickel or Cobalt Titanides, N. Tanaka, T. Sekino and K. Niihara*, Osaka University, Japan, *Nagaoka University of Technology, Japan

Fabrication of Single-Nanosized Metal Particle Monodispersed Solutions and their Multidimension Drawing with a Ink Jet Printer, *S. Itano, T. Nakayama, S. Seino, T. Sekino, T. Kusunose, M. Nagashima, S. Shinoda, H. Suematsu, K. Niihara, International Symposium on Eco-Materials Processing & Design, Holiday Inn Crowne Plaza Hotel, Chengdu, China, Jan. 8-11, 2006.

Pressureless Sintering of Aluminum Nitride/Boron Nitride with High Thermal Conductivity, N. Sakayanagi, *T. Kusunose, T. Nakayama, K. Niihara, and T. Sekino, International Symposium on Eco-Materials Processing & Design, Holiday Inn Crowne Plaza Hotel, Chengdu, China, Jan. 8-11, 2006.

Contributions to International Conferences and Journals

- Tohru Sekino The International Symposium on Eco-Materials Processing and Design (Organizing Committee)
- Tohru Sekino 11th International Conferences on Modern Materials and Technologies (CIMTEC 2006) (Organizing Committee)
- Tohru Sekino The 7th Pacific Rim Conference on Ceramics and Glass Technology (Co-Chair)
- Tohru Sekino Materials Integration (Editorial Committee)

Publications in Domestic Meetings

The Ceramic Society of Japan	17 papers
Japan Society of Powder and Powder Metallurgy	4 papers
The Magnetics Society of Japan	1 paper
Society of Nano Science and Technology	4 papers

Academic Degrees

Bachelor Degree of Engineering

- Yoshinobu Fabrication and Properties of Non-oxide Material Added SiC
- Suzuki Composites
- Asuka Molecular Adsorption and Photocatalysis of Titania Nanotube

Hayashi

Master Degree of Engineering

Yoshitaka	Fabrication of Rare-earth Cobalt Oxide Semiconductors and Their
Saijo	Thermoelectric Properties
Tomonori	Fabrication and Evaluation of the Novel Thin Film of Elastomer
Shibata	Based Nanocomposite with Pressure Sensing Function
Tsukuru	Fabrication and Property Evaluation of ZrO ₂ /CNT/Metal Multi-phase
Mizuguchi	Nanocomposite

Doctor Degree of Engineering

Ari T.	Fabrication and Characterization of Zirconia-based Nanocomposites
Hirvonen	Ceramics for Novel Coating System
Norihito	Fabrication and Evaluation of Intermetallic Particles Dispersed
Tanaka	Tetragonal Zirconia-based Composite Materials

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

Tohru Sekino	Development of Rare-Earth - Transition Metal Complex Oxide Thermoelectric Materials and Their Mechanisms Elucidation	¥1,800,000
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Grant-in-Aid for Scientific Research on Special Research Fellow

Satoshi Seino	Radiation-Induced Synthesis of Single-Nanosized Composite Nanoparticles with Improved Functionality.	¥1,100,000
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Entrusted Research

Tohru Sekino	NEDO (Materials Nanotechnology Program, Nanocoating Project)	Development of Nanocomposite Coating by In-situ Structuralization.	¥5,565,000
Tohru Sekino	Osaka Industry Promotion Agency	Feasibility Study on the Development of Water Flow Detection System using Nanocomposite Pressure Sensor	¥987,000

Cooperative Research

Tohru Sekino	Sumitomo Electric Industries, Ltd.	Basic Studies on Ceramic-Polymer Composites	¥1,051,000
Tohru Sekino	Tomoe Works Co. Ltd.	Development of Novel Nanocomposites and Their Processing	¥420,000
Tohru Sekino	Shiga Prefecture	Studies on the Development of Thermoelectric Materials	¥0

Koichi Niihara Takafumi Kusunose	Tokuyama Corporation	Development of AlN/BN Nanocomposites with High Fracture Toughness and High Strength	¥3,000,000
Takafumi Kusunose	Sumitomo Electric Industries, Ltd.	Synthesis of Phosphor Exited by Electron or Electric Field	¥1,000,000

Other Research Funds

Tohru Sekino	NEDO (Industrial Technology Research Grant Program in 2004)	Hyper-functionalization of Oxide Nanotube and Its Application for Environmentally-harmonized Systems	¥16,289,000
Takafumi Kusunose	NEDO (Industrial Technology Research Grant Program in 2001)	Application of BN Dispersed Nanocomposites in Fields of Semiconductor Manufacturing Equipment and Biomaterial	¥8,372,000
Tohru Sekino	Japan Science and Technology Agency	Seeds Fostering Research in 2005 Mechanical Properties Enhancement of CNT-dispersed Conductive Ceramic Nanocomposites	¥2,000,000

Department of Advanced-Energy Material

Professor: Katsumi TANIMURA
Associate Professor: Shin'ichiro TANAKA
Designated Research Assoc.: Ei'ichi INAMI,
Graduate Students: Junji Tsuruta, Yoshiaki Sugita, Kazunori Ichihashi,
Taku Ichibayashi
Support Staffs: Sachiyo NOZAWA,
Masanobu NUNOGAKI

Outlines

For fabricating highly functional nano-structured devices in future technology, it is essential to establish the ways to control structures and compositions of materials in atomic levels. In this department, we aim to establish the fundamentals for controlling the ***atomic binding in epitaxial processes*** 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 at solid excited state,
- 2) ultrafast carrier dynamics on semiconductor surfaces,
- 3) excitation-induced structural changes of semiconductor surfaces,

As topics in the first category, we have studied the primary processes of the dynamics of the photoinduced phase transition in quasi-one dimensional organic crystals. 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, femtosecond laser-induced phase transformation of graphite to a new phase of diamond is a very recent topic we have studied.

Current Research Programs

1. Dynamics of Photoinduced Phase Transition in Quasi-One Dimensional Organic Crystals

The purpose of this subject is to elucidate the mechanisms of photoinduced phase transitions characteristic of quasi one-dimensional organic crystals. The real-time dynamics, studied by femtosecond time-resolved studies, give crucial information for establishing microscopic understanding of the mechanisms. Topics studied in this year and the main results obtained are summarized below.

2. Excitation-Induced Instability on Semiconductor Surfaces

By using STM for revealing the structural changes on surfaces from atomic level, together with the femtosecond non-resonant ionization spectroscopy, which enables us to detect desorbed neutral species simultaneously with high sensitivity, we have studied

the laser-induced electronic processes of structural changes and desorption for Si(111)-(7x7), Si(001)-(2x1), Si(111)-(2x1), GaAs(110)-(1x1) and InP(110)-(1x1) surfaces. For all surfaces studied, the laser-induced electronic excitation results in surface structural changes associated with bond breaking of constituent atoms incorporated in the intrinsic surface structures. Based on the extensive experimental results for these semiconductor surfaces, we have established a unified theoretical mechanism of the instability this year, that can describe quantitatively the efficiency of surface bond breaking successfully. The mechanism is based on the two-hole localization of valence holes at an intrinsic surface sites.

Not only by laser excitation but also low-energy electron beams in the range of 10-100 eV can induce structural instability on semiconductor surfaces. We have studied the instability of Si(111)-(7x7) to prove experimentally that the surface plasmon is responsible for the structural change via two-hole localization mechanism, similar to the case of laser-induced instability.

3. Ultra-fast surface carrier dynamics on Si(001)-(2x1) studied by femtosecond two-photon photoelectron spectroscopy

We have studied the electron dynamics on the surfaces by means of two-photon photoelectron spectroscopy in order to elucidate the dynamics of photogenerated surface carriers, which play crucial roles in the photoinduced atomic processes on solid surfaces. Use of femtosecond laser pulses 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 150-fs temporal width has opened a new breakthrough for studying the dynamics extensively. By probing both the electrons in the bulk conduction band and those in surface-specific states of the Si(001)-(2x1) surface, we have found an ultrafast electron-hole recombination via surface localized state 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 surface un-occupied state of D_{down} shows a strong excitation-wavelength dependent feature.

4. Highly functional Surface-layer formation by Means of Charged-particle Irradiation and Plasma Processing

We have developed a multiplex surface processing for creating “a new type metal ceramics” which have the properties of high thermal loading. 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 constructing moving electrodes, which make it possible of ion-beam irradiation and plasma processing for the same samples without breaking high vacuum condition. The electrodes has given a reasonable performance in intensity and in stability.

Publications

Original Papers

Time-resolved two-photon photoelectron spectroscopy of carrier dynamics on the Si(001)-(2x1) surface, S. Tanaka and K. Tanimura, Surf. Sci. 593, (2005) 26-31.

Structural instability of Si(111)-(7x7) induced by low-energy electron irradiation, Y. Sugita, H. Horiike, J. Kanasaki, and K. Tanimura, Surf. Sci. 593, (2005) 168-172.

Formation and Clustering of Surface Vacancies under Electronic Excitation on Semiconductor Surfaces, J. Kanasaki, Physica B 376-377, (2005) 834-840.

International Conferences

Formation of Clustering of Surface Vacancies under Electronic Excitation on Semiconductor Surfaces (Invited). *J. Kanasaki, The 23rd International Conference on Defects in Semiconductors, Awaji, Japan, July 24-29, 2005.

Photoinduced Structural Instability on Semiconductor Surfaces (Invited). K. Tanimura, The 23rd European Conference on Surface Science, Berlin, Germany, Sept. 4-9, 2005.

Surface Carrier Dynamics on Si(001)-(2x1) Studied by Time-Resolved Two-Photon Photoelectron Spectroscopy with Tunable Femtosecond Excitation Lasers. T. Ichibayashi, S. Tanaka, and K. Tanimura, The 23rd European Conference on Surface Science, Berlin, Germany, Sept. 4-9, 2005.

Laser-Induced Removal of Fragmentary Intact Sheets and Transformation into New Structural Phases on Graphite (0001) Surface. J. Kanasaki and K. Tanimura, The 23rd European Conference on Surface Science, Berlin, Germany, Sept. 4-9, 2005.

Differential STM Image Analysis of Adatom Vacancies on Si(111)-(7x7) Surfaces. J. Kanasaki and K. Tanimura, The 23rd European Conference on Surface Science, Berlin, Germany, Sept. 4-9, 2005.

Photoinduced Graphite-to-"Diamond" Phase Transition. K. Tanimura, Gordon Research Conference on Ultrafast Phenomena in Cooperative Systems, Santa Ynez Valley, California, USA, Feb. 5-10, 2006.

Structural Analysis on High Density H (D) Absorbed Nano-size Pd for Hydrogen Storage Materials. Y. Arachi, S. Huichimura, A. Omura, M. Nunogaki, T. Asai, S. Yamaura, A. Inoue and Y. Arata, The 15th International Conference on Solid State Ionics, Baden-Baden, Germany, July 2005.

Hydrogen Absorbing Process in Nano-Composite Pd/ZrO₂ for Hydrogen Storage Materials. Y. Arachi, S. Emura, A. Omura, M. Nunogaki, T. Asai, S. Yamaura, A. Inoue, Y. Arata, Functional

Materials for the 21st Century, Edinburgh, UK, July, 2005.

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Publications in Domestic Meetings

Physical Society of Japan	15 papers
Japan Society of Applied Physics	1 papers

Academic Degrees

Bachelor Degree of Engineering

N. Haruna	Ultrafast carrier dynamics on semiconductor surfaces
K. Kimura	Femtosecond-laser induced structural phase transitions of graphite to diamonds

Master Degree of Engineering

J. Tsuruta	Photoinduced structural instability of compound semiconductor surfaces
T. Ichibayashi	Surface carrier dynamics on semiconductor surfaces by tunable femtosecond 2ppe technique
Y. Sugita	Structural instability of Si(111)-(7x7) induced by low-energy electron beam excitation

Sponsorship

Grand-in-Aid for Scientific Research (B)

K. Tanimura	Study of excited-state properties of quasi-two dimensional semiconductor surfaces	¥17,600,000
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Grand-in-Aid for Scientific Research (C)

S. Tanaka	Ultra-fast carrier dynamics on semiconductor surfaces by means of time-resolved femtosecond 2ppe technique	¥700,000
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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.

Achievements

- Development of chemical sensors detecting CAG trinucleotide repeat
- Proposal of new motif for nucleic acid recognition
- SNP-detecting method with remarkable simplicity and rapidity
- A new method labeling PCR products with enantiomeric DNA
- Derivatization of fusicoccane diterpenoids to have anti-cancer activity
- Reverse chemogenomics on intracellular signal transductions
- Synthesis of biologically-active heteroaromatic compounds
- Development of p-type and n-type semiconductors for organic electronics
- Construction of molecular wires with switching and insulation-covering functions
- Construction of molecular machines “molecular muscles” and “molecular valves” based on permethylated cyclodextrins
- Beam-controlled chemistry of DNA
- Multi-laser multi-step photochemistry
- Photocatalytic reactions of TiO_2
- Photochemical control of protein function
- Synthesis and application of isoxazoline/isoxazole hybrid-type asymmetric ligands
- Immobilization of multicomponent consisting asymmetric catalysts
- Functionalized nanoparticle as an asymmetric catalyst
- Development of spiro chiral ionic liquids

Department of Regulatory Bioorganic Chemistry

Professor:	Kazuhiko Nakatani
Research Associate:	Da-Yang Zhou, Masaki Hagihara, Chikara Dohno (From Oct. 16)
Technical Staff:	Fumie Takei
Post Doctoral Fellow	Tao Peng, Jinhua Zhang
Graduate Student	Gosuke Hayashi
Research Assistance	Mika Oku

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 Programs

Molecular Design of Ligands Selectively Binding to Trinucleotide Repeat

DNA trinucleotide repeats, particularly CXG, are common within the human genome. Expansion of trinucleotide repeats is associated with a number of disorders, including Huntington's disease, spinobulbar muscular atrophy, and spinocerebellar ataxia. In these cases, the repeat length is known to correlate with decreased age of onset and disease severity. Repeat expansion of (CAG)_n, (CTG)_n, and (CGG)_n trinucleotides may be related to the increased stability of alternative DNA hairpin structures consisting of CXG/CXG triads with X-X mismatches. Small molecule ligands that selectively bound to CAG repeats could provide an important probe for determining repeat length and an important tool for investigating the in vivo repeat extension mechanism. We have discovered that naphthyridine-azaquinolone (NA) was a ligand for CAG repeats and could be used as a diagnostic tool for determining repeat length. We show by NMR spectroscopy that binding of NA to CAG repeats induces extrusion of a cytidine nucleotide from the DNA helix.

Studies on Novel Motif for DNA Recognition

We discovered a novel molecular ligand naphthyridine carbamate dimer (NC) that bound to the CGG/CGG triad. The exclusive 2:1 stoichiometry of NC-binding to the CGG/CGG triad was confirmed by the measurements of cold spray ionization time-of-flight mass spectrometry (CSI-TOF MS) and UV absorption titration experiments. The cytosine in the NC-bound CGG/CGG triad was susceptible to the subsequent chemical cleavage reaction initiated by hydroxylamine and hot piperidine. Upon treating the NC-bound CGG/CGG triad, DNA oligomer was selectively cleaved at the site of cytosine in

the triad, indicating that the guanine-cytosine base pairing in the triad was broken up upon NC-binding. CSI-TOF MS measurements also suggested that the 2:1 NC-CGG/CGG complex was produced in the (CGG)_n repeat. A large conformational change of d(CGG)₁₀ observed in CD measurements upon binding with NC supported the hairpin formation. NC could be a useful molecule for studying not only the repeat expansion mechanism but also the nucleobase-ligand interactions on the biologically important repeat sequence.

Development of Rapid, Simple, and Cheap Methods of Mutation Detection

Typing of the single nucleotide polymorphisms (SNPs) in an individual genome against sets of predetermined disease-related SNPs is necessary to achieve personalized medicine. Besides the methods exploiting the sequence specific reactions of enzymes, the challenge toward novel SNP typing methods based on the organic chemistry draw attention to the molecular systems that emit fluorescence in an allele specific manner. Regarding the convenience and the simplicity of the assay, typing methods using fluorescent molecules would be particularly effective if the covalent modification of the probe DNA were not required, and if all four nucleotide bases could be analyzed by one unique fluorescent molecule. To address these issues, we have investigated a method exploiting the allele specific C-bulge probe as a scaffold to recruit a fluorescent molecule directly neighboring the SNP site. Our laboratory has discovered N,N'-(3-aminopropyl)-2,7-diamino-1,8-naphthyridine (DANP), which selectively and strongly bound to the C-bulge with an exclusive 1:1 binding stoichiometry. We discovered that the profile in the fluorescence change of DANP for the allele specific C-bulge probes hybridized to the target DNA clearly determined the allele type of the predetermined SNP site.

Novel PCR Method with Enantiomeric DNA

Polymerase Chain reaction (PCR) is indispensable for current biotechnology, and is a still growing technique by integrating new concepts to meet the increasing demands for the innovative PCR applications. We have discovered the L-DNA tagged PCR (LT-PCR) that enables us to code the PCR products with a defined sequence of mirror image DNA (L-DNA) tag. A primer used in LT-PCR was tethered at the 5' end with a sequence tag of L-DNA. The L-DNA tag did not interfere the PCR and was ignored by Taq DNA polymerase. Thus, the product of LT-PCR is the duplex DNA tethering a L-DNA sequence tag. Without separation, purification, and denaturation, LT-PCR products could be directly hybridized onto a microarray where the complementary L-DNA to the sequence tag was immobilized. Combining with allele-specific PCR, LT-PCR offers a practical method of SNP typing on L-DNA-immobilized surface-plasmon-resonance (SPR) array. Integration of L-DNA technology into PCR, microarray, and other DNA-based techniques would extend the reach of current biotechnology and molecular biology.

Publications

Original Papers

Binding of Naphthyridine Carbamate Dimer to the (CGG)_n Repeat Resulted in the

Disruption of the G-C Base Pairing, T. Peng, K. Nakatani, *Angew. Chem. Int. Ed.* 44 (2005) 7280-7283.

Small-molecule ligand induces nucleotide flipping in (CAG)_n trinucleotide repeats, K. Nakatani, S. Hagihara, Y. Goto, A. Kobori, M. Hagihara, G. Hayashi, M. Kyo, M. Nomura, M. Mishima, C. Kojima, *Nature Chemical Biology* 1 (2005) 39-43.

N,N'-Bis(3-aminopropyl)-2,7-diamino-1,8-naphthyridine stabilized a single pyrimidine bulge in duplex DNA, H. Suda, A. Kobori, J. Zhang, G. Hayashi, K. Nakatani, K. Bioorg. Med. Chem. 13 (2005) 4507-4512.

A new ligand binding to G-G mismatch having improved thermal and alkaline stability, T. Peng, T. Murase, Y. Goto, A. Kobori, K. Nakatani, *Bioorg. Med. Chem. Lett.* 15 (2005) 259-262.

Thermally Induced Helical Conformational Change in Poly(aryl isocyanide)s with Optically Active Ester Groups, F. Takei, K. Onitsuka, S. Takahashi, *Macromolecules* 38 (2005) 1513-1516.

Application of small-angle X-ray scattering utilizing X-ray anomalous dispersion to nano-structure analysis, M. Sugiyama, Y. Soejima, K. Hara, F. Takei, K. Itoh, K. Mori, T. Fukunaga, *Transactions of the Materials Research Society of Japan* 30 (2005) 855-858.

Review Papers

Diagnosis of Huntington Disease by Chemical Sensor, K. Nakatani, *Bionics*, 2005.

ESI-MS: An Effective Tool for Analyzing Ligand-DNA Interactions, K. Nakatani, *Pharmacia*, 41 (2005), 1076-1080.

International Conferences

Mismatch Binding Ligands Discovery and Applications (Invited), *K. Nakatani, The 12th Japan-Korea Seminar on Organic Chemistry, Tokyo, Japan, September 13-14, 2005.

Small Molecular Ligand Selectively Binding to Cytosine Bulge in DNA: Application for The Fluorescent Detection of Genetic Mutations (Invited), *K. Nakatani, The 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Small ligands that can induce a structural change in human telomere DNA, *M. Hagihara, K. Nakatani, The 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Thermally induced helical conformational change in poly(aryl isocyanide)s, *F. Takei, K. Onitsuka, S. Takahashi, K. Nakatani, The 2005 International Chemical Congress of

Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Small ligands that can induce a structural change in human telomere DNA, *M. Hagihara, K. Nakatani, 4th 21st Century COE "Towards Creating New Industries Based on Inter- Nanoscience" International Symposium, Toba, Mie, Japan, November 18-19, 2005.

Cobalt-catalyzed aminative cyclocarbonylation of alkynylimines, *D.-Y. Zhou, K. Onitsuka, S. Takahashi, K. Nakatani, The 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Application for The Fluorescent Detection of Genetic Mutation using N,N'-bis(3-aminopropyl)-2,7-diamino-1,8-naphthyridine, *F. Takei, J. Zhang, K. Nakatani, 4th 21st Century COE "Towards Creating New Industries Based on Inter- Nanoscience" International Symposium, Toba, Mie, Japan, November 18-19, 2005.

Publications in Domestic Meetings

85 th Japan Chemical Society Meeting:	3 papers
32 nd Symposium on Nucleic Acids Chemistry in Japan:	4 papers
54 th Symposium on Polymer Science:	1 papers
Annual Meeting on Chemical Life Science:	2 papers

Sponsorship

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

K. Nakatani	Molecular Design of Drugs regulating the higher order structure of trinucleotide repeat DNA	¥15,340,000
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Grant-in-Aid for Scientific Research on Priority Area

K. Nakatani	Suppression of repeat expansion by CAG-binding ligand	¥4,800,000
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Grant-in-Aid for Scientific Research on Exploratory Research

K. Nakatani	Development of Drugs that targeting the suppression of on set of Huntington Disease	¥1,600,000
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Other Research Fund

K. Nakatani	Health and Labor Sciences Research Grants for Research on Advanced Medical Technology from Ministry of Health	Studies on the SNP-detecting device based on mismatch binding ligands	¥43,545,000
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Department of Organic Fine Chemicals

Professor:	Nobuo KATO
Associate Professor:	Junko OHKANDA (from Jun. 1)
Research Associates:	Hajime NITTA, Tomikazu KAWANO
Post Doctoral Fellow:	Bulbule VIVEK (until Jun. 30)
Graduate Students:	Masamitsu HIRAOKA, Erika KAJITANI, Hitoshi KAJIYA, Akinobu TAKEDA, Yoshimi YANO, Takahiko YOSHINO, Takatsugu INOUE, Ichiro IMADA, Taro ENOMOTO, Masato HIRANO, Shinnosuke MACHIDA
Research Student:	Takayoshi KOBE
Support 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 Programs

1. Synthesis of Fusicoccin Derivatives Having Differentiation-Inducing Activity

We have found that cotylenin (CN) induces functional and morphological differentiation of human myeloid leukemia cells (HL-60). However, fusicoccin (FC), structurally closely related to CN, was less efficient in spite of the fact that FC and CN have identical activities on plant tissues. To clarify the structural requirements, we have synthesized several derivatives of FC. Detailed Structure-Activity-Relationship studies lead a conclusion that the 12-OH of FC interferes activity. And, therefore, this hydroxy group must be eliminated to have differentiation-inducing activity. We have succeeded in synthesizing FC derivatives, of which activities are as potent as that of CN.

2. Synthesis of Stable Antagonists and Antagonists of Autoinducer-2 in Bacterial Quorum-Sensing

Bacteria can communicate with members of their own species and others, known as quorum-sensing, by use of secreted molecules. Among the autoinducers, type II autoinducer (AI-2) is highly labile. Therefore, we have designed and synthesized a chemically-stable AI-2 agonist, of which quorum-sensing activity has been confirmed by the bioluminescence assay using *Vibrio harveyi* strain BB152. We have also synthesized several antagonists of AI-2 as well.

3. Design, Synthesis, and Functional Evaluation of Hybrid Geranylgeranyl-

transferase-I Inhibitors that Recognize Interior and Exterior Protein Surfaces

Low-molecular-weight compounds, which bind to protein exterior surfaces and potentially mimic native protein-protein interactions, are expected to show high binding affinity to the target protein. In this project a new series of hybrid inhibitors against geranylgeranyltransferase-I, an enzyme that has been receiving intense attention due to its potential as a target for new antitumor drug discovery, were designed and synthesized. The hybrid molecules were derived from the traditional peptidomimetic motif which was attached to a gallic acid derivative containing phenylalanine residues by an appropriately lengthed alkyl linker for simultaneous binding to the interior and exterior surface of the enzyme. The synthetic compound inhibits approximately 70% of GGTase-I activity at 3 μ M in vitro. This inhibition potency is almost equivalent to that of GGTI-2154, a potent, commercialized peptidomimetic inhibitor.

4. One-Pot Synthesis of 3-Bromoimidazo[1,2-*a*]pyridine Derivatives Accompanied by Dimethylsulfoxide Oxidation

Imidazo[1,2-*a*]pyridine (IP) derivatives have received considerable attention in the fields of organic chemistry and medicinal chemistry. Recently, a report has also documented left-right patterning defects in zebrafish embryos with SCH28080, which also contains an IP framework. IP derivatives with these attractive properties possess a key functional group at the 3-position of the framework. Therefore, development of an efficient synthetic route for 3-bromoimidazo[1,2-*a*]pyridines under mild conditions is worth to be investigated. We have succeeded in the development of a novel method for the preparation of 3-bromoimidazo[1,2-*a*]pyridines by the reaction of 2-aminopyridine derivatives with an excess amount of α -bromoketones in dimethyl sulfoxide.

5. Developing Methods for Lipase-Catalyzed Regio-Selective Acylation of Epigallocatechin gallate, A Green Tea Catechin

Epigallocatechin gallate (EGCG) is one of major green tea extracts that has been suggested to possess potent antiviral effects on RNA viruses such as human immunodeficiency virus type-1 (HIV-1) and Influenza. Enhancing the antiviral effect of EGCG should allow us to explore antiviral drugs for wide variety of RNA viruses. However the poor chemical stability and the cellular permeability of EGCG lowered its antiviral effect in vivo. To solve these problems, we developed a method to prepare EGCG acyl-derivatives by lipase-catalyzed reactions. Synthesized EGCG acyl-derivatives were found to have higher stabilities (>10-fold) under physiological conditions and showed higher antiviral effects (> 4 fold) on Influenza A/PR8/34/H1N1 compared to EGCG. (collaborated with Dr. Kunihiro Kaihatsu, research associate of Department of Analytical Molecular Chemistry)

Publications

Original Papers

Synthesis of indenothiophenone derivatives by cycloaromatization of non-conjugated thienyl tetraynes, T. Kawano, H. Inai, K. Miyawaki, and I. Ueda: *Tetrahedron Lett.*, 46 (2005) 1233-1236.

Triple-Stranded Helicates as a Synthetic Template: Synthesis of Pyridine-Containing Macrocyclic Compounds, T. Kawano, M. Nakanishi, T. Kato, and I. Ueda: Chem. Lett., 34 (2005) 350-351.

Inhibiting Transcription of Chromosomal DNA with Antigene Peptide Nucleic Acids, B. A. Janowski, K. Kaihatsu, K. E. Huffman, J. C. Schwartz, R. Ram, D. Hardy, C. R. Mendelson and D. R. Corey: Nature Chemical Biology, 1 (2005) 210-215.

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Patents

Aryl acyl thioharnstoff and the related chemical compound which are substituted; inhibitor of virus duplication, A. Phadke, Avinashi, D. Chen, M. Deshpande, A. Thurkauf, X. Wang, Y. Shen, C. Liu, J. Quinn, J. Okanda, S. Lee, JP2005330284.

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Method for Manufacturing Acylated Derivative of Epigallocatechin Gallate, K. Kaihatsu, S.D. Fuller, T Kobe, and N. Kato, PCT-JP2006-304788.

International Conferences

Mammalian GGTase-I Inhibitors: A solution Phase Combinatorial Approach and Structure-based Design of Hybrid Inhibitors (Invited), *J. Ohkanda, 21st Conference on Combinatorial Chemistry, Japan 2005, Tokyo, Japan, Sep. 21-22, 2005.

Peptidomimetic Inhibitors for Geranylgeranyltransferase-I: Structure-based Design and Solution Phase Combinatorial Approach (Poster), *J. Ohkanda, A. D. Hamilton, and N. Kato, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Forth International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Interfering RNA Virus Membrane Fusion By A Green Tea Catechin Extract, Epigallocatechin Gallate (Poster), *K. Kaihatsu, S. D. Fuller, and N. Kato: 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Forth International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Fusicoccane Diterpenoids Having Differentiation-inducing Activity on Human Myeloid

Leukemia Cells: Studies on Structural Requirements, *N. Kato, H. Nitta, T. Yoshino, Y. Honma, and T. Sassa: The 2005 International Chemical Congress of Pacific Basin Societies, Hawaii, USA, Dec. 15-20, 2005.

Solid-phase organic synthesis of epoxides by using arylsulfide resin (Poster), *T. Kawano, and N. Kato: The 2005 International Chemical Congress of Pacific Basin Societies, Hawaii, USA, Dec. 15-20, 2005.

Synthesis of autoinducer-2 agonists and antagonists in bacterial quorum-sensing (Poster), *M. Hiraoka, Y. Yano, T. Kawano, H. Hirakawa, A. Kobayashi, T. Hirata, A. Yamaguchi, N. Kato: The 2005 International Chemical Congress of Pacific Basin Societies, Hawaii, USA, Dec. 15-20, 2005.

Publications in Domestic Meetings

National Meeting of Chemical Society of Japan	10 papers
Congress of Heterocyclic Chemistry	1 paper
Heterocyclic Chemistry Forum	1 paper
Symposium on Biomolecular Chemistry	1 paper
Japan Society for Bioscience, Biotechnology, and Agrochemistry	1 paper

Sponsorship

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

N.Kato	Chemogenomic Approach to Clarify the Intracellular Signal Transductions	¥3,200,000
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Grant-in-Aid for Scientific Research in Special Area (2)

N.Kato	Analysis and Control of Intracellular Signal Transductions by Use of Diterpene Glycosides as Tools	¥3,400,000
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Grant-in-Aid for Scientific Research (A) (1)

N.Kato	Gene-Cloning of Fungal and Plant Terpene Synthases and Its Usage for the Production of Useful Compounds	¥1,100,000
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Other Research Funds

J. Ohkanda	Hayashi Memorial Foundation for Female Natural Scientists	Design and Synthesis of Hybrid Inhibitors that Recognize both Interior and Exterior Protein Surfaces	¥1,500,000
K.Kaihatsu	Venture Business Support Program, Osaka University	Developing Anti-Avianflu Drugs with Green Tea Catechin Derivatives	¥750,000

Department of Organic Molecular Materials

Professor:	Yoshio ASO
Associate Professor:	Takahiro KANEDA
Research Associate:	Yutaka IE
Research Assistant:	Kaori ASANO
Post Doctoral Fellow:	Aihong HAN
Invited Researcher:	Muhammad Mizanur RAHMAN
Graduate Students:	Nobukazu NEGISHI, Yoshikazu UMEMOTO, Wakana YAMAMOTO, Tetsuro KAWABATA, Susumu TSUDA, Setsuko ISHIOKA, Masaru ENDO, Liu FENG
Under Graduate Students:	Masashi NITANI, Tomoya HIROSE
Support Staff:	Misayo IMAI

Outlines

The main subject in the Department of Organic Molecular Materials is development of novel molecular-based materials with promising electronic and photoelectric properties for molecular electronics and highly organized supermolecules for supramolecular machines, which is based on the study of the relationship between molecular structure and physical properties to elucidate and control the functions. We have focused our research on the design, synthesis, and properties of (1) novel extended conjugation systems with switching or self-association functions for electronic and photoelectric materials, (2) fully insulated nano-scale conjugated molecules for promising molecular wires, and (3) supermolecules composed of permethylated cyclodextrins and various π -systems especially oligothiophenes, azobenzenes, stilbenes, and tolans. These nano-scale molecular materials have potential use as a fundamental framework for molecular electronic devices.

Current Research Programs

1. Molecular Electronics Materials

We have developed organic materials for n-type organic field-effect transistors. It has been known that the introduction of perfluoroalkyl groups into π -conjugated systems dramatically increases n-type character. We have synthesized hexafluorocyclopenta[c]thiophene and its-based oligothiophenes. Their electronic absorptions, X-ray analysis and redox potentials indicated that the ring fusion of hexafluorocyclopentane unit to both β -sites of thiophene ring not only keep the planarity between consecutive thiophene rings but also increases n-type character.

Donor-acceptor linked oligothiophene, which incorporated with an imidazolium salt as a switching unit, was synthesized. The fluorescence measurement showed that the fluorescence intensity was found to be dependent on the counter anion. This result indicates that the degree of electron transfer can be controlled by the influence of counter anions.

We have synthesized the branched oligothiophenes with the juncture of 1,3,5-

trisubstituted benzene ring for development of high carrier-mobility materials in a film. The NMR spectra of the compounds with several junctures showed the significant dependence of chemical shifts of the aromatic protons on both the concentration and the temperature. The association constants and thermodynamic parameters determined from the NMR data revealed an increasing association properties with increasing the number of branch points as well as the length of oligothiophenes. Moreover, MALDI-TOF MS revealed a series of clear ion peaks of the associated species together with the strong molecular-ion peak. The thin-film field-effect transistors fabricated by spin coating from a solution of the branched oligothiophene showed reasonably good p-type characteristics.

2. Molecular Wires

We have been preparing molecular wires for building up nanoelectronic devices, with the use of the 24-mer of oligothiophenes (24T) with ca. 10 nm in length having insulating coverage around the oligomer chain. We firstly prepared the thiophene-monomer unit with bulky t-butyldiphenylsilyl groups, and then a series of its oligomers was synthesized by repeated oxidative coupling reactions. The X-ray analysis of 4T revealed that the oligomeric backbone of 4T is completely insulated by the bulky t-butyldiphenylsilyl 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 electrode and we have succeeded in synthesis of 4T, 8T, and 24T with terminal thiol anchor groups for metal electrodes.

3. Molecular Machines

We have developed design and construction of molecular machines based on [n]supercyclodextrins defined as cyclic n-mers of hermaphroditic cyclodextrin derivatives. The supercyclodextrins are a new class of interlocked supermolecules organized by a mechanical bond and have potential use as a fundamental framework for assembling nanoscale molecular devices.

Publications

Original Papers

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Photophysical Properties of Oligo(2,3-thienyleneethynylene)s, Y. Oseki, M. Fujitsuka, M. Hara, X. C. Cai, Y. Ie, Y. Aso, and T. Majima: *J. Phys. Chem. B*, 109 (2005) 10695-10698.

Syntheses, Structures, Spectroscopic Properties, and pi-Dimeric Interactions of [n.n]Quinquethiophenophanes, T. Sakai, T. Satou, T. Kaikawa, K. Takimiya, T. Otsubo, and Y. Aso: *J. Am. Chem. Soc.*, 127 (2005) 8082-8089.

Extensive Quinoidal Oligothiophenes with Dicyanomethylene Groups at Terminal Positions as Highly Amphoteric Redox Molecules, T. Takahashi, K. Matsuoka, K. Takimiya, T. Otsubo, and Y. Aso: *J. Am. Chem. Soc.*, 127 (2005) 8928-8929.

Effect of Substituents on Charge Carrier Dynamics in Thiophene Oligomers, A. Acharya, Y. Koizumi, S. Seki, A. Saeki, S. Tagawa, Y. Ie, and Y. Aso: *J. Photochem. Photobio. A*, 173 (2005) 161-168.

Control of Photoinduced Energy- and Electron-Transfer Steps in Zinc Porphyrin-Oligothiophene-Fullerene Linked Triads with Solvent Polarity, T. Nakamura, J. Ikemoto, M. Fujitsuka, Y. Araki, O. Ito, K. Takimiya, Y. Aso, and T. Otsubo: *J. Phys. Chem. B*, 109 (2005) 14365-14374.

Oligothiophene-multifullerene Linkage Molecules as High Performance Photovoltaic Materials, N. Negishi, K. Takimia, T. Otsubo, Y. Harima, and Y. Aso: *Synth. Metals*, 125 (2005) 125-128.

Synthesis and Spectral Properties of a Highly Soluble Push-Pull Type of Quinoidal Thiophenes, T. Takahashi, K. Takimiya, T. Otsubo, and Y. Aso: *Org. Lett.*, 7 (2005) 4313-4316.

Rhodium-Catalyzed C-H– CO– Olefin Coupling Reactions. A Chelation-Assisted Direct Carbonylation at the ortho C-H Bond in the Benzene Ring of 2-Arylpyridines, N. Chatani, T. Uemura, T. Asaumi, Y. Ie, F. Kakiuchi, and S. Murai: *Can. J. Chem.*, 83 (2005) 755-763.

Polyether-Bridged Sexithiophene as a Complexation-Gated Molecular Wire for Intramolecular Photoinduced Electron Transfer, T. Oike, T. Kurata, K. Takimiya, T. Otsubo, Y. Aso, H. Zhang, Y. Araki, and O. Ito: *J. Am. Chem. Soc.*, 127 (2005) 15372-15373.

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Fullerene-tethered Oligothiophenes as Advanced Molecular Electronics Materials, T. Otsubo, Y. Aso, and K. Takimiya: *Pure Appl. Chem.*, 77 (2005) 2003-2010.

Books

Molecular Wires, Y. Aso, *The Fifth Series of Experimental Chemistry*, 28, The Chemical Society of Japan, Maruzen (2005) 1-27.

Patents

Oligothiophenes based on Hexafluorocyclopenta[c]thiophene Monomer Unit, Y. Ie, Y. Aso, Y. Umemoto, and M. Ueda, JP2005-261284

Fluorinated Compounds and Their Synthesis, Fluorinated Polymer, Organic Thin Films, and Organic Thin Film Devices, Y. Ie, Y. Aso, M. Nitani, and M. Ueda, JP2006-045768

Polymers Consisting of Condensation Units with Fluorocyclopentane Ring and Aromatic Ring and Their Organic Thin Films and Organic Thin-Film Devices, Y. Ie, Y. Aso, Y. Umemoto, and M. Ueda, JP2006-066729

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Synthesis and their properties of blanché oligothiophenes (Poster), *N. Negishi, Y. Ie, T. Kaneda, and Y. Aso, International Symposium on Molecular Conductors 2005 (ISMC 2005) "Novel functions of molecular conductors under extreme conditions", Hayama, Japan, July 17-21, 2005.

Synthesis and Properties of Branched Oligothiophenes (Poster), *Y. Aso, N. Negishi, Y. Ie, and T. Kaneda, 11th International Symposium on Novel Aromatic Compounds, St. John's, Canada, August 14-18, 2005.

Synthesis and Self-association Properties of Branched Oligothiophenes (Poster), *N. Negishi, Y. Ie, T. Kaneda, and Y. Aso, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Mie, Japan, November 18-19, 2005.

Synthesis and Properties of Hezafluorocyclopenta[c]thiophene-based Oligothiophenes towards n-Type Semiconductors (Poster), *Y. Ie, Y. Umemoto, T. Kaneda, and Y. Aso, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Mie, Japan, November 18-19, 2005.

Photophysical properties of polyether-bridged oligothiophenes as gated molecular wires (Poster), *T. Kurata, K. Koyama, I. Doi, T. Oike, K. Takimiya, T. Otsubo, and Y. Aso, 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, USA, December 15-20, 2005.

Fullerene-tethered oligothiophenes as novel photovoltaic materials (Poster), *M. Narutaki, M. Toguchi, S. Handa, K. Takimiya, T. Otsubo, Y. Harima, N. Nagishi, and Y. Aso, 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, USA, December 15-20, 2005.

Permethylated α -cyclodextrin-based molecular valves (1): Synthesis and photochemical behavior of a Janus rotaxane (Poster), *S. Tsuda, G. Fukuhara, T. Fujimoto, Y. Aso, and T. Kaneda, 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, USA, December 15-20, 2005.

Permethylated α -cyclodextrin-based molecular valves (2): The vent size of interlocked cyclic pentamers is controlled by solvent (Poster), *S. Ishioka, S. Tsuda, Y.

Development and electronics application of modified long oligothiophenes (Invited),
*Y. Aso, N. Negishi, A. Han, Y. Ie, and T. Otsubo, 2005 International Chemical
Congress of Pacific Basin Societies, Honolulu, USA, December 15-20, 2005.

Synthesis of branched oligothiophenes and their properties (Poster), *N. Negishi, Y. Ie, T. Kaneda, and Y. Aso, 2005 International Chemical Congress of Pacific Basin Societies, Honolulu, USA, December 15-20, 2005.

Synthesis and properties of hexafluorocyclopenta[c]thiophene-based oligomers (Poster),
*Y. Ie, T. Kaneda, and Y. Aso, 2005 International Chemical Congress of Pacific Basin
Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Synthesis and Properties of Oligomers Containing Hexafluorocyclopenta[c]thiophene (Poster), *Y. Umemoto, Y. Ie, T. Kaneda, and Y. Aso, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Suita, Japan, February 8-9, 2006.

Permethylated alpha-cyclodextrin-based molecular valves (1): Synthesis and photochemical behavior of a Janus rotaxane (Poster), *S. Tsuda, G. Fukuhara, T. Fujimoto, Y. Aso, and T. Kaneda, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Suita, Japan, February 8-9, 2006.

Permethylated alpha-cyclodextrin-based molecular valves (2): The vent size of interlocked cyclic pentamers is controlled by solvent (Poster), *S. Ishioka, S. Tsuda, Y. Aso, and T. Kaneda, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Suita, Japan, February 8-9, 2006.

Synthesis and Self-association Properties of Branched Oligothiophenes (Poster), *N. Negishi, Y. Ie, T. Kaneda, and Y. Aso, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Suita, Japan, February 8-9, 2006.

Development and Electronics Application of Modified Long Oligothiophenes (Invited),
*Y. Aso, The 2nd Taiwan-Japan Conference on Molecular Architecture of Organic
Compounds for Functional Designs, Fukuoka, Japan, March 24-25, 2006

Y. Aso 22nd International Symposium on the Organic Chemistry of Sulfur
(Organizing Committee)

Y. Aso	The Seventh International Symposium on Functional π -Electron Systems (Organizing Committee)
Y. Aso	12th International Symposium on Novel Aromatic Compounds (Organizing Committee, Financial Chair)
Y. Aso	SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams (Organizing Committee)
Y. Ie	SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams (Executive Committee)

Publications in National Meetings

The Chemical Society of Japan	8 papers
Symposium on Structural Organic Chemistry	6 papers
The Society of Polymer Science, Japan	2 papers

Academic Degrees

Master degree of Engineering

T. Kawabata	Synthesis and Properties of Oligothiophenes Molecular Wire Bearing an Imidazolium Salt as Switching Unit
S. Tsuda	Functionalization of Rotaxanes based on Guest-branched Cyclodextrin
Cyclodextrin	Permethylates

Sponsorship

Grant-in-Aid for Scientific Research (B)

Y. Aso	Function-Accumulated Extended-Conjugation Systems Based on Oligothiophenes and Their Novel Functions	¥4,100,000
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Grant-in-Aid for Scientific Research on Priority Areas (2)

Y. Aso	Electron-Transport Materials Based on Extended-Conjugation Systems and Their Novel Functions	¥2,200,000
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Entrusted Research

Y. Aso	Japan Science and Technology Agency	Synthesis of Insulated Molecular Wires	¥1,040,000
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Cooperative Research

Y. Aso	Sumitomo Chemical	Development of Materials for Organic Electronics	¥3,700,000
Y. Ie	Co., Ltd.		

Other Research Funds

Y. Aso	CREST, Japan Science and Technology Agency	Construction of Nano-electronic Devices Based on Precise Molecular Design	¥7,310,000
Y. Ie	Toso Award in Synthetic Organic Chemistry, Japan	Development of Perfluoroalkyl-bridged Aromatic Compounds and its Application to Luminescent Metal Complexes	¥500,000
Y. Ie	Kansai Research Foundation for Technology Promotion	Synthesis and Properties of Hexafluorocyclopenta[c]-thiophene-based Oligomers	¥70,000
Y. Ie	21 COE	Development of Organic Materials and STML Technique for Organic Luminescent Nano-device	¥1,000,000
N. Negishi	21 COE	Synthesis and Characteristics of Dendritic Oligothiophene/[60]-fullerene Linkage Molecules	¥500,000

Department of Molecular Excitation Chemistry

Professor:	Tetsuro MAJIMA
Associate Professor:	Mamoru FUJITSUKA
Research Associates:	Sachiko TOJO, Kiyohiko KAWAI (-2005.10.15), Takashi TACHIKAWA (2005.11.16-)
Visiting Professor:	Jin-Zhong XIANG (2005.5.10-11.11)
Visiting Associate Professors:	Akira SUGIMOTO, Dae Won CHO
Post Doctoral Researchers:	Xichen CAI, Takashi TACHIKAWA (-2005.11.15), Tadao TAKADA, Kohji NAKAYAMA,
Researchers:	Chunyan RIM, Shi-Cong CUI
Graduate Students:	Takumi KIMURA, Masanori SAKAMOTO, Yosuke OSEKI, Shingo SAMORI, Yasuko OSAKADA, Kazuya NAITO, Hangxiang WANG, Yoshiaki ASANOI, Mitsue OKADA
Undergraduate Students:	Ken HARADA, Sho YAMADA
Support 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 Programs

1. 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. We clarified the photo-cleavage of C-O bond via the higher triplet excited states of various organic compounds such as naphthalene, benzophenone and acetophenone by using two-color two-laser flash photolysis. Furthermore, we found C-Si bond can also be cleaved by excitation to the higher triplet state. We also investigated the excited state properties of ketyl radical of various compounds. Transient absorption spectra of excited ketyl radical were observed for the first time. We found that the excited ketyl radical of azaxanthone shows D₂-fluorescence, which violates the Kasha's rule. In addition, we found the electron transfer from excited ketyl radical.

2. TiO₂ Photocatalytic Reactions

One-electron oxidation of various aromatic compounds such as aromatic sulfides and biphenyl derivatives, adsorbed on the surface of TiO₂ powder slurried in acetonitrile has been investigated by time-resolved diffuse reflectance spectroscopy. We directly observed the formation of MV^{•+} generated from the one-electron reduction reactions with carbon dioxide radical anion (CO₂^{•-}), which is generated from the one-electron reduction reactions of HCO₂⁻ with the photogenerated h⁺, in the colloidal TiO₂ aqueous solution. It is indicated that the CO₂^{•-}, which is desorbed from the surface, reacts with MV²⁺ via a homogeneous electron transfer process in the bulk solution. We also studied the photocatalytic oxidation reactivities of the photogenerated h⁺ during the UV or Vis laser flash photolysis of S- and C-doped TiO₂ powders. The oxidation reactions of substrates by h⁺ generated during the 355-nm laser photolysis of the TiO₂ powders increased in the order of the pure > S-doped > C-doped TiO₂. On the other hand, no oxidation reaction was observed during the 430-nm laser photolysis of the S- and C-doped TiO₂ powders, although charge carriers were sufficiently generated under excitation. The mobility and potential energy of h⁺ trapped at the doping sites would have significant influence on the efficiency of the one-electron oxidation reactions of organic molecules adsorbed on the S- and C-doped TiO₂ powders.

3. Photochemistry of DNA

DNA site-specifically modified with probe molecules such as photosensitizer, molecules which radical ions have high extinction coefficient, fluorophore, were chemically synthesized. Based on the laser flash photolysis of the probe-modified DNA, physical and chemical properties of DNA were investigated. Through the direct measurements of the hole transfer in DNA, it was revealed that hole transfer process in DNA is coupled with proton transfer. By controlling the hole transfer process in DNA,

we successfully produced a long-lived charge-separated state with a quantum yield of up to 26%. A combination of laser flash photolysis kinetic studies and quantitative HPLC analyses of photosensitized DNA damage for photosensitizer-modified DNA were performed and it was clearly shown that hole transfer promotes photosensitized DNA damage and consecutive adenine sequences serve as potential targets in photosensitized DNA damage. Using the fluorophore-modified DNA, the microenvironmental changes in major and minor grooves of DNA upon B- to A-DNA conformational transition were revealed. We also succeed to determine the dynamics of the end-to-end contact of ssDNA by monitoring the formation rate of pyrene dimer radical cation.

• Photochemical Regulation of Enzymes

Photochemical regulation of enzymes by controlling the protein-protein interaction and peptide bond cleavage was investigated by introducing photoremovable, photoisomerizable, and photodegradable molecules into the specific positions of enzymes. Dimer interface of an endonuclease *Bam*HI was site-selectively photofunctionalized using photoremovable 2-nitrobenzyl derivatives and photoisomerizable azobenzene derivatives for suppressing the enzymatic activity. By photoactivation of the molecules, the enzyme recovered the activity, and the level of the activity was regulated by adjusting the photoirradiation time. Photochemical activation of an apoptosis-related caspase-3 was also examined. A photodegradable 2-nitrophenylglycine was incorporated into the specific position in the peptide chain. The photofunction group introduced to caspase-3 perfectly suppressed the activity without photoirradiation, and the irradiation rapidly produced the active form of the enzyme. These studies indicate that the combination of the selective photofunctionalization of the enzymes and photoirradiation are one of the reliable methods for practical control of the enzymes. The photofunctionalized enzymes can be introduced into a cell by attaching a protein-transduction domain and would be applied for induction of apoptosis by selective photoirradiation.

Publications

Original Papers

Remarkable Reactivities of Xanthone Ketyl Radicals in the Excited State Compared with that in the Ground State, M. Sakamoto, X. Cai, M. Hara, M. Fujitsuka, and T. Majima: *J. Am. Chem. Soc.*(Commun.) 127[11] (2005) 3702-3703.

Kinetics of Transient End-to-End Contact of Single-Stranded DNAs, K. Kawai, H. Yoshida, A. Sugimoto, M. Fujitsuka, and T. Majima: *J. Am. Chem. Soc.* 127[38] (2005)

13232-13237.

Fast Exciton Migration in Porphyrin-Functionalized Polypeptides, M. Fujitsuka, M. Hara, S. Tojo, A. Okada, V. Troiani, N. Solladié, and T. Majima: *J. Phys. Chem. B* (Commun.) 109[1] (2005) 33-35.

Inhibition of the formation and decay of core-stilbene radical cations by the dendron-phenoxy groups during the photoinduced electron transfer, M. Hara, S. Samori, X. Cai, S. Tojo, T. Arai, A. Momotake, J. Hayakawa, M. Uda, K. Kawai, M. Endo, M. Fujitsuka, and T. Majima: *J. Phys. Chem. B* 109[2] (2005) 973-976.

Hofmeister Effects on the Electron Transfer Reactions of 1-Pyrenesulfonic Acid Radical Cation with Nucleophilic Anions in Nafion Membrane, T. Tachikawa, R. Ramaraj, M. Fujitsuka, and T. Majima: *J. Phys. Chem. B* 109[8] (2005) 3381-3386.

Formation of Highly Stabilized Intramolecular Dimer Radical Cation and π -Complex of $[3_n]$ Cyclophanes ($n = 3, 5, 6$) during Pulse Radiolysis, M. Fujitsuka, S. Samori, M. Hara, S. Tojo, S. Yamashiro, T. Shinmyozu, and T. Majima : *J. Phys. Chem. B* 109[16] (2005) 3531-3534.

Photophysical Properties of Oligo(2,3-Thienyleneethynylene)s, Y. Oseki, M. Fujitsuka, M. Hara, X. Cai, Y. Ie, Y. Aso, and T. Majima: *J. Phys. Chem. B* 109[21] (2005) 10695-10698.

Efficient emission from charge recombination during the pulse radiolysis of electrochemical luminescent substituted quinolines with donor-acceptor character, S. Samori, M. Hara, S. Tojo, M. Fujitsuka, S.-W. Yang, A. Elangovan, T.-I. Ho, and T. Majima: *J. Phys. Chem. B*. 109[23] (2005) 11735-11742.

Exclusion of Aromatic Radical Cations from Cyclodextrin Nanocavity Studied by Pulse Radiolysis, T. Tachikawa, S. Tojo, M. Fujitsuka, and T. Majima: *J. Phys. Chem. B* 109[37] (2005) 17460-17466.

Ultrafast Photoinduced Intramolecular Charge Separation and Recombination Processes in the Oligothiophene-Substituted Benzene Dyads with Amide Spacer, Y. Oseki, M. Fujitsuka, D. W. Cho, A. Sugimoto, S. Tojo, and T. Majima, *J. Phys. Chem. B*. 109[41] (2005) 19257-19262.

Single-Molecule Fluorescence Imaging of the Remote TiO_2 Photocatalytic Oxidation, K. Naito, T. Tachikawa, M. Fujitsuka, and T. Majima: *J. Phys. Chem. B* (Lett.) 109[49] (2005) 23138-23140.

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Contribution to International Conferences

T. Majima, International Symposium on “Chemistry, Biological Chemistry, and Material Science towards Creating New Science and Industry based on Inter-Nanoscience” 2005 (CBMS2005) (Chairperson)

T. Majima, 2004 Korea-Japan Symposium on Frontier Photoscience “Photochemistry and Nanotechnology” (Chairperson)

T. Majima, PACIFICHEM 2005 (Session organizer)

Publications in Domestic Meetings

Photochemistry Meeting	7 papers
Radiation Chemistry Meeting	11 papers
Advanced Radiation Chemistry Meeting	3 paper
Japan Photomedical Science and Photobiology	1 paper
85th Japan Chemical Society Meeting	13 papers
Surface Photochemistry Meeting	18 papers

Academic Degrees

Doctor Degree of Engineering

M. Sakamoto, Studies on Excited Transient Species using Multi-Color Multi-Laser

K. Nakayama, Studies on DNA Conformational Transition Using Modified Nucleobases

Master Degree of Engineering

Y. Osakada, Consecutive Adenine Sequences are Potential Targets in Photosensitized DNA Damage

K. Naito, Single-Molecule Fluorescence Imaging of the Remote TiO₂ Photocatalytic Oxidation

H. Wang, Self-Assembly and its Structure of Chemically Modified Tobacco Mosaic Virus (TMV) Coat Protein (CP)

Sponsorship

Grand-in-Aid for Scientific Research (S)

T. Majima Nanoscience of Photofunctionalized DNA
¥46, 400, 000

Grand-in-Aid for Scientific Research in Special Area (2)

T. Majima Fundamental Science and Technology of ¥10,600,000
Photofunctional Interfaces

Grand-in-Aid for Basic Scientific Research

T. Majima Formation of Carbon Nanotubes Arrays based on ¥2,400,000

DNA Self-assembly

Grand-in-Aid for Scientific Research (C)

M. Fujitsuka	Construction and Application of Hybrid Biomolecular Devices	¥3,400,000
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Grand-in-Aid for Encouragement of Young Scientists (B)

M. Endo	Apoptosis and its Application to Cancer Therapy Based on Photofunctional Biomolecules	¥800,000
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Grand-in-Aid for Scientific Research in Special Area (2)

M. Endo	Fundamental Science and Technology of Photofunctional Interfaces	¥2,600,000
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Grand-in-Aid for Scientific Research for Young Scientist

X. Cai	Development of Multi-laser Chemistry to Molecular Devices, Medical Treatment, and Environmental Science	¥1,500,000
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Grand-in-Aid for Scientific Research for Young Scientist

T. Takada	High Efficient Formation of Long-lifetime Charge Separated State in DNA and its Application to DNA Molecular Devices	¥900,000
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Grand-in-Aid for Scientific Research for Young Scientist

T. Tachikawa	Mechanism of Charge Separation and DNA Damage of TiO ₂ -DNA Nanoconjugates	¥1,100,000
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Grand-in-Aid for Scientific Research for Young Scientist

T. Kimura	Hydration of DNA Structure Studied by Dynamic Stokes Shift	¥1,100,000
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Department of Synthetic Organic Chemistry

Professor:	Hiroaki SASAI
Associate Professor:	Kiyotaka ONITSUKA
Research Associates:	Junko ICHIHARA, Doss JAYAPRAKASH
Specially Appointed Research Associate:	Kazuhiro TAKENAKA
Post Doctoral Fellows:	Mahesh L. PATIL, Gan Bahadur BAIJRACHARYA
Research Assistants:	Kouji YONEZAWA, Gabr Randa Kassem MOHAMED
Guest Researchers:	Naveen Kumar MANGU
Graduate Students:	Takahiro KAWASE, Cilamkoti Venkat Laxman RAO, Priti Sharad KORANNE, Tetsuya TSUJIHARA, Naohito INOUE, Kouichi TANAKA, Akira HAYASHI, Takashi HARA, Tomoko HIROTA, Junichi YOGO, Haruki OKUDA, Tomomi KATAYAMA, Takayuki SHIROMOTO, Atsushi HORII
Research Student:	Yuu ITANO
Support Staff:	Misuzu TANNO, Miho OHAMA

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 Programs

1. Development Multifunctional Asymmetric Catalysts

Multifunctional asymmetric catalysts such as La-Li₃-tris(binaphthoxide) (LLB) complex and Al-Li-bis(binaphthoxide) complex (ALB) function like an enzyme by activating two different substrates to facilitate a chemical reaction. In a similar manner, a homo-dinuclear catalyst should be able to activate two identical substrates in a homolytic coupling reaction. Chiral dinuclear vanadium(IV) complexes with axially chiral skeletons have been synthesized and found to promote the enantioselective oxidative coupling of 2-naphthol derivatives through a dual activation mechanism affording the product with up to 94% ee. The dual activation mechanism in this system was supported by the kinetic analysis and catalyst loading effects.

A new double-activation catalysis for the Morita-Baylis-Hillman (MBH) reaction of an α,β -unsaturated ketone and an aldehyde has also been established by the combined use of multifunctional asymmetric complexes and tributylphosphine ((*n*-Bu)₃P). The above asymmetric catalyst is found to accelerate the enantioselective MBH reaction to afford the adduct in good chemical yield with up to 99% ee.

2. Development Multifunctional Asymmetric Organocatalysts

The aza-MBH reaction is a C-C bond-forming reaction of activated alkenes with imines catalyzed by Lewis bases, such as amines or phosphines, to give highly functionalized allylic amines. Two types of chiral bifunctional organocatalysts for enantioselective aza-MBH reaction of α,β -unsaturated carbonyl compounds with *N*-tosylimines, which possess Brønsted acid unit and Lewis base unit, have also been developed. The enantioselective reactions promoted by the chiral organocatalysts proved to be deeply influenced by the position of the Lewis base unit on the BINOL skeleton. Especially, in the (*S*)-3-(*N*-isopropyl-*N*-3-pyridinylaminomethyl)BINOL catalyzed aza-MBH reaction, the acid-base functionalities are required for not only the activation of the substrate but fixing the conformation of the organocatalyst.

3. New Asymmetric Spiro-type Ligands

So far we have developed a new type of chiral bis(isoxazoline) ligand with spiro[4.4]nonane skeleton (SPRIXs). Pd(II)-SPRIXs catalyst is quite effective to promote highly enantioselective reactions such as tandem cyclization of dialkenylalcohols with up to 95% ee. For the improvement of SPRIX, novel spiro-type ligands which contain both isoxazole and isoxazoline ring were designed. Among the synthesized ligands, the hybrid ligand bearing isoxazole and isoxazoline ring with spiro[5.4]decane skeleton showed great affinity towards Pd(II) salts and the resulting chiral Pd(II)-hybrid ligand complex mediated the catalytic asymmetric tandem cyclization of dialkenylalcohols in higher yield with comparable enantioselectivity. The lack of acceleration effects with oxazoline ligands clearly shows the crucial role of isoxazolines/isoxazoles in the above reactions.

4. Development Chiral Spiro Ionic Liquids and Quaternary Ammonium Salts

Ionic liquids have proved to be good alternatives for conventional solvents as they offer recyclable and greener reaction media. Spiro imidazolium salts, spiro pyridinium salts and spiro ammonium salts have been designed and synthesized for use as chiral ionic liquids and chiral phase transfer catalysts respectively.

5. Stereoselective Reactions with Planar-Chiral Cyclopentadienyl Complexes

The reaction of planar-chiral cyclopentadienyl-ruthenium complexes with *t*-butyl isocyanide resulted in the diastereoselective formation of isocyanide complexes under kinetic control (up to >99%de). The reaction with phenyl acetylene followed by the treatment with alumina gave acetylide complexes diastereoselectively (up to >99%de). The planar-chiral cyclopentadienyl-ruthenium complexes served as effective catalysts for the kinetic resolution of racemic allyl carbonates in asymmetric allylic alkylation.

6. Precise Polymerization with Transition-Metal Complexes

Polymerization of aryl isocyanides possessing chiral ester groups with NiCl₂ at room temperature produced helical polymers, of which helical sense selectivity was not so high. Heating of the polymer solution resulted in the increase in the helical sense selectivity. ¹³C NMR studies suggested that the isomerization around the C=N bonds at higher temperature led to the increase in the stereoregularity of the main chain, which was the origin of the helical structural change.

7. Efficient Solvent-free Catalytic Oxidation System Using Green Solid Disperse

Phase

The search for environmentally benign alternatives to the conventional reaction process using organic solvents has been of great significance in green chemistry. We have developed a new approach to solvent-free catalytic oxidation system using 'green solid disperse phase'. We have developed an efficient catalytic solid-phase system for epoxidations that uses cetylpyridinium dodecatungstate ((CetylPy)₁₀[H₂W₁₂O₄₂]) catalyst/fluorapatite (FAP) disperse phase with a solid urea-hydrogen peroxide complex (urea-H₂O₂). The system was reusable and retained its high catalytic activity, although the catalyst was not fixed on the solid-phase. The high efficiency in the solid system is considered to be due to a new non-degraded peroxo species that retains the framework of the parent cluster.

Molecular oxygen as well as hydrogen peroxide is an environmentally benign and low waste oxidant. We developed a solid-phase-oxidation-system using FAP disperse phase and Keggin vanadomolybdophosphoric acid (H_{3+n}PV_nMo_{12-n}O₄₀:PV_n) with molecular oxygen as a new green catalytic reaction system. The system was efficiently and repeatedly used for solvent-free oxidative dehydrogenation of α -terpinene to *p*-cymene under mild conditions with 1 atm of molecular oxygen.

Publications

Original Papers

Spiro Crown Ethers Bearing (S)-1,1'-Spirobiindanes as Chiral Backbones, K. Yonezawa, M. L. Patil, H. Sasai, and S. Takizawa, *Heterocycles*, 66 [1] (2005) 639-644.

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Micelle-Derived Polymer Supports for Enantioselective Catalysts, S. Takizawa, M. L. Patil, F. Yonezawa, K. Marubayashi, H. Tanaka, T. Kawai, and H. Sasai, *Tetrahedron Lett.*, 46 [7] (2005) 1193-1197.

Enantioselective Morita-Baylis-Hillman (MBH) Reaction Promoted by a Heterobimetallic Complex with a Lewis Base, K. Matsui, S. Takizawa, and H. Sasai, *Tetrahedron Lett.*, 46 [11] (2005) 1943-1946.

Thermally Induced Helical Conformational Change in Poly(aryl isocyanide)s with Optically Active Ester Groups, F. Takei, K. Onitsuka, and S. Takahashi, *Macromolecules*, 38 [4] (2005) 1513-1516.

Diastereoselective Formation of Ruthenium-Isocyanide and -Acetylide Complexes with Planar-Chiral Cyclopentadienyl-Phosphine Ligands, Y. Matsushima, K. Onitsuka, and S. Takahashi, *Organometallics*, 24 [11] (2005) 2747-2754.

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Effective Forms of Hydroxyapatite Disperse Phase in Solvent-Free Epoxidation System, K. Iteya, Y. Sasaki, S. Itoh, and J. Ichihara, *Phosphorus Res. Bull.*, 19 (2005) 142-146.

Book

Organometallic Dendrimers (in Japanese), K. Onitsuka, In *Dendritic Polymers*, M. Kakimoto, K. Aoi, M. Kawa, N. Kurita, K. Kawano, K. Naka, T. Matsunaga Ed., NTS, (2005) 404-460.

Patents

Preparation of Optically Active Spirobis(isoxazoline) Derivatives and their Transition Metal Complexes as Asymmetric Catalysts, H. Sasai, K. Wakita, T. Kato, M. A. Arai, T. Shinohara, and S. Takizawa, JP2006076939 (2006).

Preparation of Optical Active Spirobis(isoxazole) Derivatives and their Transition Metal Complexes as Asymmetric Catalysts, H. Sasai, K. Wakita, T. Kato, M. A. Arai, T. Shinohara, and S. Takizawa, JP2006076915 (2006).

Preparation of N-Spiro Chiral Quarternary Ammonium Salts and their Use as Phase-Transfer Catalysts in Asymmetric Reactions, A. Shimomoto, K. Yonezawa, S. Takizawa, and H. Sasai, JP2006076911 (2006).

Preparation of Spiro Imidazoliums and their Salts as Ionic Fluids, M.L. Patil, C. V. L. Rao, S. Takizawa, and H. Sasai, JP2006076887 (2006).

Preparation of Chiral Spiro Compounds as Phase-Transfer Catalysts and their Use for Asymmetric Alkylation, K. Yonezawa, A. Shimomoto, S. Takizawa, and H. Sasai, JP2006070001 (2006).

Novel Organic Molecular Catalyst Having Binaphthol Skeleton and Processes for Producing the Same and Application Thereof, H. Sasai, S. Takizawa, and K. Matsui, US2006009646 (2006).

Novel Organic Molecular Catalyst Having Binaphthol Skeleton and Processes for Producing the Same and Application Thereof, H. Sasai, S. Takizawa, and K. Matsui, JP200628021 (2006).

Process of Manufacture of Catalyst for Asymmetric Synthesis, M. Shibasaki, H. Sasai, and Y. Tahara, JP2005028363 (2005).

Preparation of Epoxides from Olefins, J. Ichihara, H. Sasaki, T. Yamaguchi, and T. Nosu, JP2005104902 (2005).

International Conferences

Metal-Bridged Polymers as Highly Enantioselective Catalysts (Poster), *S. Takizawa, H. Sasai, N. Inoue, D. Jayaprakash, The 13th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS13), Geneva, Switzerland, Jul. 17-21, 2005.

Dinuclear Vanadium Complexes with Dual Activation: Enantioselective Homolytic Coupling Reaction of 2-Naphthols (Poster), *H. Sasai, H. Somei, Y. Asano, T. Yoshida, T. Katayama, S. Takizawa, The 13th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS13), Geneva, Switzerland, Jul. 17-21, 2005.

Development of Novel Chiral Ligands Bearing Spiro Skeleton (Oral), P. S. Koranne, T. Tsujihara, T. Shinohara, S. Takizawa, *H. Sasai, Palermo, Italy, the 20th International Congress of Heterocyclic Chemistry, Jul. 31-Aug. 5, 2005.

Synthesis and Stereoselective Reactions of Planar-Chiral Cyclopentadienyl-Ruthenium Complexes (Invited), *K. Onitsuka and S. Takahashi, 7th International Symposium on Biotechnology, Metal Complexes and Catalysis (BMC-VII), Beijing, China, Aug. 17-20, 2005.

Novel Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman (aza-MBH) Reaction (Poster), *K. Matsui, S. Takizawa, H. Sasai, The 3rd International Symposium on Integrated Synthesis 2005 (ISIS-3), Osaka, Japan, Sep. 30-Oct. 1, 2005.

Rational Design and Synthesis of Novel Chiral Spiro Type Ligands (Poster), * P. S. Koranne, T. Tsujihara, J. Yogo, S. Takizawa, H. Sasai, The 3rd International Symposium on Integrated Synthesis 2005 (ISIS-3), Osaka, Japan, Sep. 30-Oct. 1, 2005.

Precise Synthesis of Organometallic Dendrimers (Invited), *K. Onitsuka and S. Takahashi, 15th International Symposium on Fine Chemistry and Functional Polymers (FCFP-XV), Shanghai, China, Oct. 17-20, 2005.

Multifunctional Asymmetric Organocatalyst (Invited), *H. Sasai, The 10th International Chemical Conference in Taipei (ICCT10), Hsinchu, Taiwan. Oct. 28-30, 2005.

Development of Enantioselective Intramolecular Aminocarbonylation Catalyzed by Pd-SPRIX (Poster), *T. Tsujihara, P. S. Koranne, J. Yogo, K. Wakita, T. Shinohara, M. A. Arai, T. Arai, S. Takizawa, K. Onitsuka, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Design and Synthesis of Novel Chiral Ionic Liquids with Spiro Skeleton (Poster), *C. V. L. Rao, M. L. Patil, K. Yonezawa, S. Takizawa, K. Onitsuka, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Synthesis of Dendritic Copper(I) Complex and its Reactivity Towards Dioxygen (Poster), *R. N. Nadaf, D. Jayaprakash, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

A Rational Approach Toward the Development of Spiro Ligands (Poster), * P. S. Koranne, T. Tsujihara, J. Yogo, S. Takizawa, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Development of Functionalized Nanoparticles Towards Targeted Drug Delivery Systems (Poster), *S. Takizawa, K. Tatematsu, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman (aza-MBH) Reaction (Invited), K. Matsui, K. Tanaka, S. Takizawa, *H. Sasai, PACIFICHEM 2005, Hawaii, USA, Dec. 15-20, 2005.

Development of Novel Chiral Spiro-Type Ligands Bearing Isoxazoline/Isoxazole Rings (Invited), P. S. Koranne, T. Tsujihara, J. Yogo, M. A. Arai, S. Takizawa, *H. Sasai, PACIFICHEM 2005, Hawaii, USA, Dec. 15-20, 2005.

New Concepts for Immobilization of Asymmetric Catalysts (Invited), *H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Development and Applications of Metal-Bridged Polymers as Asymmetric Catalysts (Poster), S. Takizawa, *N. Inoue, H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Development of Effective Enzyme Mimics Utilizing Dendrimers (Poster), *D. Jayaprakash, R. N. Nadaf, H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Trinuclear Ruthenium-Acetylide Complexes with Tri(ethynylphenyl)amine-Bridge: A New Building Block for Multi-Step Redox Active Organometallic Macromolecules (Poster), *K. Onitsuka, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Syntheses and Properties of Transition-Metal Acetylide Dendrimers (Invited), *K. Onitsuka, PACIFICHEM 2005, Hawaii, USA, Dec. 15-20, 2005.

Phosphovanadomolybdate/Fluorapatite Solid-Phase System for Aerobic Oxidative Dehydrogenation (Poster), K. Iteya, Y. Sasaki, S. Itoh, J. Ichihara, The 10th Japan-Korea Symposium on Catalysis, Matsue, Japan, May 10-13, 2005.

High Efficiency of Hydrogen Peroxide in Fluorapatite Solid-Phase Epoxidation System (Poster), K. Sato, Y. Sasaki, J. Ichihara, The 10th Japan-Korea Symposium on Catalysis, Matsue, Japan, May 10-13, 2005.

Solvent-Free H₂O₂-Epoxidation in Tungstate/Hydrotalcite Solid-Phase System (Poster), S. Hoshi, Y. Sasaki, S. Yamaguchi, T. Nosu, J. Ichihara, The 10th Japan-Korea Symposium on Catalysis, Matsue, Japan, May 10-13, 2005.

Effective Forms of Hydroxyapatite Disperse Phase in Solvent-Free Epoxidation System, K. Iteya, Y. Sasaki, S. Itoh, J. Ichihara (Poster), 5th International Symposium on Inorganic Phosphate Materials '05, Kasugai, Japan, Sep. 6-8, 2005.

Participation of New Active Species in Epoxidation with Cetylpyridinium Dodecatungstate /FAP /Urea-H₂O₂ System, *J. Ichihara, Y. Sasaki, 5th World Congress on Oxidation Catalysis, Sapporo, Japan, Sep. 25-30, 2005.

Green Solid-Phase Epoxidation System: Participation of New Peroxo-Nanocluster of Polyoxometalate Catalyst (Poster), *J. Ichihara, K. Iteya, S. Hoshi, K. Momoi, Y. Sasaki, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams (SIS-2006), Osaka, Japan, Feb. 8-9, 2006.

Publications in Domestic Meetings

The 4th Symposium on Reaction Control of Dynamic Complexes	1 paper
The Chemical Society of Japan	18 papers
The 1st Symposium on Ionic Liquid	1 paper
Symposium on Organometallic Chemistry	2 papers
Symposium on Combinational Chemistry	1 paper
Congress of Heterocyclic Chemistry	2 papers
Symposium on Progress in Organic Reactions and Syntheses	1 paper
The Society of Polymer Science, Japan	1 paper
Symposium on Organic Synthesis	1 paper
Symposium of Green Sustainable Chemistry	2 paper
Catalysis Meeting	1 paper
The 1st Symposium on Creation of Biologically Functional Molecules	1 paper

Academic Degrees

Master Degree of Science

N. Inoue	Development and Application of Novel Chiral Metal-Bridged Polymer Catalyst
K. Tanaka	Development of Novel Bifunctional Organocatalyst for aza-Morita-Baylis-Hillman Reaction
A. Hayashi	Diastereoselective Reaction of Planner-Chiral Cyclopentadienyl-Ruthenium Complex with 2-Pyridylmethanimine
T. Hara	Development of Diastereoselective Nitroaldol Reaction

T. Hirota	Development and Application of Novel Chiral Spiro Quaternary Ammonium Salts	
J. Yogo	Optical Resolution of Spiro Bis(isoxazoline) Ligand	

Doctor Degree of Science

K. Yonezawa	Development of Spiro Chiral Backbone for Enantioselective Reaction	
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Sponsorship

Grant-in-Aid for Scientific Research (2)

H. Sasai	Development of Enantioselective Cascade Reaction	¥2,900,000
H. Sasai	Development of Artificial Enzyme with Synergistic Multicooperation in Active Sites	¥2,000,000

Grant-in-Aid for Basic Research (C)

J. Ichihara	Solvent-free catalytic oxidation system on environmentally benign solid-disperse-phase	¥2,000,000
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Grant-in-Aid for JSPS Fellows

H. Sasai	Development and Application of Novel Asymmetric Spiro Catalysts	¥1,500,000
H. Sasai	Polymer-Supported Artificial Enzyme with Dendritic Systems	¥ 800,000

Other Research Fund

H. Sasai	Yamada Science Foundation	Development of Enzyme-like Asymmetric Bifunctional Organocatalyst	¥2,000,000
K. Onitsuka	Tanaka Kikinzoku Co. Ltd.	Development of New Phosphorescent Iridium Complexes Applicable to Organic EL Devices	¥ 500,000
K. Onitsuka	Izumi Science and Technology Foundation	Syntheses and Functionalities of Organometallic Dendrimers Directed toward Novel Functional Materials	¥1,000,000
K. Onitsuka	Research Foundation for Materials Science	Syntheses and Functions of Nano-sized Organometallic Molecules	¥ 800,000
K. Onitsuka	The Ogasawara Foundation for the Promotion of Science & Engineering	Development of Functional Polymers with Rigid Helical Structures	¥ 1,200,000

Department of Analytical Molecular Chemistry

Professor: Tetsuro MAJIMA
Research Associate: Yoshio TAKAI
Kunihiro Kaihatsu

Outlines

The department of analytical molecular chemistry was newly founded in April 2004. The department is intended to study current analytical molecular chemistry based on the theory, methodology, and techniques about important subjects on molecular chemistry, material chemistry, life science, and environmental chemistry. The department partly contributes to supporting work of materials analysis center of ISIR.

Current Research Programs

TiO₂ photocatalytic reaction studied by solid-state high-resolution NMR

With collaboration to materials analysis center of ISIR, solid-state high-resolution NMR measurement was applied for elucidation of properties of substrates adsorbed on the TiO₂ surface and the TiO₂ photocatalytic reaction mechanism. ¹H and ¹³C solid-state high-resolution NMR spectra of several catechols adsorbed on the TiO₂ surface was measured before and after photoirradiation at the wavelength of the CT band. The photocatalytic degradation mechanism of catechols at the TiO₂ surface was interpreted in terms of the interfacial charge recombination reaction with conduction band electrons.

Host-guest chiral recognition studied by MS Spectrometry

Enantiomer excess of chiral carboxylic acid was determined by ESI-MS Spectrometry.

Inhibition of Chromosomal Transcription with Peptide Nucleic Acids (PNAs)

Collaborating with Department of Organic Fine Chemicals, we designed antigene Peptide Nucleic Acid (agPNA), a DNA/RNA analogue, to target the transcription starting sites for a human hormone receptor within the chromosomal DNA. We succeeded to control the transcription level of Human Progesterone receptor using agPNAs (details are written in the report of Department of Organic Fine Chemicals).

Developing Methods for Lipase-Catalyzed Regio-Selective Acylation of Epigallocatechin gallate, A Green Tea Catechins, and Application of EGCG Acyl-Derivatives for Antiviral Reagents

Collaborating with Department of Organic Fine Chemicals, we developed a method for lipase-catalyzed acylation of Epigallocatechin gallate (EGCG), a major green tea extract. By using this technology, we succeeded to enhance the chemical stability of EGCG under physiological conditions and its antiviral effects on Influenza (details are written in the report of Department of Organic Fine Chemicals).

Publications

Original Paper

Inhibiting Transcription of Chromosomal DNA with Antigene Peptide Nucleic Acids, B. A Janowski, K. Kaihatsu, K. E. Huffman, J. C. Schwartz, R. Ram, D. Hardy, C. R. Mendelson and D. R. Corey: Nature Chemical Biology, 1 (2005), 210-215.

Patent

“Method for Manufacturing Acylated Derivative of Epigallocatechin Gallate”, K. Kaihatsu, S.D. Fuller, T Kobe, and N. Kato, PCT-JP2006-304788

International Conferences

Interfering RNA Virus Membrane Fusion By A Green Tea Catechin Extract, Epigallocatechin Gallate (Poster), *K. Kaihatsu, S. D. Fuller, and N. Kato: Fourth 21 Century COE International Symposium “Toward Creating New Industry Based on Inter-Nanoscience”, Mie, Japan, November 18-19, 2005.

Publications in Domestic Meetings

The Chemical Society of Japan	6 papers
The Mass Spectrometry of Japan	4 papers
Others	2papers

Sponsorship

Osaka University	(Venture Business Support Program)	
K. Kaihatsu	Developing Anti-Avianflu Drugs with Green Tea Catechin Derivatives.	¥750,000

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 (Advanced Reasoning 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.

Achievements

- Theory of role and ontology development environment
- Systematization of functional knowledge using ontological engineering and its deployment
- Systematization of Learning/Instructional theories and learning support systems
- Analysis of collaborative learning interaction and meta-cognitive skill modeling
- Authoring task ontology and an innovative architecture of an authoring system
- Mobile user modeling for task-oriented mobile service navigation
- 3D modeling and visualization
- 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 acquisition from human experts
- Knowledge discovery from graph structured data
- Information retrieval under various data format
- Discovery of time dependent law equations from data
- Derivation of association rules for data with numeric attributes

Department of Knowledge Systems

Professor:	Riichiro MIZOGUCHI
Associate Professor:	Yoshinobu KITAMURA
Research Associate:	Munehiko SASAJIMA
Specially Appointed	
Research Associate:	Yusuke HAYASHI (from Dec. 1)
Post Doctoral Fellow:	Daniele Allard
Graduate Students:	Eiichi SUNAGAWA, Masataka TAKEUCHI, Yusuke KOJI, Jonathan Touitou(from 2004 Oct. to 2005 Sep.), Shinya TARUMI, Mesbahy HOUDA, Naoya WASHIO
Undergraduates:	Tetsuya IIDA, Masanori OOKUBO
Support 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 Programs

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 Ohmsha 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. Furthermore, API functionality and compliance with WWW standard has been augmented. Concerning theoretical issues, further refinement of Role theory has been done.

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 production company. In 2005, we developed a modeling framework for integration of functional knowledge with fault knowledge and a knowledge transform system for interoperability between them. The evaluation made by collaborative research with industry showed its considerable effect on comprehensiveness of fault knowledge. Next, we extended our ontology to include various non-device types of function (This work was awarded in an academic conference). Then, we investigated mapping of our ontology with existing other functional taxonomy.

3. Task Ontology for Intelligent Tutoring System

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 a comprehensive ontology of Education of Informatics in high school and an intelligent authoring support system based on the ontology and a reference model for explaining existing metacognition learning systems.

4. Model-based Knowledge Management Support Environment

We continue to learn during our lifetimes. As researchers, for example, we learn basic knowledge through ‘book learning’, acquire up-to-date knowledge from the literature, develop original knowledge for ourselves, and then disseminate it to society. In this sense, we can share the idea that “life is a continuous process of learning.” “Learning” in a wide sense includes various forms of learning: for example, workplace learning, life-long learning, organizational learning, and so on. Along a similar line of thought, this research aims to develop a model of learning in a wide sense. Needless to say, we are all vaguely conscious of a similar model in our own minds which we apply to increase awareness of social relations among organization members; however, that model is implicit and not systemic in most cases. We propose a model called a “dual loop model”, which shows how intellect is formed in individual life in organizations and works as a fundamental component of a learning support platform. The dual loop model indicates an ideal relation between individual activity and organizational activity and clarifies roles of individuals, activities, and documents as a vehicle for intellectual communication in organizational learning. In this research project, we have been developing an IT platform, Kfarm, to develop users’ pro-found social intellectual awareness in organization. We have developed a knowledge management system for disclosure of the organizational knowledge to the outside world. The latest results include implementation of a supporting system for designing a collaboration field optimized for both learning and practicing together with an explanation function of the design rationale of the field.

5. 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. By quality, we mean whether the information corresponds to the needs of the users or not. Necessity of information lies in a task, not in a domain. 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. Additionally we have been developing ontologies necessary for the modeling.

Publications

Original Papers

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A Framework for Organizing Role Concepts Based on their Dependencies on Contexts (In Japanese): E. Sunagawa, K. Kozaki, Y. Kitamura and R. Mizoguchi, Transactions of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 461-472.

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Formal Ontology and Extensions of Order-Sorted Logic (In Japanese): K. Kaneiwa and R. Mizoguchi, Transactions of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 387-395.

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The Role of Ontological Engineering for AIED Research, Riichiro MIZOGUCHI, Computer Science and Information Systems, Vol.2, No.1, (2005) 31-42,

Systematic Description of the Goal of IT Education based on Ontology Theory (In Japanese): T. Kasai, H. Yamaguchi, K. Nagano and R. Mizoguchi, IEICE TRANSACTIONS on Information and Systems (Japanese Edition), J88-D-I, [1], (2005)

3-15.

Reviewed Papers

A Present State of Ontology Development Tools (In Japanese): K. Kozaki and R. Mizoguchi, Journal of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 407-714.

Editor's Introduction to "Ontology and Its Applications" (In Japanese): R. Mizoguchi, Journal of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 739.

Book

Ontology Engineering (In Japanese): R. Mizoguchi, Ohmsha, (2005)

International Conferences

How to Build an Ontology: Examples and Guidelines, (Invited) *R. Mizoguchi, International Workshop on Applications of Semantic Web Technologies for E-Learning (SW-EL), Banff, Canada, Oct. 2, 2005.

Ontology Engineering and its Application to Technical Knowledge Sharing, (Invited) *R. Mizoguchi, 16th International Conference on Applications of Declarative Programming and Knowledge Management, INAP2005, Fukuoka, Japan, Oct. 22, 2005.

Ontological Engineering, (Invited) *R. Mizoguchi, The Sixth Symposium on Natural Language Processing 2005 (SNLP 2005), Chiang Rai, Thailand, Dec. 14, 2005

Ontological Engineering and ITS Research, (Invited) *R. Mizoguchi, The First International Conference on Digital Media and Learning, Bangkok, Thailand, March 13, 2006.

Functional Metadata Schema for Engineering Knowledge Management, *Y. Kitamura, N. Washio, Y. Koji and R. Mizoguchi, The Workshop on Activities on Semantic Web Technologies in Japan, The 14th International World Wide Web Conference (WWW2005), Chiba, Japan, May 10, 2005.

An Ontological Model of Device Function and its Deployment for Engineering Knowledge Sharing, Y. Kitamura, Y. Koji, and R. Mizoguchi, The First Workshop FOMI 2005 - Formal Ontologies Meet Industry, Castelnuovo del Garda (VR), Italy, June 9-10, 2005.

Developing Ontology-based Applications using Hozo, *K. Kozaki, Y. Kitamura and R. Mizoguchi, The Fourth IASTED International Conference on Computational Intelligence (CI2005), Calgary, Canada, July 4-6, 2005.

What Do You Mean by to Help Learning of Metacognition?, *M. Kayashima, A. Inaba

and R. Mizoguchi, The 12th Artificial Intelligence in Education (AIED2005), Amsterdam, The Netherlands, July 18-22, 2005.

Goal Transition Model and Its Application for Supporting Teachers based on Ontologies, *T. Kasai, H. Yamaguchi, K. Nagano and R. Mizoguchi, The 12th Artificial Intelligence in Education (AIED2005), Amsterdam, The Netherlands, July 18-22, 2005.

Making Learning Design Standards Work with an Ontology of Educational Theories, *V. Psyche, J. Bourdeau, R. Nkambou, and R. Mizoguchi, The 12th Artificial Intelligence in Education (AIED2005), Amsterdam, The Netherlands, July 18-22, 2005.

Ontology-based Transformation from an Extended Functional Model to FMEA, *Y Koji, Y Kitamura, and R Mizoguchi, The 15th International Conference on Engineering Design (ICED '05), Melbourne, Australia, Aug. 15-18, 2005.

An Order-Sorted Quantified Modal Logic for Meta-Ontology, *K. Kaneiwa, and R. Mizoguchi, The International Conference on Automated Reasoning with Analytic Tableaux and Related Methods (TABLEAUX 2005), Koblenz, Germany, Sep. 14-17, 2005.

A Framework for Organizing Role Concepts in Ontology Development Tool: Hozo, *E. Sunagawa, K. Kozaki, Y. Kitamura, and R. Mizoguchi, Roles, an Interdisciplinary Perspective: Ontologies, Programming Languages, and Multiagent Systems, The AAAI Fall Symposium, Arlington, Virginia, USA, Nov. 4-6, 2005.

Toward Task Ontology-based Modeling for Mobile Phone Users' Activity (Poster), *M. SASAJIMA, Y. KITAMURA, T. NAGANUMA, S. KURAKAKE and R. MIZOGUCHI, International Semantic Web Conference (ISWC2005), Galway, Ireland, Nov. 6-10, 2005.

Hozo: an Ontology Development Environment -Treatment of "Role Concept" and Dependency Management - (Poster), *K. Kozaki, E. Sunagawa, Y. Kitamura, and R. Mizoguchi, The 4th International Semantic Web Conference (ISWC2005), Galway, Ireland, Nov. 6-10, 2005.

A Multi Modal Supporting Tool for Multi Lingual Communication by Inducing Partner's Reply, *K. Imoto, M. Sasajima, T. Shimomori, N. Yamanaka, M. Yajima and Y. Masai, The International Conference on Intelligent User Interfaces (IUI2006), Sydney, Australia, Jan. 29 - Feb. 1, 2006.

Development of Ontology-based Knowledge Integration and Management System for Nanotechnology (Poster), *K. Kozaki, Y. Kitamura and R. Mizoguchi, Handai Nanoscience and Nanotechnology International Symposium, Icho Kaikan, Osaka University, Japan, Jan. 30 - Feb. 1, 2006.

Contributions to International Conferences and Journals

Riichiro Mizoguchi	European Project on SEKT (Steering committee member)
Riichiro Mizoguchi	Semantic Web Science Association (Vice-president)
Riichiro Mizoguchi	The 2 nd European Semantic Web Conference (ESWC2005) (PC member)
Riichiro Mizoguchi	The 2005 IFIP International Conference on Intelligence in Communication Systems (INTELLCOMM 05) (PC member)
Riichiro Mizoguchi	Second IFIP Conference on Artificial Intelligence Applications and Innovations (AIAI2005) (PC member)
Riichiro Mizoguchi	Third International Conference on Knowledge Capture (K- CAP 2005) (PC member)
Riichiro Mizoguchi	LORNET Conference I2LOR 2005 (PC member)
Riichiro Mizoguchi	Third IEEE International Workshop on Wireless and Mobile Technologies in Education (WMTE 2005) (PC member)
Riichiro Mizoguchi	Fourth international semantic web conference (ISWC2005) (Posters and demo chair)
Riichiro Mizoguchi	The 5th IEEE International Conference on Advanced Learning Technologies (ICALT2005) (PC member)
Riichiro Mizoguchi	The 14th International World Wide Web Conference (WWW2005) Educational track (Vice chair)
Riichiro Mizoguchi	The 13th International Conference on Computers in Education (ICCE2005) (PC member)
Riichiro Mizoguchi	International Artificial Intelligence in Education Society (Executive Committee member)
Riichiro Mizoguchi	Asia-Pacific Society for Computer in Education (APSCE) (Board member)
Riichiro Mizoguchi	International Journal of Applied Ontology (Editorial board)
Riichiro Mizoguchi	International Journal of Artificial Intelligence in Education (Editorial board)
Riichiro Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
Riichiro Mizoguchi	International Journal of Web Semantics (Editorial board)
Riichiro Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	9 papers
The institute of Electronics, information and communication engineers	1 paper
The society of chemical engineers, Japan	1 paper
The Japan society of mechanical engineers	1 paper

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas (2)

R. Mizoguchi	Management and Utilization of Knowledge Contents of Design and Manufacturing based on Function	¥5,100,000
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Grant-in-Aid for Scientific Research (A) (2)

R. Mizoguchi	Development of a Theory-Aware Authoring Workbench	¥9,600,000
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Grant-in-Aid for Encouragement of Young Scientists (B)

Y. Kitamura	Research on functional ontologies for sharing functional design knowledge	¥1,200,000
Y. Hayashi	Development of competency-oriented intellect disclosure engine based on organizational intellect model	¥1,689,432

Grant-in-Aid for JSPS Fellow

R. Mizoguchi	Ontological Modeling of Second Language Learning Interferences and an Experimental Computer Application	¥1,200,000
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Other Allocations

R. Mizoguchi	Human-Centered Semantic Web	¥2,720,000
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Entrusted Research

R. Mizoguchi	Galaxy Express Corporation	MEXT IT Program e-Science Project Building a support system for operating a large-scale system using advanced IT	¥1,050,000
R. Mizoguchi	The Society of Chemical Engineers, Japan	Surveillance Study for Development of Structured Knowledge Platform for Nano-particle and Nano-carbon (1) Brush up of Basic Systems and Information Gathering about Nano-particle and Nano-carbon to expand the Contents	¥2,100,000

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
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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	Sumitomo Wiring Systems, Ltd.	Development of a tool for technical knowledge systematization	¥3,000,000

Department of Intelligent Media

Professor:	Yasushi YAGI
Associate Professor:	Yasuhiro MUKAIGAWA
Research Associate:	Ryusuke SAGAWA
Designated Researchers:	Tomio ECHIGO, Wang JUNQIU, Radu ORGHIDAN
Designated Research Associate:	Yasushi MAKIHARA
Graduate Students:	Nobuya AOKI, Kazuaki KONDO, Hai VU, Tetsuji HAGA, Ngo Thanh Trung, Kensuke UEDA, Suchit PONGNUMKUL, Masaya TAKATSUJI, Hiroyuki NOGUCHI, Nanaho OSAWA, Hidetoshi MANNAMI, Yuichiro KOJIMA, Kohei SUMINO
Undergraduates:	Takuro SAKAI, Yuya NAKAMORI, Yoshifumi NISHIOKA, Kazuya TAKEI
Support Staff:	Masako KAMURA, Noriko YASUI, Yuko NAKAZAWA

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 Programs

1. Spectral Reflectance Estimation of Outdoor Scene Considering Daylight Changes

Nowadays, many studies about multi-spectral imaging are done for object recognition and computer graphics. We propose a method of spectral reflectance estimation of outdoor scenes considering daylight changes. Illumination of outdoor scenes is assumed to be a weighted linear combination sunlight and skylight, and the relation between the two lights is obtained by a pair of sunny and shady area in the same object. Then, we cluster the whole region into regions with the same spectral reflectance by checking whether difference of observed spectra is represented by changing the weights for the two lights. Finally, spectral reflectance and the weights are re-estimated with all data in each cluster. We made experiments about spectral reflectance estimation of outdoor scenes and confirmed that the spectral reflectance is stably estimated for the same object under different illumination conditions.

2. Video Analysis of Small Intestine using a Capsule Endoscope

A capsule endoscope is a small capsule equipped with an endoscopic camera and a radio transmitter. The capsule swallowed by a patient moves in the peristaltic movement and takes images of the small intestine. As it is hard for a traditional endoscope to examine the small intestine, the capsule endoscope is a promising choice to examine digestive organs. As the direction of the camera frequently changes frame by frame, a medical doctor sometimes cannot recognize which direction the camera looks toward. This paper describes the method to improve the viewability by stabilizing a center position of the small intestine. Using low brightness area and rugae of the small intestine as feature quantities, we classified the state of the small intestine, estimated the center position, and displayed by moving it to the center of the screen. Additionally, it is worth analyzing the movement of the small intestine which is poorly understood so far. This paper also describes a method to detect shrinkage, which is a characteristic movement of the small intestine, occurred by the peristaltic movement. We detect a scene that the intestine shrinks by computing the change of feature quantities. By applying our method to the image sequence of the capsule endoscope, we validated that our method can detect the shrinkage of the small intestine correctly.

3. Deformable Registration for Generating Dissection Image of an Intestine from Annular Image Sequence

Examination inside an intestine by an endoscope is difficult and time consuming, because the whole image of the intestine cannot be taken at one time due to the limited field of view. Thus, it is necessary to generate a dissection image, which can be obtained by extending the image of an intestine. We acquire an annular image sequence with an omnidirectional or wide-angle camera, and then generate the dissection image by mosaicing the image sequence. Though usual mosaicing techniques transform an image by perspective or affine transformations, these are not suitable for our situation because the target object is a generalized cylinder and the camera motion is unknown a priori. Therefore, we propose a novel approach for image registration that deforms images by a two-dimensional-polynomial function whose parameters are estimated from optical flow. We evaluated our method by registering annular image sequences and we successfully generated dissection images, as presented in this paper.

4. Calibration of Endoscopic Imaging System - Analysis of Image Distortion and Illumination Distribution -

An endoscopic imaging system has unique characteristics. In particular, an image distortion and a non-uniform illumination distribution should be analyzed. In this research, we analyze these two problems existing in the endoscope images. In terms of the image distortion, we propose a method for calibrating the image distortion of wide-angle lenses by using structured-light patterns. In our method, the structured light patterns are displayed on a flat display to make a mapping function between an image coordinate system and a display coordinate system. This approach has two advantages. First, it is easier to find correspondences between the image and display coordinates around the edge of a camera image. Second, since we can easily construct a dense map, a simple linear interpolation is enough to create an undistorted image. Furthermore, our method is not restricted by distortion parameters because we can directly generate the map. We have evaluated the accuracy of our method, and as a result an error becomes smaller than a result of a parameter fitting. As for the analysis of the non-uniform

illumination distribution, we construct an illumination distribution model as the sum of point light sources which have different illumination distributions. In this research, we determine camera and light positions beforehand to make it easy to construct the model. We have actually measured the illumination distribution of the endoscope which has two light sources, and confirmed the effectiveness of our method.

5. Adaptive Dynamic Range Camera with Transmissive/Reflective Liquid Crystal

Wide Dynamic Range Image (WDRI) is needed for capturing scenes which include drastic lighting changes. This paper presents a method to widen the dynamic range of a camera with liquid crystal. The system consists of a camera and a liquid crystal plane placed in front of the camera. By controlling the attenuation rate of the liquid crystal, scene radiance can be controlled adaptively. After controlling the radiance, the original scene radiance can be derived from attenuation rate of the liquid crystal and the radiance obtained by the camera. There are two types of liquid crystal plane; transmissive one and reflective one. Their different features are as follows; Transmissive liquid crystal plane can be used easily, but its contrast ratio is reduced because the driving circuit exists between elements. Reflective liquid crystal plane achieves a higher contrast ratio, but its size tends to be larger because it needs a beam splitter for separating the rays. Since each of them has both merits and demerits, we construct two systems; one with transmissive liquid crystal, the other with reflective liquid crystal. In case of the system with the transmissive liquid crystal, a masking effect blurs because the focus point does not exist on the transmissive filter. Though the masking effect blurs, the scene radiance is derived if a blurring function is known. We calculate the blurring function from real data and evaluate the preciseness of the calculated function by comparing with Gaussian function. As a result, we verify that the calculated function can obtain the scene radiance more precisely. In case of the system with reflective liquid crystal, a masking effect does not blur because the focus point exists on the reflective surface. In this system, the radiance control can be done for each pixel independently. We show the result of controlling the radiance and WDRI obtained by calculating the original scene radiance.

6. Approaching Object Detection using Hierarchical Images by Compound Omnidirectional Sensor

This paper proposes a method to detect an approaching object with a compound omnidirectional sensor. Some previous works proposed a method on real-time detection of near objects using the corresponding points for infinity range with the compound omnidirectional sensor. However, it was troublesome to calibrate the camera and the mirrors to get the corresponding points. In addition, the method could not detect the approach of the objects. Therefore, we construct a catadioptric system with a single orthogonal projection camera and paraboloidal mirrors to save from the troublesome calibration. Moreover, based on the characteristics that the detectable distance gets shorter as the resolution of input image gets lower, we propose a method of detecting the approaching objects using hierarchical images with various resolutions. First, we construct the hierarchical scaled images from the input image, and apply the near objects detection to each scaled image to get the quantized distance. Next, we track the detected objects sequentially and detect the approach of the object by checking changes of the quantized distance. Finally, we made the experiments for objects placed at

various distance using 3-level hierarchical images, and confirmed the quantized distance was correctly detected.

6. Development of Mobile Omni-Alarm using Compound Omnidirectional Sensor

A compound stereo sensor, which consists of a single camera with multiple convex mirrors, has been proposed for surveying omnidirection at once and detecting near objects. However, a real mobile system, including an image processing function, has not been realized. In this paper, a new mobile omni-alarm system is introduced which has been developed for realizing omnidirectional observation, mobility, and real time processing. We developed a stand-alone system with a small and lightweight body by incorporating a small computer with newly designed sensors in order to realize a mobile security alarm. In the system, the camera and six convex parabolic mirrors are used for taking omnidirectional images, and the small computer is used for processing the images to detect near objects. When the system detects objects, the direction is immediately notified to a user by voice. Experimental results show that such a small mobile sensor has a certain ability of detecting near objects and processing images in real time. We confirmed the availability as a security sensor of the developed system.

7. Adaptive Displaying Deformable Dissection Image of Intestine by Changing Point of Interest

This paper proposes adaptive displaying method for a dissection image of intestine. A method was proposed to get a panoramic image by mosaicing, which deforms and connects a sequence of images. Though an input image without image processing is better for the inspection by a medical doctor, a panoramic image created with the mosaic method includes a lot of image processing, because each of frames is deformed based on the first frame and overwritten sequentially. Therefore, our proposed method creates a panoramic image, which is created for a point of interest, and display a part of the image near by the point without image processing. Our method consists of following three points: 1.Create a panoramic image, which is deformed as to a base frame, 2.Sort images to make the base frame seen on the top of images, 3.Change the scope of original images to create a panoramic image of different view direction. We achieved interactive deformation and rendering by implementing these methods with a graphics hardware.

8. Mirror Localization of Catadioptric Imaging System using Multiple Parallel Lights of Constant Angle

This paper describes a method of mirror localization to calibrate a catadioptric imaging system. While the calibration of a catadioptric system includes the estimation of various parameters, we focus on the localization of the mirror. We propose a method that uses multiple parallel lights of constant angle to simplify the geometry of projection to estimate the position of the mirror and so does not restrict the position and shape of the mirror. We omit the translation between a camera and calibration objects from the parameters to be estimated by observing two parallel lights of constant angle. Since we obtain the constraints about the angle between them, we can compute the error between the model of the mirror and the measurements. The position of the mirror is estimated by minimizing the error. Finally, we evaluate the accuracy of our method by simulation.

Publications

Original Papers

Iconic Memory-Based Omnidirectional Route Panorama Navigation, Yasushi Yagi, Kousuke Imai, Kentaro Tsuji, Masahiko Yachida, IEEE Transactions on Pattern Analysis and Machine Intelligence, 27[1] (2005) 78-87.

Adaptively Merging Large-Scale Range Data with Reflectance Properties, Ryusuke Sagawa, Ko Nishino, Katsushi Ikeuchi, IEEE Transactions on Pattern Analysis and Machine Intelligence, 27[3] (2005) 392-405.

International Conferences

Stereo Vision with a Single Camera and Multiple Mirrors, *E. Mouaddib, R. Sagawa, T. Echigo, Y. Yagi, IEEE International Conference on Robotics and Automation, Barcelona, Spain, Apr. 18-22, 2005.

Non-isotropic Omnidirectional Imaging System for an Autonomous Mobile Robot, *K Kondo, Y. Yagi, M. Yachida, 2005 IEEE International Conference on Robotics and Automation, Barcelona, Spain, Apr. 18-22, 2005.

Development of a Networked Robotic System for Disaster Mitigation - Test Bed Experiments for Remote Operation Over Rough Terrain and High Resolution 3D Geometry Acquisition -, K. Yoshida, K. Nagatani, K. Kiyokawa, Y. Yagi, T. Adachi, H. Saitoh, H. Tanaka, H. Ohno, the 5th International Conference on Field and Service Robotics, North Queensland, Australia, Jul. 29-31, 2005.

Calibration of Lens Distortion by Structured-Light Scanning, *R. Sagawa, M. Takatsuji, T. Echigo, Y. Yagi, 2005 IEEE/RSJ International Conference on Intelligent Robots and Systems, Edmonton, Canada, Aug. 2-6, 2005.

Real Time 3D Environment Modeling for a Mobile Robot by Aligning Range Image Sequences, *R. Sagawa, N. Osawa, T. Echigo, Y. Yagi, British Machine Vision Conference 2005, Oxford, UK, Sep. 5-8, 2005.

Calibration and Performance Evaluation of Omnidirectional Sensor with Compound Spherical Mirrors, *Y. Kojima, R. Sagawa, T. Echigo, Y. Yagi, the 6th Workshop on Omnidirectional Vision, Camera Networks and Non-classical cameras, Beijing, China, Oct. 21, 2005.

Deformable Registration for Generating Dissection Image of an Intestine from Annular Image Sequence, *S. Pongnumkul, R. Sagawa, T. Echigo, Y. Yagi, In Computer Vision for Biomedical Image Applications, Beijing, China, Oct. 21, 2005.

Strategy for Displaying the Recognition Result in Interactive Vision, *Y. Makihara, J. Miura, Y. Shirai, N. Shimada, the 2nd Int. Workshop on Language Understanding and Agents for Real World Interaction, Singapore, Singapore, Nov. 23-24, 2005.

Matching Gait Image Sequences in the Frequency Domain for Tracking People at a Distance, R. Sagawa, Y. Makihara, T. Echigo, Y. Yagi, the 7th Asian Conference on Computer Vision, Hyderabad, India, Jan. 13-16, 2006.

Adaptive Display Speed Control for Diagnosis of Capsule Endoscopic Images, Y. Yagi, T. Arakawa, K. Higuchi, M. Shiba, K. Yagi, R. Sagawa, V. Hai, *T. Echigo, the 5th International Conference on Capsule Endoscopy, Florida, USA, Mar. 6-7, 2006.

Two or more mirrors for the omnidirectional stereovision?, *E. Mouaddib, R. Sagawa, T. Echigo, Y. Yagi, the 2nd IEEE-EURASIP International Symposium on Control, Communications, and Signal Processing, Marrakech, Morocco, Mar. 13-15, 2006.

Real-Time Transmission of 3D Video to Multiple Users via Network, *T. Koyama, Y. Mukaigawa, Y. Kameda, Y. Ohta, IAPR Workshop on Machine Vision Applications 2005, Tsukuba Science City, Japan, May 16-18, 2005.

Probabilistic Framework for Intelligent Filming by Switching Temporarily Locked Pan-Tilt Cameras, *B. Hicham, Y. Kameda, Y. Mukaigawa, Y. Ohta, IAPR Workshop on Machine Vision Applications 2005, Tsukuba Science City, Japan, May 16-18, 2005.

Coordination of Appearance and Motion Data for Virtual View Generation of Traditional Dances, *Y. Kamon, R. Yamane, Y. Mukaigawa, T. Shakunaga, the 5th International Conference on 3-D Digital Imaging and Modeling, Ottawa, Canada, Jun. 13-16, 2005.

Classification of Photometric Factors Based on Photometric Linearization, *Y. Mukaigawa, Y. Ishii, T. Shakunaga, the 7th Asian Conference on Computer Vision, Hyderabad, India, Jan. 13-16, 2006.

Analysis of Response Performance Characteristics for Identification Using a Matching Score Generation Model, *T. Maeda, M. Matsushita, K. Sasakawa, Y. Yagi, 5th International Conference on Audio- and Video-Based Biometric Person Authentication, Hilton Rye Town, NY, USA, Jul. 20-22, 2005.

Contributions to International Conferences and Journals

Y. YAGI	IEEE International Conference on Intelligent Robots and Systems 2006 (Program Committee Members)
Y. YAGI	IEEE International Conference on Robotics & Biomimetics 2006 (Program Co-Chairs)
Y. YAGI	Asian Conf. on Computer Vision 2006 (Program Committee Members)
Y. YAGI	European Conf. on Computer Vision 2006 (Program Committee Members)
Y. YAGI	Computer Vision and Pattern Recognition 2006 (Program

	Committee Members)
Y. YAGI	Asian Conference on Computer Vision 2007 (Program Chair)
Y.	Computer Vision and Pattern Recognition 2005 (Program
MUKAIGAWA	Committee Members)
Y.	Asian Conf. on Computer Vision 2006 (Program Committee
MUKAIGAWA	Members)
Y.	European Conf. on Computer Vision 2006 (Program Committee
MUKAIGAWA	Members)
Y.	Computer Vision and Pattern Recognition 2006 (Potential Paper
MUKAIGAWA	Reviewer)

Publications in Domestic Meetings

Information Processing Society of Japan	17 papers
The Institute of Electronics, Information and Communication Engineers	5 papers
The Japan Society of Naval Architects and Ocean Engineers	1 paper

Academic Degrees

Doctor Degree for Information Science

Tetsuji Haga	Intruder Surveillance Technology for Outdoor Scenes based on Spatio-temporal Motion Features
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Master Degree of Information Science

Hiroyuki Noguchi	Spectral Reflectance Estimation of Outdoor Scene Considering Daylight Changes
Kensuke Ueda	Video Analysis of Small Intestine using a Capsule Endoscope
Suchit Pongnumkul	Deformable Registration for Generating Dissection Image of an Intestine from Annular Image Sequence
Masaya Takatsuji	Calibration of Endoscopic Imaging System - Analysis of Image Distortion and Illumination Distribution -
Hidetoshi Mannami	Adaptive Dynamic Range Camera with Transmissive/Reflective Liquid Crystal

Sponsorship

Grant-in-Aid for Scientific Research (S)

Y. Yagi	Wearable Omnidirectional Stereo Surveillance System	¥8,720,000
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Grant-in-Aid for Young Scientists (A)

Y. Mukaigawa	Full measurement of spatially varying BRDF and its advanced application	¥8,284,000
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Grant-in-Aid for Young Scientists (B)

R. Sagawa	Research on 3-D Modeling of Deformable Tubes	¥1,800,000
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Other Research Funds

Y. Yagi	Japan Science and Technology Agency (JST) Development of medical technology using omnidirectional vision	¥39,000,000
Y. Yagi	Strategic Information and Communications R&D Promotion Programme, Multimedia Information Search by Teleoperated Robot Network in a Disaster Site	¥1,950,000

Department of Architecture for Intelligence

Professor: Masayuki NUMAO
Associate Professor: Satoshi KURIHARA
Research Associate: Koichi MORIYAMA
Research Associate(Specially Appointment): Ken-ichi FUKUI (From July.1)
Graduate Students: Roberto LEGASPI, Md. Nazmul HUDA, Kazushi
NAKAMURA, Minoru KAWANO, Yuya HASHIMONO,
Nagayoshi YAMASHITA, Norihiro IMANAKA, Toshinori
KAWASAKI, Motoki KONISHI
Undergraduate Students: Naofumi YASUBA, Seiichi HONDA, Mitsuhiro
MATSUMOTO
Special Research Students: Hideki NAKAYAMA
Support Stuff: 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. Web-based Learning Environments, and 3. Instructional Design Support for Collaborative Learning.

Current Research Programs

1. 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.

2. 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.

3. 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.

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International Conferences

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A Cluster-based Predictive Modeling to Improve Pedagogic Reasoning, *R. Legaspi, R. Sison, K. Fukui, and M. Numao. Proc. IADIS International Conference on Cognition and Exploratory Learning in Digital Age. Porto, Portugal. Dec. 14-16, 2005.

Contributions to International Conferences and Journals

M. Numao	New Generation Computing (Area Editor)
M. Numao	8th Annual Symposium on Japanese-American Frontiers of Science (Co-chair of Planning Group)
M. Numao	1st Annual Symposium on Japanese-French Frontiers of Science (Planning Group Member)
M. Numao	The Nineteenth International Joint Conference on Artificial Intelligence (IJCAI 05) (Reviewer)
M. Numao	The 22nd International Conference on Machine Learning (ICML2005) (Program Committee)
M. Numao	The 16th European Conference on Machine Learning (ECML 2005) (Program Committee)
M. Numao	The 9th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD 2005) (Program Committee)
M. Numao	The 4th International Joint Conference on Autonomous Agents and Multi Agent Systems (AAMAS 2005) (Program Committee)
M. Numao	The 5th International Joint Conference on Autonomous Agents and Multi Agent Systems (AAMAS 2006) (Program Committee)
M. Numao	The 9th Pacific Rim International Conference on Artificial Intelligence (PRICAI 2006) (Program Committee)
S. Kurihara	The First International Workshop on Agent Network Dynamics and Intelligence (ANDI) (Program Committee)
S. Kurihara	The Second International Workshop on Biologically Inspired Approaches to Advanced Information Technology (BioADIT) (Program Committee)
S. Kurihara	The IEEE/WIC/ACM International Conference on Web Intelligence (WI) (Program Committee)
S. Kurihara	The IEEE/WIC/ACM International Conference on Intelligent Agent Technology (IAT) (Program Committee)
S. Kurihara	The Second International Workshop on Networked Sensing Systems (INSS) (Program Committee)

S. Kurihara	Joint Workshop on Massively Multi-Agent Systems and Challenges in the Coordination of Large Scale Multi-agent Systems (MMAS/LSMAS) (Program Committee)
S. Kurihara	The 4th International Joint Conference on Autonomous Agents and Multi Agent Systems (AAMAS) (Program Committee)
S. Kurihara	Workshop on Emergent Intelligence on Networked Agents (WEIN) (Organizer)
S. Kurihara	Seventh International Workshop on Multi-Agent-Based Simulation (MABS) (Program Committee)
S. Kurihara	The 12 th International Joint Conference on Artificial Intelligence (IJCAI) (Program Committee)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence:	3 papers
The Institute of Electronics, Information and Communication Engineers	2 paper

Academic Degrees

Doctor Degree of Information Science

Roberto Legaspi	A Cluster Knowledge-based Predictive Model Learning Framework for a Tutoring Agent to Self-improve its Pedagogic Reasoning
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Master Degree of Information Science

Y. Hashimoto	Individual <i>KANSEI</i> Acquisition Mechanism in a Music Structure
N. Yamashita	Summarization of the Web Documents using Link Analysis by Block Model

Bachelor Degree of Engineering

N. Yasuba	Analysis of People Movements by Hierarchal Clustering of Motion Detections
S. Honda	Personal Tracking by Infrared Sensor Network
M. Matsumoto	Design and Evaluation of Q-Learning Agent in U-Mart

Sponsorship

Cooperative Research

M. Numao	Brains Corporation	¥3, 000, 000
S. Kurihara	NTT Communication Science Labs.	Multiagent Algorithm for Ubiquitous Systems ¥1, 000, 000

Department of Advanced Reasoning

Professor:	Hiroshi MOTODA
Associate Professor:	Takashi WASHIO
Research Associate:	Kouzou OHARA
Post Doctoral Fellows:	Chien Phu NGUYEN, Alexandre TERMIER
Graduate Students:	Fuminori ADACHI, Yuki MITSUNAGA, Akira MOGI Kotaro NAKANISHI, Hong Tao LU, Viet Phuong NGUYEN
Research Students:	Kiyoto TAKABAYASHI, Hadiyanto
Under Graduate Students:	Kentaro KIDO, Kenta Fukata
Supporting Staffs:	Kana KOYAGI, Hiroko OKADA

Outlines

Being able to reason is fundamental to the intelligent activities of human beings. We humans create new ideas and entities based on our internal knowledge resource acquired by both external facts and past experiences. However, there is a cognitive and psychological limit in our information processing capability. Humans are very good at reasoning and interpreting a small amount of data be it semantically or syntactically, but are very poor at extracting useful/meaningful information in a short period of time from a huge amount of data. Our laboratory's research focus is on exploring various methods of mining/discovering informative knowledge from massive data using mathematical constraints, heuristic and statistical search techniques. During this year, we have worked on 1) derivation of association rules for data with numeric attributes, 2) knowledge discovery from graph structured data, 3) discovery of time dependent law equations from data, and 4) information retrieval under various data format.

Current Research Programs

1. Derivation of association rules for data with numerical attributes

Basket Analysis is to derive frequently co-occurred symbolic features and the relations among them, i.e., association rules. However, its applicability is limited to some narrow field since most of practical data are mixtures of symbolic and numerical features. In this regard, the extension of Basket Analysis to make it applicable to the data containing numerical features is expected to highly widen the application area of data mining. Our laboratory has worked on this topic in the last few years and obtained the following achievements.

1. An approach to discretize numerical feature data into symbolic feature data was developed. The data are preprocessed by this approach and applied to Basket Analysis. This approach enables to apply Basket Analysis to the data containing numerical features under a certain rough discretization, i.e., approximation, of numerical data.
2. A drawback of the above approach is to lose some detailed information contained

in the original numerical feature data though the discretization, and this induces the loss of accuracy and the miss of the association rules. In this regards, we investigated some principles and algorithms to search association rules in a more rigorous manner without introducing numerical discretization, and established monotonic interval density measure to mine quantitative association rules in the framework of Basket Analysis.

3. The aforementioned monotonic interval density measure has been implemented into a tool program named QFIMiner for quantitative frequent itemset mining, and its performance has been tested in practical conditions. Moreover, a new classification approach based on the quantitative frequent itemset mining has been developed, and its performance has been tested. The performance of these approaches demonstrated significant practicality in both efficiency and accuracy.

In this year, the tool program QFIMiner for quantitative frequent itemset mining has been significantly improved. The performance achieved the world top level in terms of both accuracy and efficiency where its efficiency is higher in an order of magnitude than the other programs developed by some overseas research groups. Moreover, the classification approach based on the quantitative frequent itemset mining has been implemented as a tool program named LSC-CAEP. The significant performance of this tool in both accuracy and interpretability has been confirmed through many realistic data in comparison with conventional classification approaches.

2. Knowledge discovery from graph structured data

There have recently been many attempts on data mining but most of them are targeted to data in the standard transaction format or the relational database format. It appears that there are no effective methods that allow us to mine a dataset that has a more complex structure. Noting that most of the knowledge and concepts we handle can be represented in a graph structure, we have been working for the knowledge discovery from graph-structured data from various perspectives over the last several years. The task of finding frequently appearing subgraphs (subgraph isomorphism) is known to be computationally hard and this is a very difficult problem to solve. The main results obtained in the past years include the followings.

1. We have developed a learning mechanism called “graph-based induction (GBI)” that discovers characteristic patterns in a graph based on a simple idea of repeated chunking of linked two nodes in the graph. We also have expanded the method to discover classification rules that can predict the root node of a tree-structured data, and applied this to command prediction which is one of the functions needed for friendly user interface and to browsing pattern discovery from WWW log data. This method has a pruning function to suppress the overfitting.
2. We have developed a framework of the conventional basket analysis to derive association rules among sub-graphs by appropriately pre-processing the graph-structured data to a standard transaction of the conventional basket analysis. This approach allows to use the well-known Apriori algorithm without any modification to a graph-structured data but it is limited to a graph where each node has a unique

label.

3. We have succeeded in dropping the requirement of the uniqueness of each node by rebuilding a completely different method called “Apriori-based Graph Mining (AGM)” that allows to handle topological structure. Graph structure is represented by adjacency matrix and isomorphic structure is efficiently disambiguated by introducing a notion of canonical form. Unlike GBI which is very fast but can only obtain approximate solutions, AGM’s search is complete and derives all frequent induced subgraphs. AGM can handle the most general class of graphs, which includes both connected/unconnected, directed/undirected graphs with colored/un-colored nodes and labeled/unlabeled links. Self-looped link is also allowed.
4. We have extended GBI to handle multi-inputs/outputs, directed/undirected graph with/without node and link labels and loop structure (including a self-loop). It is not capable of handling non-connected graph. The method was verified to work as expected using artificially generated data. The repeated pairwise chunking does not by any means ensure the optimal solutions. It only extracts frequently appearing patterns in an approximate manner. However, its time complexity is shown to be almost linear to the size of graph.
5. In order to make AGM more efficient, further improvement was made to the data structure and the algorithm, i.e., extension of code expression representing a graph, change of the definition of the canonical form and the improvement of the search method. This accelerated the execution speed by two order of magnitude. In fact, the past AGM needed much computation time to analyze the subgraph co-occurrence in the molecular substructures of chemical compounds having mutagenesis and carcinogenesis. With this improvement, it is now possible to solve this problem within a tractable time.
6. Extensive improvement was also made on GBI without losing its merit of greedy approach. Two separate criteria were introduced one for generating chunks and the other for extracting chunks. Repeated chunking is based on frequency measure but a different measure such as class separability measure can now be used to select good set of chunks. Further, canonical labelling was introduced to identify whether two subgraphs that are generated by different chunking history are indeed isomorphic. With this enhancement, both directed and undirected graphs are now uniformly treated. The most important improvement was to adopt a beam search to expand the search space, which is quite effective in reducing the omitted important patterns.
7. We applied GBI to a real world medical dataset of hepatitis B and C, and went through all the phases of data mining: data preprocessing, conversion to graphs, extraction of typical subgraphs, evaluation by medical expert, and repeated this cycle four times. During the course of analysis, we made an improvement such as biasing the chunking direction, the need that really came from actual practice.
8. We proposed a new method of building a classifier DT-GBI for a graph structured data using GBI recursively at each node of a decision tree and applied it to a

preliminary study of hepatitis data analysis.

9. We extended the adjacency matrix elements which are basic graph representation in AGM to explicitly represent edge labels in a graph. By this extension, generic, efficient and complete mining of frequent subgraphs which include edges having various labels has been enabled.
10. AcGM has been developed which can mine frequent generic subgraphs and frequent connected subgraphs not limited to frequent induced subgraphs. This has been achieved by introducing biases to constrain join operation to generate candidate frequent subgraphs in AGM's search. Especially, the connected subgraph mining is very efficient, and highly practical result in application to Bioactive Compounds Analysis has been obtained.
11. B-AGM has been developed which can mine frequent sub-ordered trees, frequent sub-unordered trees, frequent subpaths and frequent subsequences not limited to frequent subgraphs. The application fields of AGM have been significantly extended by this development.
12. We extended AGM to do a complete search reflecting the 3 dimensional sub-graph structure taking into account the 3 dimensional coordinates of vertices in the graph.
13. The algorithms of the aforementioned AcGM and B-AGM have been further improved to enable very fast data mining of the structures. With this improvement, AcGM and B-AGM are now one of the fastest complete graph mining tools.
14. Moreover, AcGM was made to be a public software to return the benefit resulted from our research to the public society.
15. We proposed a standard of PMML (Predictive Model Markup Language) to represent graph structured data. PMML is a subset of XML. The current graph mining tools in public support a graph representation only dedicated to each tool. This is the significant difficulty in sharing the graph data and their mined results. However, with our proposal, a powerful environment becomes available for flexibly combining and using many tools and system in graph mining.
16. We performed an extensive analysis of the hepatitis dataset which was provided by Chiba University Hospital using DT-GBI, and succeeded in predicting the level of fibrosis, type of hepatitis (B or C), and effectiveness of interferon therapy with a reasonably good accuracy using only the results of the safe and inexpensive blood inspection.
17. We proposed an algorithm that approximately solves the subgraph isomorphism problem.
18. We proposed a graph mining method called CI-GBI (Chunkingless Graph-Based Induction), which is an extension of GBI and can find overlapping patterns that GBI

cannot find. With this improvement, CI-GBI can solve a crucial problem that GBI has, i.e., possibility of overlooking important subgraphs due to inappropriate chunking order.

19. We developed a decision tree learner DT-CI-GBI that employs CI-GBI instead of GBI, and applied it to the analysis of the hepatitis dataset.
20. The characteristics of the subgraph search in the aforementioned B-AGM have been theoretically analyzed, and its generic completeness has been proved.
21. A language to represent graph, GML(Graph Markup Language), based on the aforementioned PMML standard has been designed, and the set of open software tools for the graph representation, the data conversion, and the AGM analysis by using GML was developed to return the benefit resulted from our research to the public society.

In this year, we proposed graph mining based statistical causal inference to analyse highly massive and complicated causal structures among gene expressions by applying AGM and AcGM to gene micro array data. We also proposed a 2-step analysis method using DT-CI-GBI for the hepatitis dataset, which 1) classifies all the patients into two groups, Typical and non-Typical, based on their average accuracy obtained by applying DT-CI-GBI to the whole dataset varying some of its configuration parameters, and 2) constructs two decision trees by applying DT-CI-GBI to each group. As a result, we confirmed that with this method, the classification accuracy can increase by about 10%. We further developed a heuristic function used as a criterion of selecting node pairs to chunk in CI-GBI, and experimentally showed its usefulness.

3. Discovery of time dependent law equations from data

Just like physicists have tried for many years to find the truth that is hidden in the experimental data by the deep insight and understood the phenomena, computer can assist in analysing a huge amount of data that are beyond the capability of human cognition and derive equations that explain the phenomena. Being able to reproduce the experimental data does not necessarily mean that the derived equations represent the first principle. We are developing a method that ensures to derive the first principle. The main results obtained up to this year include the followings.

1. We have developed a theory of first principle discovery and implemented it to a working system that can discover multiple simultaneous equations under experimental setting. Notion of scales of the experimental data and an interesting property that is deduced by dimensional analysis are the basis of the method. These two together with simple mathematics can constrain the form of admissible relations among the variables.
2. We have extended the above approach to derive equations from observed data where no active experimentation is allowed. This extension expands the scope of the application areas of our approach to various practical domains. The manipulation of quantities is not possible, under the environment of passive observation, to obtain

numeric data from which to extract the relations among quantities. We introduced a technique to emulate virtual experiments to identify the relations among quantities within a given set of observed data. The final system works for passively observed phenomena for which nothing is known about the equation formulae that are needed to describe them and no knowledge of dimensions of the variables involved is available. It can handle a system that is described by several equations and many variables. The simulation results indicate that the method is noise resistant.

3. We have developed a method that can enhance the reliability of the obtained equations using two different sets of quantities for the same phenomenon and the information of scale-types of the quantities.
4. An approach to discover a complex law equation model consisting of simultaneous equations was developed when only the passive observation is available. This work investigated the mathematical properties of invariance, symmetry and lattice structure of a simultaneous equation, and established a principle to figure out the number of equations governing the observed data simultaneously and the configuration of quantities in the equations. Based on the principle, an algorithm to derive law based simultaneous equations from data is developed and implemented. Its high ability to discover the complex models for the data obtained from a process plant and a social phenomenon has been confirmed.
5. We investigated some principles to discover time dependent law equations which are differential equations reflecting the dynamics of the objects. The equations are discovered based on the observed time series data of quantities associated with the objects.

In this year, a method to identify state variable numbers required to represent the objective system of the observed time series data, a method to reason the scale-types of state variables based on the scale-types of observed variables, a method to search candidate simultaneous time differential equations governing the state variables and a method to evaluate the accuracy of the searched candidate equations have been established. These have been implemented into a simultaneous time differential law equation discovery system named SCALETRACK which discovers the equations from the observed time series data, and its performance has been evaluated through simulation data. Its ability has been confirmed to discover law equations representing time dependent dynamics of complex systems including chaos.

4. Information retrieval under various data format

Massive data having various formats such as text, movie, sound, coded data and data specific to each application are being accumulated in computers and their networks. However, information retrieval systems such as search engines remain within the keyword based text search approach. Though some new retrieval methods specific to each data format such as movies and sounds have been proposed, these new retrieval methods can hardly handle many data formats newly borne year by year. We have started developing a new generic retrieval approach that is independent of data format, and the following results have been obtained.

1. A framework has been developed that enables the generic retrieval of various data format under a single principle.
2. The principle is based on the use of the fast Fourier transform having a mathematical nature of transformation invariance which enables the robust retrieval against the various similar byte sequences to be retrieved.
3. The retrieval algorithm based on this principle has been applied to the keyword based retrieval on text data files and the binary data based retrieval on binary data files of a word processor. In both cases, good performance of the proposed approach has been confirmed.
4. The performance evaluation has been conducted on many more different kinds of binary document data sets, and the efficiency of the retrieval program has been improved. By removing redundant retrieval in the algorithm, the speed of the retrieval has been increased more than 10 times.
5. The program has been extended to enable binary data having two dimensional structure such as picture image data. Only slight extension was required for this purpose because of the essential generality of this approach in nature.
6. A collaborative research has been conducted with an industrial company to remove spam mails from a massive set of e-mail data by retrieving only spam mails which have a large variety of unformatted documents based on the aforementioned techniques.

In this year, the aforementioned techniques have been applied to discover time dependent law equations from numeric data. To discover credible and generic law equations, the equations should be searched based on numeric time series data generated from many similar dynamics. These similar dynamics data must be acquired by the retrieval from massive numeric time series database. Our retrieval technique has been combined with the simultaneous time differential law equation discovery system named SCALETRACK for this objective, and the extended SCALETRACK has been developed. It discovered law equations having higher credibility in one order of magnitude and efficiently focused on law equations having high generality.

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Computation-time efficient and robust attribute tree mining with DRYADEPARENT, *A. Termier, M.C. Rousset, M. Sebag, K. Ohara, T. Washio and H. Motoda, The 3rd

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SCALETRACK: A System to Discover Dynamic Law Equations Containing Hidden States and Chaos, *T. Washio, F. Adachi and H. Motoda, The 8th International Conference on Discovery Science (DS'05), Singapore, Oct.8-11, 2005.

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Decision Tree Construction by Chunkingless Graph-Based Induction for Graph-Structured Data, P. C. Nguyen, *K. Ohara, A. Mogi, H. Motoda and T. Washio, The First International Workshop on Mining Complex Data (MCD'05), Houston, Texas, USA, Nov.27, 2005.

Contributions to International Conferences and Journals

H. Motoda	Intelligent Data Analysis: An International Journal(Editorial Board)
H. Motoda	Advanced Engineering Informatics (Editorial Board)
H. Motoda	International Journal of Human-Computer Studies (Editorial Board)
H. Motoda	Knowledge and Information Systems: An International Journal (Editorial Board)
H. Motoda	Discovery Science Conference (Steering Committee, Chair)
H. Motoda	Algorithmic Learning Theory Conference (Steering Committee)
H. Motoda	Pacific-Asia Conference on Knowledge Discovery & Data Mining (Steering Committee, Chair)
H. Motoda	Pacific Rim International Conference on Artificial Intelligence (Steering Committee)
H. Motoda	The 8 th International Conference on Discovery Science (Conference Chair)
H. Motoda	The 9 th Pacific-Asia Conference on Knowledge Discovery & Data Mining (Conference Chair)
H. Motoda	The 2 nd International Workshop on Mining Complex Data (MCD'06) (Program Committee)
H. Motoda	The 6 th International Conference on Data Mining (ICDM'06) (Program Committee)
H. Motoda	The 16 th International Symposium on Methodologies for Intelligent Systems (ISMIS2006) (Program Committee)
H. Motoda	The International Workshop on Feature Selection for Data Mining: Interfacing Machine Learning with Statistics (FSDM2006) (Program Committee)
H. Motoda	The 23 rd International Conference on Machine Learning (ICML-2006) (Senior Program Committee)

H. Motoda	The 10 th Pacific-Asia Conference on Knowledge Discovery & Data Mining (PAKDD06) (Program Committee)
H. Motoda	The 15 th International Conference on Inductive Logic Programming (ILP2005) (Program Committee)
H. Motoda	The 5 th IEEE International Conference on Data Mining (ICDM2005) (Program Committee)
H. Motoda	The 11 th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD2005) (Program Committee)
H. Motoda	The 10 th International Conference on Rough Sets, Fuzzy Sets, Data Mining, and Granular Computing (RSFDGrC2005) (Program Committee)
H. Motoda	The 16 th European Conference on Machine Learning (ECML) (Area Chair, Program Committee)
H. Motoda	The 9 th European Conference on Principles and Practice of Knowledge Discovery in Databases PKDD (Area Chair, Program Committee)
H. Motoda	The 22 nd International Conference on Machine Learning (ICML-2005) (Area Chair, Program Committee)
H. Motoda	The Symposium on Abstraction, Reformulation and Approximation (Program Committee)
H. Motoda	The 9 th Pacific-Asia Conference on Knowledge Discovery & Data Mining (PAKDD05) (Program Committee)
H. Motoda	International Workshop on Feature Selection for Data Mining Interfacing Machine Learning with Statistics (FSDM2005) (Program Committee)
H. Motoda	The 4 th Workshop on Multi-Relational Data Mining (MRDM-2005) (Program Committee)
H. Motoda	Workshop on Foundation of Semantic Oriented Data and Web Mining (Program Committee)
T. Washio	New Frontiers in Artificial Intelligence: Proceeding of the 20th Annual Conference of the Japanese Society for Artificial Intelligence (Editorial Board)
T. Washio	Special Issue on Applications Eligible for Data Mining, Journal of Advanced Engineering Informatics (Editorial Board)
T. Washio	New Frontiers in Artificial Intelligence: Proceeding of the 19th Annual Conference of the Japanese Society for Artificial Intelligence (Editorial Board)
T. Washio	Advances in Mining Graphs, Trees and Sequences, Frontiers in Artificial Intelligence and Applications (Editorial Board)
T. Washio	Special Issue on Mining Graphs, Trees and Sequences (MGTS), Journal of Fundamental Informatica (Editorial Board)
T. Washio	The 11 th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD07) (Workshop Chair)
T. Washio	The 9 th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD05) (Tutorial Chair)
T. Washio	The 10 th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD) (Program Committee)

T. Washio	The 17 th European Conference on Machine Learning (Program Committee)
T. Washio	Knowledge Management (KM) track of the ACM 15th Conference on Information and Knowledge Management (CIKM-2006) (Program Committee)
T. Washio	The 16 th International Conference on Inductive Logic Programming (ILP2006) (Program Committee)
T. Washio	The 23 rd International Conference on Machine Learning (ICML2006) (Program Committee)
T. Washio	The 9 th Pacific Rim International Conference on Artificial Intelligence (PRICAI06) (Program Committee)
T. Washio	The 3 rd International Workshop on Mining Graphs, Trees and Sequences (MGTS-2005) (Program Committee)
T. Washio	The 17 th European Conference on Machine Learning (ECML05) (Program Committee)
T. Washio	The 2005 IEEE/WIC/ACM International Joint Conference on Web Intelligence and Intelligent Agent Technology (WI/IAT 2005) (Program Committee)
T. Washio	The 23 rd International Conference on Machine Learning (ICML2005) (Program Committee)
T. Washio	The 15 th International Conference on Inductive Logic Programming (ILP05) (Program Committee)
T. Washio	The 4 th Workshop on Multi-Relational Data Mining (MRDM-2005) (Program Committee)
T. Washio	The 15 th International Symposium on Methodologies for Intelligent Systems (ISMIS2005) (Program Committee)
T. Washio	The 9 th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD05) (Program Committee)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	10 papers
Information Processing Society of Japan	1 paper
The Operations Research Society of Japan	1 paper
Joint Symposium of Japan Pharmaceutical Manufacturers Association and The Institute of Statistical Mathematics	1 paper

Academic Degrees

Doctor Degree of Engineering

F. Adachi	A Study for Scientific Law Equation Discovery based on Passive Observation Data
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Master Degree of Engineering

Y. Mitsunaga	A Study for a Mining Principle of Quantitative Frequent Itemsets and its Implementation
A. Mogi	Development of a Graph Mining Method based on Pseudo Chunking and Its Application to Medical data

Sponsorship

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

H. Motoda	Constructive Induction of Useful Attributes from Complex Structured Data	¥7,100,000
T. Washio	Development of Data Mining Method for 3-dimensional Graph Structured Data and Its Application to Identification System of Bioactive Molecules	¥4,500,000

Grant-in-Aid for Exploratory Research

T. Washio	Development of Fast and Complete Search Method of Numeric Association Rules and Its Application to Medication Rule Discovery	¥1,600,000
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Grant-in-Aid for Young Scientists (B)(2)

K. Ohara	Development of Domain Adaptive Data Mining System using Personalization Techniques	¥2,000,000
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Grant-in-Aid for JSPS Special Research Fellows

A. Termier	Efficient Algorithm for Finding Patterns from a Large Amount of Structured Data	¥1,200,000
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Division of Biological Sciences

Outlines

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. Single-molecule imaging of membrane proteins reconstituted in an artificial planar bilayer.
3. Developments of novel microdevices for highly sensitive detection of biological reactions.
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 quinoxinoproteins
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

Achievements

- Single-molecule manipulation of F-type H⁺ ATPases
- Single-molecule imaging of H⁺ ATPase or multidrug exporter molecules in artificial planar membrane
- Imaging of transport vesicle formation on an artificial membrane at a single molecule level
- Development of microdevices for single-molecule analysis of restriction enzyme assay
- Determination of the crystal structure of bacterial major multidrug exporter AcrB
- Site-directed mutagenesis studies based on the crystal structure of AcrB
- Indole-sensing mechanism on the up-regulation of drug exporter genes in *E. coli*
- Analysis of regulation network on bacterial multidrug exporters
- Investigation of xenobiotic exporters from *Salmonella enterica* serovar Typhimurium and their roles on virulence
- Analysis of ABCA5 knock-out mice, a novel ABCA subfamily transporter
- Studies on the sphingosine-1-phosphate export mechanism from platelet
- Identification of novel mammalian RND-type transporters
- Structural and kinetic studies on the catalytic mechanism of copper/topa quinone-containing amine oxidase
- Biochemical and molecular biological studies on the role of an iron-sulfur protein in posttranslational modification of quinoxinoprotein amine dehydrogenase

- Mitochondrial transport is promoted by FEZ1 in neurites of NGF-differentiated PC12 cells
- Novel functions of a splice variant of a RING-IBR protein RBCK1 in transcriptional regulation and proteasomal protein degradation
- Hepatitis B virus envelope pre-S peptide applicable for the human liver-specific protein delivering system

Department of Structural Molecular Biology

Professor:	Katsuyuki TANIZAWA
Associate Professor:	Shun'ichi KURODA
Research Associate:	Kenji TATEMATSU
Post Doctoral Fellows:	Andrés D. MATURANA, Atsuko UEDA, Joo-Hee JUNG, Hiroyasu KADOYA (2005.11~), Nobuo YOSHIMOTO (2006.1~)
Research Assistants:	Yoshimi MAEKAWA (~2005.6), Yoko MATSUSHITA, Ayako TORIKAI (2005.6~7), Kumiko HAZAMA (2005.7~), Takae TOYOSHIMA (2005.9~), Noriko MATSUNAGA (2005.9~), Noriko SHIKAKU (2005.10~), Shino HASHIMOTO (2006.1~), Kazuyo SADAMOTO (2006.1~)
Graduate Students:	Nobuo YOSHIMOTO (~2005.12), Kazutoshi ONO, Takeshi MURAKAWA, Nobuyuki BOKUI, Junko IKUTA, Masami ISHIDA, Takeshi KASUYA, Minobu TANI, Hiroyuki TONOI
Support Staff:	Mayumi MURATA

Outlines

The primary research of this department continues to focus on the biochemical and molecular biological studies on various functional proteins, with particular emphasis on the amino acid-metabolizing enzymes. The active-site structures and catalytic functions of amino acid residues in several interesting enzymes are being investigated by means of affinity labeling, site-directed mutagenesis, various spectroscopies, and X-ray crystallography. One of the recent conspicuous findings is the copper ion-dependent, post-translational modification mechanism for the biogenesis of the topa quinone cofactor in copper amine oxidase. In addition, this department started to 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 hollow bio-nanoparticles 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 Programs

1. Structural and Kinetic Studies on the Catalytic Mechanism of Copper/Topa Quinone-containing Amine Oxidase.

A key step decisively affecting the catalytic efficiency of copper amine oxidase is stereospecific abstraction of substrate α -proton by a conserved Asp residue. We analyzed this step by pre-steady-state kinetics using a bacterial enzyme and

stereospecifically deuterium-labeled substrates, 2-phenylethylamine and tyramine. A small and temperature-dependent kinetic isotope effect (KIE) was observed with 2-phenylethylamine, whereas a large and temperature-independent KIE was observed with tyramine in the α -proton abstraction step, showing that this step is driven by quantum mechanical hydrogen tunneling rather than the classical transition-state mechanism. Furthermore, an Arrhenius-type preexponential factor ratio approaching to a transition-state value was obtained in the reaction of a mutant enzyme lacking the critical Asp. These results provide strong evidence for enzyme-enhanced hydrogen tunneling. X-ray crystallographic structures of the reaction intermediates revealed a small difference in the binding mode of distal parts of substrates, which would modulate hydrogen tunneling proceeding through either active or passive dynamics.

2. Biochemical and Molecular Biological Studies on the Role of an Iron-Sulfur Protein in Posttranslational Modification of Quinohemoprotein Amine Dehydrogenase.

Quinohemoprotein amine dehydrogenase (QHNDH) of *Paracoccus denitrificans* contains a peptidyl quinone cofactor, cysteine tryptophylquinone (CTQ), as well as intra-peptidyl thioether crosslinks between Cys and Asp/Glu residues within the smallest γ -subunit of the $\alpha\beta\gamma$ heterotrimeric protein. A putative [Fe-S]-cluster-binding protein (ORF2 protein) encoded between the structural genes for the α - and γ -subunits of QHNDH in the *n*-butylamine utilizing operon likely belongs to a Radical SAM (S-Ado-Met) superfamily that includes many proteins involved in vitamin biosynthesis and enzyme activation. In this study, the role of ORF2 protein in the biogenesis of QHNDH has been explored. While the wild-type strain of *P. denitrificans* produced an active, mature enzyme upon induction with *n*-butylamine, a mutant strain, in which the *ORF2* gene had been mostly deleted, neither grew in the *n*-butylamine medium nor showed QHNDH activity. When the mutant strain was transformed with an expression plasmid for the ORF2 protein, *n*-butylamine-dependent bacterial growth and QHNDH activity were restored. Site-specific mutations in the putative [Fe-S]-cluster- or SAM-binding motifs in the ORF2 protein failed to support bacterial growth. The α - and β -subunits were both detected in the periplasm of the mutant strain, whereas the γ -subunit polypeptide was accumulated in the cytoplasm and stained negatively for redox-cycling quinone staining. MALDI-TOF mass spectrometric analysis revealed that the γ -subunit isolated from the mutant strain had not undergone posttranslational modification. These results unequivocally show that the putative [Fe-S]-cluster- and SAM-binding ORF2 protein is necessary for the posttranslational processing of γ -subunit, most likely participating in the formation of the intra-peptidyl thioether crosslinks.

3. Mitochondrial Transport Is Promoted by FEZ1 in Neurites of NGF-Differentiated PC12 Cells.

The presence of mitochondria in the distal part of neuron, *i.e.*, dendrites and axon, is crucial to maintain both cell functions and survival. Mitochondria in neuron are transported from soma to axon and dendrites with the help of motor proteins along the microtubules network. The mitochondrial transport and localization are tightly and finely regulated by second messengers and biosignaling proteins. Fasciculation and elongation protein zeta-1 (FEZ1) is 45-kDa protein with four coiled-coiled domains.

FEZ1 interacts with protein kinase C ζ , and efficiently promotes the neurite elongation in the rat pheochromocytoma PC12 cells. Moreover, FEZ1 rescues both abnormal neuronal morphology and locomotory defect caused by *Caenorhabditis elegans unc-76* mutations, indicating FEZ1 is tightly related to axonal guidance. In this study, we are aiming to elucidate how FEZ1 promotes axonal outgrowth in mammalian neurons. During the NGF-induced neurite outgrowth of PC12 cells, expression of endogenous FEZ1 is strongly enhanced. Suppression of FEZ1 expression using specific RNA interference (RNAi) strongly inhibits the NGF-induced neurite elongation. The NGF-induced FEZ1 is found in both cytoplasm and neurites and co-localized mostly with mitochondria. Moreover, FEZ1 and mitochondria co-migrate along the outgrowing neurites of PC12 cells. Immunoprecipitation experiments revealed that FEZ1 binds tubulin and an anterograde-directed motor protein kinesin but not with the retrograde-directed motor protein dynein. The RNAi down-regulation of FEZ1 expression does not alter the distribution of mitochondria but efficiently inhibits the anterograde movement of mitochondria in NGF-treated PC12 cells. Thus, these observations strongly suggest that FEZ1 is an essential modulator of the anterograde but not retrograde transport of mitochondria along the outgrowing neurites and axons. In conclusion, FEZ1 might play an essential role for axonal outgrowth during neuronal differentiation by regulating the axonal transport of mitochondria.

4. Novel Functions of a Splice Variant of a RING-IBR Protein RBCK1 in Transcriptional Regulation and Proteasomal Protein Degradation.

RBCK1 (RBCC protein interacting with PKC $\underline{1}$), a member of the RING-IBR protein family, possesses both transcriptional and ubiquitin ligase activities. The protein shuttles between the nucleus and the cytoplasm by the activities of nuclear export and localization signals (NES and NLS) contained within its amino acid sequence. RBCK2, a splice variant of RBCK1, lacks the RING-IBR domain and possesses no transcriptional activity, while it represses the RBCK1-mediated transcriptional activity by forming an RBCK1-RBCK2 complex. We have recently demonstrated that RBCK2 plays two distinct roles in transcriptional regulation and proteasomal protein degradation. First, RBCK2 is predominantly localized in the cytoplasm by the function of two Leu-rich nuclear export signals (NESs). A NES-disrupted RBCK1, mostly localized in the nucleus, is translocated to the cytoplasm by the overexpression of RBCK2. This finding indicates that RBCK2 serves as a cytoplasmic tethering protein for RBCK1 and regulates its transcriptional activity. Second, RBCK2 links a poly-ubiquitin chain with the poly-ubiquitin chain-recognizing subunit S5a of the 26S proteasome, and thereby promotes the proteasomal degradation of a poly-ubiquitinated protein. This observation strongly suggests that RBCK2, like Rad23, serves as a scaffold for a poly-ubiquitinated protein and the 26S proteasome. Other RING-IBR proteins (*e.g.*, Parkin) and various RING proteins (*e.g.*, BRCA1, BARD1, RNF8) also accompany with splice variants lacking the RING-IBR domain and the RING domain, while the function of these splice variants has so far been unsettled. Based upon the results obtained in the present studies, it is assumed that these splice variants may control the intracellular localization and/or the functions of parental proteins by protein-protein interaction.

5. Hepatitis B Virus Envelope Pre-S Peptide Applicable for the Human Liver-Specific Protein Delivering System.

Human hepatitis B virus (HBV) is known to infect specifically human hepatocyte, causing hepatocellular carcinoma. HBV has three envelope proteins, large (L), middle (M), and small (S), which share the C-terminal 226 amino acids called S domain. L protein has 2 extra peptides called pre-S1 and pre-S2 in its N terminus, M protein only the pre-S2 peptide. Pre-S1 (21-47) is suggested necessary for hepatocyte specific binding. Pre-S2 may enable envelope proteins to penetrate the hepatocyte plasma membrane, although major aspects of HBV-specific hepatocyte attachment, the way to enter the cell and to deliver genetic information to the nucleus remain obscure. We have investigated these points using pre-S1, pre-S2, and pre-S(1+2) peptides fused to GFP (Green Fluorescent Protein). When GFP-pre-S1 and GFP-pre-S(1+2) were applied *in vitro*, GFP-derived fluorescent was predominantly detected in human hepatoma-derived cells and only faintly in non-hepatic cells in the case of GFP-pre-S(1+2). On the other hand, GFP-pre-S2-derived fluorescence was observed in all cell lines. In addition, using a xenograft model of nude mice carrying NuE, human hepatoma cells, we found that only GFP-pre-S(1+2) could be accumulated in human liver-derived tumors after systemic intravenous administration. These results indicate that GFP-fused pre-S(1+2) peptide behaves as human liver-specific homing peptide *in vivo*, revealing its usefulness for the human liver-specific protein delivering system.

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Original Papers

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Nuclear-cytoplasmic Shuttling of a RING-IBR Protein RBCK1 and Its Functional Interaction with Nuclear Body Proteins, K. Tatematsu, N. Yoshimoto, T. Koyanagi, C. Tokunaga, T. Tachibana, Y. Yoneda, M. Yoshida, T. Okajima, K. Tanizawa, and S. Kuroda: J. Biol. Chem., 280 (2005) 22937–22944.

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The Specific Delivery of Proteins to Human Liver Cells by Engineered Bio-Nanocapsules, D. Yu, C. Amano, T. Fukuda, T. Yamada, S. Kuroda, K. Tanizawa, A. Kondo, M. Ueda, H. Yamada, H. Tada, and M. Seno: FEBS J., 272 (2005) 3651–3660.

Identification of FEZ1 as a Protein That Interacts with JC Virus Agnoprotein and Microtubules: Role of Agnoprotein-Induced Dissociation of FEZ1 from Microtubules in Viral Propagation, T. Suzuki, Y. Okada, S. Semba, S. Orba, S. Yamanouchi, S. Endo, S. Tanaka, T. Fujita, S. Kuroda, K. Nagashima, and H. Sawa: J. Biol. Chem., 280 (2005) 24948–24956.

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Effective Gene Therapy Conducted by Nanotechnology, J. H. Jung, and S. Kuroda: Kagaku, 60 [1] (2005), 23–25.

Innovative Nanocarrier: Pinpoint DDS using Hollow Bio-nanoparticles, A. Kondo, S. Kuroda, K. Tanizawa, M. Seno, and M. Ueda: Bioindustry, 22 [5] (2005), 22–27.

Pinpoint DDS using Hollow Bio-nanoparticles, A. Kondo, S. Kuroda, K. Tanizawa, M. Seno, and M. Ueda: Chemical Engineering, 50 [5] (2005), 23–28.

Bio-nanocapsules Facilitating Cell- and Tissue-Specific Gene Transfer, T. Yamada, M. Seno, M. Ueda, A. Kondo, K. Tanizawa, and S. Kuroda: Seibutsukougaku-kai Zasshi, 83 [8] (2005), 380–383.

Novel Medical Technology Using Bio-nanocapsules, S. Kuroda: Bioscience and Bioindustry, 63 [9] (2005), 589–590.

Development of Bio-nanocapsule and Its Application for Cosmetics, S. Kuroda: FRAGRANCE JOURNAL, 11 (2005), 22–28.

BEACLE Corp., S. Kuroda: Bioindustry, 22 [4] (2005), 88–95.

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Books

Protein Self-processing, T. Okajima and K. Tanizawa: *in* Protein Science—Structure, Property, Function (Y. Goto, K. Kuwajima, and K. Tanizawa, Eds.), Kagaku-Dojin (2005), 351–362.

Mechanism of Intracellular Signal Transduction: Scaffold Proteins and Protein Kinases, S. Kuroda: *in* Protein Science—Structure, Property, Function (Y. Goto, K. Kuwajima,

and K. Tanizawa, Eds.), Kagaku-Dojin (2005), 519–530.

Dictionary of Nano-biotechnology (T. Yamane and T. Matsunaga, Eds.) S. Kuroda, Techno-system Corp (2005).

Patents

“Peptide Array for Detection of Protein Kinase Activity” K. Tatematsu, M. Kyou, Y. Katayama, T. Sonoda, Y. Inoue, and K. Inamori: JP2005-297337.

“Screening Method for Receptor-binding Materials” A. Kondo, S. Kuroda, M. Ueda, J. Ishii, H. Fukuda, K. Tatematsu, and T. Yamasaki: JP2005-96184.

“Drugs for the Treatment of Cancer and Their Production” M. Seno, H. Tada, T. Fukuda, S. Kuroda, K. Tanizawa, A. Kondo, M. Ueda, and H. Hamada: JP2005-84438.

“Efficient Methods for Incorporating Materials into Bio-nanocapsules” S. Kuroda, A. Ueda, and M. Nagita: JP2005-267573.

“Efficient Purification Methods of Bio-nanocapsules” S. Kuroda, M. Maekawa, and M. Nagita: JP2006-35666.

International Conferences

Bionanocapsules for Pinpoint Drug and Gene Delivery –A Hybrid of Virus and Liposome– (Invited), S. Kuroda, International Workshop Improving Gene and Drug Delivery to the Heart, University of Geneva Medical School, Geneva, Switzerland, August 1–2, 2005.

High-throughput Drug Screening System Using Yeast Displaying System (Invited), S. Kuroda, Enzyme Engineering XVIII, Engineering Conference International, Hotel Hyndai, Gyeong-ju, Korea, October 10–15, 2005.

Novel Oral Vaccine System Using Lactobacillus Surface Displaying System (Invited), S. Kuroda, Human Science Forum (Kinki Bio-industry Association), Intex Osaka, Osaka, Japan, October 19–21, 2005.

Active-site Structure of Copper Amine Oxidase Probed by Three Hydrazine Derivatives Reactive with the TPQ Cofactor (Oral), T. Murakawa, T. Okajima, M. Taki, Y. Yamamoto, S. Kuroda, H. Hayashi, and T. Tanizawa, International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Awaji, Hyogo, Japan, November 6–11, 2005.

Reaction Mechanism of Bacterial Copper Amine Oxidase: X-ray Crystal Structures of Catalytic Intermediates with Reduced Forms of the TPQ Cofactor (Poster), T. Okajima, T. Murakawa, S. Kuroda, and K. Tanizawa, International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Awaji, Hyogo, Japan, November 6–11, 2005.

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Involvement of a [Fe-S]-binding Protein in the Biogenesis of Quinohemoprotein Amine Dehydrogenase (Poster), T. Okajima, K. Ono, M. Tani, S. Kuroda, and K. Tanizawa, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

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Nano-scale Structure of Copper Amine Oxidase Probed by Three Hydrazine Derivatives Reactive with the TPQ Cofactor (Poster), T. Murakawa, T. Okajima, M. Taki, Y. Yamamoto, S. Kuroda, H. Hayashi, and K. Tanizawa, Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Hepatitis B Virus Envelope pre-S Peptide as a Useful Human Liver-specific Homing Peptide (Poster), T. Kasuya, A. Ueda, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Cell Signaling Machineries of Novel Differentiation Factors for Neural Crest-derived Cells, NELL1 and NELL2 (Poster), N. Bokui, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Pinpoint Drug and Gene Delivery System Using ZZ-displaying BIO-nanocapsule and Targeting Molecular-fused IgG Fc Protein (Poster), H. Tono, H. Tada, A. Ueda, T. Kasuya, K. Tatematsu, T. Okajima, A. Kondo, M. Senno, M. Ueda, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Development of Functionalized Nanoparticles towards Targeted Drug Delivery Systems (Poster), S. Takizawa, and K. Tatematsu, 4th 21st Century COE “Towards Creating New

Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Involvement of a Hypothetical [Fe-S]-binding Protein in the Biosynthesis of Quinohemoprotein Amine Dehydrogenase (Invited), K. Tanizawa, Gordon Research Conference on Protein Derived Cofactors, Radicals and Quinones, Ventura, California, U.S.A., January 22–27, 2006.

Active-site Structure of Copper Amine Oxidase Probed by Three Hydrazine Derivatives Reactive with the TPQ Cofactor (Poster), T. Murakawa, T. Okajima, M. Taki, Y. Yamamoto, S. Kuroda, H. Hayashi, and K. Tanizawa, Gordon Research Conference on Protein Derived Cofactors, Radicals and Quinones, Ventura, California, U.S.A., January 22–27, 2006.

Involvement of a Hypothetical [Fe-S]-binding Protein in the Biosynthesis of Quinohemoprotein Amine Dehydrogenase (Poster), K. Ono, M. Tani, T. Okajima, D. Sun, V. L. Davidson, S. Kuroda, and K. Tanizawa, Gordon Research Conference on Protein Derived Cofactors, Radicals and Quinones, Ventura, California, U.S.A., January 22–27, 2006.

Reaction mechanism of bacterial copper amine oxidase: X-ray crystal structures of catalytic intermediates with reduced forms of the TPQ cofactor (Poster), T. Okajima, T. Murakawa, S. Kuroda, and K. Tanizawa, Handai Nanoscience and Nanotechnology International Symposium, Suita, Osaka, Japan, January 30–February 1, 2006.

In Vivo Pinpoint Gene/Drug Delivery System Using Bionanocapsules (Invited), S. Kuroda, The International Symposium for 20th Anniversary of Biotechnology Center, Chungnam University, Chungnam University, Taejeon, Korea, February 15, 2006.

Publications in Domestic Meetings

Japanese Biochemical Society	3 papers
The Molecular Biology Society of Japan	1 paper
Bimonthly Meeting of Vitamin B Committee	2 papers

Academic Degrees

Doctor Degree of Science

N. Yoshimoto	Novel Functions of a Splice Variant of a RING-IBR Protein RBCK1 in Transcriptional Regulation and Proteasomal Protein Degradation
T. Murakawa	Structural and Kinetic Studies on the Catalytic Mechanism of Copper/Topa Quinone-containing Amine Oxidase

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas (C) (2)

S. Kuroda	Development of New Pinpoint Gene Delivery System Using Nanoparticles Fused with Bio-recognition Molecule.	¥8,100,000
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Grant-in-Aid for Scientific Research (21st Century COE)

K. Tatematsu	Development of Functionalized Nanoparticles towards Targeted Drug Delivery Systems	¥1,000,000
N. Bokui	Cell Signaling Machineries of Novel Differentiation Factors for Neural Crest-derived Cells, NELL1 and NELL2	¥500,000
J. Ikuta	Mitochondrial Transport Is Promoted by FEZ1 in Neurites of NGF-Differentiated PC12 Cells	¥500,000
T. Murakawa	Quantum Mechanical Hydrogen Tunneling in Bacterial Copper Amine Oxidase Reaction	¥500,000

Health and Labour Sciences Research Grants

S. Kuroda	Development of Bio-Nanocarriers for Pinpoint Drug Delivery System and Its Application for Cancer Therapy	¥4,500,000
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Cooperative Research

S. Kuroda	As One Corp.	Development of Screening Method for Agonists and Receptors Using Combinatorial Biochemistry	¥37,050,000
S. Kuroda	Beacle Inc.	Development of Hollow Bio-nanocapsule Applicable to Tissue/Cell-specific Targeting and Imaging	¥210,000
K. Tatematsu	Bio-Leaders Japan, Ltd.	Production and Development of New Live Bacterial Vaccines	¥405,000

Entrusted Research

K. Tanizawa	Japan Society for the Promotion of Science	Survey and Research on the Academic Trends in Biological Sciences	¥3,500,000
K. Tanizawa	Mitsubishi Electric Company, Ltd. (NEDO)	Analysis of Intracellular Signal Networks for Industrial Application of Genomics	¥4,200,000
K. Tanizawa	Japan Science and Technology Agency (CREST)	Creation of Functional Materials/ System that Utilize Nano Biotechnology for Realizing a Noninvasive Medical Treatment System:	¥11,950,000

		Novel Cell-selective Gene Delivery System Using Intracellular Signal-responsive Molecular System	
K. Tanizawa	Bio-oriented Technology Research Advancement Institution (BRAIN)	Development of Innovative and Hypersensitive Bio-sensing Technology Using Yeast-derived Bio-nanocapsule	¥21,805,000
S. Kuroda	Ministry of Education, Culture, Sports, Science, and Technology	Protein 3000 Project	¥3,000,000
S. Kuroda	Osaka Science and Technology Center (Ministry of Economy, Trade and Technology)	Development of Proteome-based High Throughput Screening System Using Combinatorial Biochemistry.	¥4,655,000
S. Kuroda	Japan Science and Technology Agency (Innovation Plaza Osaka)	Development of Hollow Nanoparticles for Pinpoint Gene/Protein/Drug Delivery to Various Tissues and Cells in Animals.	¥30,000,000
Other Research Funds			
K. Tanizawa	Vitamin B Committee	Research on Built-in Cofactors	¥250,000
K. Tanizawa	Applied Enzyme Association of Japan	Biogenesis and Catalytic Function of Peptide Built-in Quinone Cofactors	¥1,000,000

Department of Single Molecule Biophysics

Professor:	Hiroyuki NOJI
Associate Professor:	Yoh WADA
Research Associate:	Kazuhito TABATA,
Specially Appointed- Research Associate:	Ryota IINO
Postdoctoral Researchers:	Daichi OKUNO, Hiroshi UENO, Liza Lam
Undergraduate Student:	Mahito MATSUNO, Junya HORIGUCHI, Masayoshi NAKATA
Research Technical Expert:	Takako NAKASHIMA, Minako AOYAMA
Secretary:	Miki WALSH
Japan Association for the Advancement of Medical Equipment Researchers:	Yuko IKO

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. Thus, we conduct quite interdisciplinary researches crossing biochemistry, nanobiotechnology, and micro/nano fabrication.

Current Research Projects

1. Single-molecule studies on a rotary molecular motor, F₁-ATPase

F₁-ATPase is the smallest rotary motor of which diameter is only 10 nm. Hydrolyzing ATP molecules, it generates rotary torque to rotate its rotary shaft against surrounding stator ring. However, its physiological function is not a rotary motor but ATP generator. Recently, we directly proved that F₁ motor molecules synthesize ATP when it is pushed in backward direction (clockwise) using single-molecule manipulation techniques and a microfabrication techniques. Thus, this motor is a nanometer-sized molecular device for mechano-chemical energy conversion. Our main theme is to reveal the molecular mechanism of F₁-ATPase. We directly observe and manipulate individual F₁-ATPase molecules under optical microscopy to see their chemical and mechanical responses.

2. Membrane protein dynamics embedded in lipid bilayer

Membrane proteins are crucial for signaltransduction, energy conversion and transport of bioactive substance such as ion, chemical, peptide and proteins. However, handling of membrane proteins is generally much more difficult than that of soluble proteins because membrane proteins are often degenerated when they are extracted from lipid bilayer and exposed to a hydrophilic environment. Therefore, dynamics of

membrane proteins has not been studied well. In this study, we developed an experimental system for real-time imaging of dynamics of single membrane proteins.

Publications

Original Papers

Temperature Alternation by an On-Chip Microheater to Reveal Enzymatic Activity of Beta-Galactosidase at High Temperatures, H.F. Arata, Y. Rondelez, H. Noji and H. Fujita: *Anal Chem.* 77 (2005) 4810-4814.

Activation of Pausing F1 Motor by External Force, Y. Hirono-Hara, K. Ishizuka, K. Jr. Kinoshita, M. Yoshida and H. Noji: *Proc. Natl. Acad. Sci. U.S.A.* 102 (2005) 4288-4293.

Highly Coupled ATP Synthesis by F1-ATPase Single Molecules, Y. Rondelez, G. Tresset, T. Nakashima, Y. Kato-Yamada, H. Fujita, S. Takeuchi and H. Noji: *Nature* 433 (2005) 773-777.

Microfabricated Arrays of Femtoliter Chambers Allow Single Molecule Enzymology, Y. Rondelez, G. Tresset, K. Tabata, H. Arata, H. Fujita, S. Takeuchi and H. Noji: *Nature Biotechnology* 3 (2005) 361-365.

Review Papers

Chemomechanical Coupling in Single-Molecule F-type ATP Synthase, R. Iino, Y. Rondelez, M. Yoshida and H. Noji: *J Bioenerg Biomembr.* 37 [76] (2005) 451-453.

Techno-Trend, Ultrasensitive Enzyme Assay using the World's Smallest Solution Chamber, H. Noji: *Biotechnology Journal* 9-10 (2005) 576-578.

Molecule Choro-Q Project, Study of the Protein Rotary Motor using Micro Solution Chamber, H. Noji, *Bionics* 8 (2005) 46-52.

Basic course, Biological Molecule Mortar – Fusion/Contact of Biology and Electronics, H. Noji, *Applied physics* 74 [7] (2005) 951-956.

Development of Single-Molecule Bioassay using Micro Solution Chamber, H. Noji, *Brain Techno News* 109 (2005) 37-40.

Single Molecule Bioassay using Micro Solution Chamber, H. Noji, Y. Rondelez, G. Tresset, H. Fujita and S. Takeuchi, *Chemistry and Micro-nano system* 3 (2005), 12-14.

International Conferences

Femtoliter chamber of Single Molecule Analysis of Biological Reactions (invited), *H. Noji, 3rd International IEEE-EMBS Special Topic Conference on Microtechnologies in Medicine and Biology, Hawaii, May 15, 2005.

Single Molecule Studies on F1-ATPase Using a Femtoliter Chamber (invited), *H. Noji and R. Iino, FASEB summer seminar, Vermont Academy, June 20, 2005

Micron-Sized Reaction Chamber for Single Biomolecule Detection (invited), *H. Noji, Bioseparation KOBE, Kobe, Japan, Aug 1, 2005

Femtoliter Reaction Chamber for Single Molecule Detection of Biological Reaction (invited), *H. Noji, UT-TUM Bilateral Symposium on Nanosciences, Tokyo, Oct 5, 2005.

Femtoliter Reaction Chamber for Single-Molecule Studies of Biological Reactions (invited), *H. Noji, Micro Total Analysis Systems, Boston, USA, Oct 11, 2005.

Temperature Dependent Angular Velocity Measurement of F1-ATPase Biomolecular Motor by Micro Fabricated Local Heating Device (Poster), *H. Arata, H. Noji and H. Fujita, Micro Total Analysis Systems, Boston, USA, Oct 9 – Oct 13, 2005.

Imaging of Heat Denaturation of Single DNA Molecules in Femtoliter Chambers on a Micro Heating Device: Toward a Single-Molecule Detection of PCR (Poster), *K. Ishizuka, H. Arata, S. Sakakihara, C. Bergaud, K. V. Tabata, Y. Rondelez, S. Takeuchi, H. Fujita and H. Noji, Micro Total Analysis Systems, Boston, USA, Oct 9 – Oct 13, 2005.

High-Speed Switching of Chemical Stimulation for Single Molecular Analysis in Continuous-flow Format (Poster), *S. W. Lee, T. Yamamoto, H. Noji and T. Fujii, Micro Total Analysis Systems, Boston, USA, Oct 9 – Oct 13, 2005.

Simultaneous Reconstitution of Multiple Planar Lipid Bilayers (Poster), *H. Suzuki, K. V. Tabata, H. Noji and S. Takeuchi, Micro Total Analysis Systems, Boston, USA, Oct 9 – Oct 13, 2005.

Femtoliter Reaction Chamber for Single-molecule Analysis of Biological Reactions (invited), *H. Noji, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Toba, Japan, Nov 19, 2005.

Femtoliter Reaction Chamber for Single Molecule Detection of Biological Reaction (invited), *H. Noji, Multi-Institutional International Symposium on 命 (mei), Hokkaido University, Japan, Dec 7, 2005.

Microdevices for Detection and Control of Biological Reaction at a Single Molecule Level (invited), *H. Noji, 21st Century COE-RCMS International Conference-Chemistry for Life - & 2nd Yoshimasa Hirata Memorial Lecture, Nagoya University, Japan, Jan 27, 2006.

Femtoliter Reaction Chamber for Single-molecule Analysis of Biological Reactions (invited), *H. Noji, 1st Workshop on Nanoscience and Nanotechnology between Sanken and CNRS, University Paris-Sud, Orsay, France, Feb 12, 2006.

New Reaction Intermediate of F1-ATPase Found at Low Temperature (Poster), *R.

Watanabe, K. Shimabukuro, M. Yoshida and H. Noji, Biophysical Society, Utah, USA, Feb 22, 2006.

Conformation of the Epsilon Subunit in F1 Forced-Rotated by Magnetic Tweezers (Poster), *E. Saita, R. Iino, Y. Yamada-Kato, H. Noji, T. Suzuki and M. Yoshida, Biophysical Society, Utah, USA, Feb 22, 2006.

Publications in Domestic Meetings

Biophysical Society of Japan	10 papers
Research Group on Polymers and Biosciences	1 paper
Surface Science Lecture Convention	1 paper
Nano-Micro Bioanalysis	1 paper
Molecular Biology Society of Japan	1 paper
Kyoto University, Workshop of Institute for Theoretical Physics Institute	1 paper
Kyoto University, Conference of Institute for Frontier Medical Sciences	1 paper
Kyoto University, Chemical COE Mini Symposium	1 paper
Institute of Electrical Engineers, Sensor Micro-machine Subdivision General Workshop	2 papers
Institute of Electrical Engineers, Sensor Micro-machine Subdivision, Bio-micro System Workshop	2 papers
Bio-energy Workshop	2 papers

Sponsorship

Grants-in-Aid for Scientific Research of Health, Labour and Welfare Ministry

Hiroyuki Noji	Development of single molecule PCR device	¥5,000,000
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Tokubetsu Kenkyuin Shorei-hi

Liza Lam	Micro-device development for single molecule DNA detection	¥400,000
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Entrusted Research

Hiroyuki Noji	Bio-oriented Technology Research Advancement Institution	Preparation of Membrane Protein and single molecule observation	¥40,000,000
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Department of Cell Membrane Biology

Professor:	Akihito YAMAGUCHI
Associate Professor:	Satoshi MURAKAMI
Research Associate:	Takahiro HIRATA
Specially Appointed- Research Associate:	Syoko NISHI
Post Doctoral Fellows:	Takashi MATSUMOTO
Graduate Students:	Nobuyoshi KOBAYASHI, Hidetada HIRAKAWA, Naoki KOBAYASHI, Satofumi HASHIMOTO, Takeshi MASAKI, Ayumi IWATA, Megumi OHIGASHI, Asuka KOBAYASHI, Sakiko SHIBATA, Hiroyuki MANSHIO, Yasuko SENDA, Yu HISANO, Aiko YONEMITSU
Research Students:	Ayumi KISHI, Eiji NIKAIDO, Li-Yuan WANG
Support Staff:	Kotoko ISE, Chiemi TAKENAKA, Reiko SATO, Mari NISHIDA

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.

In this year, we have succeeded to determine the crystal structure of the substrate-bound form of the xenobiotic efflux transporter AcrB. The substrate-bound AcrB was an asymmetric trimer. Only one substrate bound to one of the three protomers, which represents the binding form. The other two protomers corresponded to the two other transport steps, access and release. One trimer crystal contained all snap shots of the three transport steps. Therefore, this crystal structure clearly indicates that AcrB mediates drug export by means of the completely novel functionally rotating binding change mechanism.

As for the regulation of xenobiotic exporter gene expression, we found that indole acts as an intracellular signal transduction molecule and induce the expression of xenobiotic exporter genes. In addition, we found that the pathogenicity of bacteria depends on the xenobiotic exporter gene expression.

As for the mammalian exporters, we advanced the analysis of a novel ABC family protein ABCA5. In addition, we proved that the secretion of sphingosine 1-phosphate from platelets is mediated by unknown membrane exporters driven by ATP hydrolysis.

Current Research Programs

1. Crystallographic and protein engineering analysis of xenobiotic exporters.

We have succeeded in determining the first crystal structure of bacterial multidrug efflux transporter AcrB in 2002. This is the first crystal structure for transporter proteins. This year, we solved the new asymmetric structure of AcrB in complex with its substrates. 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 ordered binding change mechanism. The crystal structure solved in 2002 also suggested direct interaction of AcrB and TolC. We are also performing the mutagenesis studies based on the crystal structure. AcrB-TolC complex by disulfide cross-linking was detected when the specific pair of cysteine mutants was co-expressed in *E. coli*. Our observation indicates that the AcrB can directly interact to TolC.

2. Studies on regulatory networks and physiological functions of xenobiotic exporters in *E. coli* and *S. typhimurium*.

We previously constructed the gene library for 37 putative drug exporters in *E. coli* and clarified that 20 genes actually encode drug exporters and confer drug-resistances. Although *E. coli* has these intrinsic 20 drug exporter genes, most of them are hardly expressed under growth conditions of the complex laboratory media. We found the signals as indole and N-acetylglucosamine that induces some drug exporter genes via two component systems and/or two-component system-independent pathway. Indole also acts as an intercellular signal transducer that depends on the cell growth stage. We believe that some of these exporters have unknown important physiological functions and we are actively pursuing it. During this reporting period, the following progress was made, 1. The growth-phase dependent expression of MdtEF exporter, 2. Fur repression on *mdtABC* and *acrD* genes, 3. Roles of indole on the virulence in EHEC cells, 4. Investigation of xenobiotic exporters from *Salmonella enterica* serovar Typhimurium and their roles on virulence. We are also studying about the regulation of MdtEF by cAMP-CRP-related system, roles of exporters in biofilm formation, and BaeSR-sensing mechanisms.

3. Identification of the exporters that mediates secretion of lipophilic signal transducing molecules.

We develop a monoclonal antibody that recognized the ABCA5 proteins and found that ABCA5 is localized in vesicle like organelle localized near the apical membrane of the thyroid cells. This localization is similar to that of thyroglobulin that is essential for thyroid hormone biosynthesis. This result suggested the possible contribution of ABCA5 protein in thyroid hormone synthesis.

We are also trying to identify a sphingosine-1-phosphate exporter(s) from platelet. We success to show that sphingosine-1-phosphate is exported with specific transporter(s), is not mediated by exocytosis, from the platelet. Using the semi-intact platelet cells and specific inhibitors for known transporters, we proposed that ABC A-type transporters may participate the export of sphingosine-1-phosphate.

Publications

Original Papers

Effect of Laser Irradiation on Enzyme Activity, S. Murakami, M. Kashii, H. Kitano, H. Adachi, K. Takano, H. Matsumura, T. Inoue, Y. Mori, M. Doi, K. Sugamoto, H. Yoshikawa and T. Sasaki: Jpn. J. Appl. Phys., 44 (2005) 8216-8218.

Direct Interaction of Multidrug Efflux Transporter AcrB and Outer Membrane Channel TolC Detected via Site-Directed Disulfide Cross-Linking, N. Tamura, S. Murakami, Y. Oyama, M. Ishiguro and A. Yamaguchi: Biochem., 44 (2005) 11115-11121.

Processing of Membrane Protein Crystal Using UV Laser Irradiation, H. Kitano, S. Murakami, H. Adachi, H. Matsumura, K. Takano, T. Inoue, Y. Mori, M. Doi and T. Sasaki: J. Biosci. Bioeng., 100 (2005) 50-53.

ABCA5 Resides in Lysosomes, and ABCA5 Knockout Mice Develop Lysosomal Disease-Like Symptoms, Y. Kubo, S. Sekiya, M. Ohigashi, C. Takenaka, K. Tamura, S. Nada, T. Nishi, A. Yamamoto and A. Yamaguchi: Mol. Cell. Biol., 25 (2005) 4138-4149.

Semiautomatic Protein Crystallization System Featuring Crystallization Solution Preparation Function, H. Adachi, H. Matsumura, T. Inoue, A. Niino, K. Takano, S. Murakami, Y. Mori and T. Sasaki: Jpn. J. Appl. Phys., 44 (2005) 6302-6303.

Femtosecond Laser Processing of Protein Crystals in Crystallization Drop, M. Kashii, H. Kitano, Y. Hosokawa, H. Adachi, Y. Mori, T. Sasaki, H. Masuhara, K. Takano, H. Matsumura, T. Inoue, S. Murakami, K. Sugamoto and H. Yoshikawa: Jpn. J. Appl. Phys., 44 (2005) L873-875.

Temperature-Screening System for Determining Protein Crystallization Conditions, H. Adachi, A. Niino, K. Takano, H. Matsumura, S. Murakami, T. Inoue, Y. Mori and T. Sasaki: Jpn. J. Appl. Phys., 44 (2005) 4080-4083.

Protein Crystal Growth Using Laser-Processed Seed Crystals, K. Takeuchi, H. Kitano, H. Adachi, Y. Mori, T. Sasaki, H. Matsumura, T. Inoue, S. Murakami, M. Doi, Y. Koga, K. Takano and S. Kanaya: Jpn. J. Appl. Phys., 44 (2005) 3177-3179.

Protein Crystallization by Combining Laser Irradiation and Solution-Stirring Techniques, H. Adachi, A. Niino, S. Murakami, K. Takano, H. Matsumura, T. Kinoshita, M. Warizaya, T. Inoue, Y. Mori and T. Sasaki: Jpn. J. Appl. Phys., 44 (2005) 1365-1366.

Genome-Wide Analyses of *Escherichia coli* Gene Expression Responsive to the BaeSR Two-Component Regulatory System, K. Nishino, T. Honda and A. Yamaguchi: J. Bacteriol., 187 (2005) 1763-1772.

Indole Induces the Expression of Multidrug Exporter Genes in *Escherichia coli*, H. Hirakawa, Y. Inazumi, T. Masaki, T. Hirata and A. Yamaguchi: Mol. Microbiol., 55 (2005) 1113-1126.

Protein Cryocrystallography using Laser-processed Crystal, H. Kitano, H. Matsumura, H. Adachi, S. Murakami, K. Takano, T. Inoue, Y. Mori, M. Doi and T. Sasaki: Jpn. J. Appl. Phys., 44 (2005) L54-L56.

Review Papers

Structure and Functions of Drug-Efflux Transporters ~Towards Overcoming Multi-Drug Resistances, S. Murakami, Kousho Kogaku News, 54 (2005) 16-20.

Books

Solve the Mysteries of Life through Protein Structures, S. Murakami, Kuba Pro, Co., Ltd., (2005) 178-190.

Protein Science, A. Yamaguchi, Kagaku-Dojin Publishing Company, Inc., (2005) 505-517.

Patents

Temperature Controller and Protein Crystallizer Utilizing the Same Apparatus, H. Adachi, T. Sasaki, Y. Mori, K. Takano, T. Inoue, H. Matsumura, S. Murakami, PCT/JP2005/000585

Process for Producing Polymer Crystal and Polymer Crystal Growing Apparatus, H. Adachi, H. Kitano, T. Sasaki, Y. Mori, K. Takano, T. Inoue, H. Matsumura, S. Murakami, NIKON Corporation, PCT/JP2005/016405

International Conferences

Crystal Structure of the Substrate Binding Form of Multidrug Exporter AcrB and the Binding Change Mechanism for the Multidrug Export (Invited), *S. Murakami, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka Univ., Japan, Feb. 8-9, 2006

Regulation of Xenobiotic Exporter Gene Expression by Environmental Response Systems in *Escherichia coli* (Invited), *H. Hirakawa and A. Yamaguchi, The 1st CNU-SANKEN Joint Symposium on Advanced Materials Science, Chungnam National Univ. Daejeon, Korea, November 1-2, 2005.

Analysis of the Mechanism of Proton Translocation through the Integral Vo Domain of the Vacuolar (H⁺)-ATPases (Invited), S. Nishi, *T. Nihai and A. Yamaguchi, 4th 21st Century COE program "Towards Creating New Industries Based on Inter-Nanoscience" International symposium, Toba, Mie, Japan, November 18, 2005.

Regulation of Xenobiotic Exporter Gene Expression and Multidrug Resistance in *Escherichia coli* (Poster), *H. Hirakawa, A. Kobayashi, T. Hirata and A. Yamaguchi,

4th 21st Century COE program "Towards Creating New Industries Based on Inter-Nanoscience" International symposium, Toba, Mie, Japan, November 18, 2005.

Structure and Function of Bacterial Multi-drug Efflux Transporter (Invited), *S. Murakami, Gordon Research Conference on Multi-Drug Efflux Systems, Magdalen college, Oxford, UK, August 28 - September 2, 2005.

Regulation of Xenobiotic Exporter Gene Expressions by Environmental Response systems in *Escherichia coli* (Poster), H. Hirakawa, A. Kobayashi, T. Kodama, T. Hirata and *A. Yamaguchi, Gordon Research Conference on Multi-Drug Efflux Systems, Magdalen college, Oxford, UK, August 28 - September 2, 2005.

Bacterial Xenobiotic Exporter World: From Molecular Structure to Physiological Implications (Invited), *A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Structure and Mechanism of Multi-drug Efflux Transporter AcrB (Invited), *S. Murakami, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Characterization of ABCA5 Protein with Its Specific Monoclonal Antibody and Knockout Mice (Poster), *M. Ohigashi, C. Takenaka, T. Nishi and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Identification of ABCA7 Protein Expression in Mouse Platelet (Poster), *S. Shibata, C. Takenaka, T. Nishi and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Distinct Secretion Mechanism of Sphingosine 1-Phosphate (Poster), *N. Kobayashi, T. Nishi, T. Hirata, A. Kihara, T. Sano, Y. Igarashi and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Localization of Novel RND-type Proteins in Culture Cells and Mice Tissues (Poster), *S. Hashimoto, Y. Kubo, T. Nishi, T. Hirata and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Identification of the Residues Involved in Substrate Recognition in RND-type Multidrug Efflux Transporter (Poster), *N. Kobayashi, N. Tamura, S. Murakami and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Molecular Design of the Super Carbenicillin Resistance AcrB (Poster), *A. Iwata, N. Kobayashi, N. Tamura, Y. Ohkawa, F. Ishibashi, S. Murakami and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Regulation of *E. coli* Drug Resistance and Pathogenicity by Indole Signaling (Poster), *H. Hirakawa, A. Kobayashi, T. Kodama, T. Honda, T. Hirata and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Regulation Mechanisms of the Growth Phase-dependent Expression of Xenobiotic Exporters in *Escherichia coli* (Poster), *A. Kobayashi, H. Hirakawa, T. Hirata and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Fur (Ferric uptake regulator) Controls the Expression of AcrD and MdtABC, Multidrug Efflux Transporters in *Escherichia coli* (Poster), *T. Masaki, H. Hirakawa, T. Hirata and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Small-Scale and Efficient Reporter Assay of *Pseudomonas aeruginosa* Quorum-Sensing System and the Evaluation of 3-oxo-C₁₂-Homoserine Lactone Analogues (Poster), *T. Hirata, A. Kobayashi, H. Hirakawa, M. Horikawa, M. Ishiguro and A. Yamaguchi, American Society of Microbiology, 105th General Meeting, Atlanta, Georgia, June 5-9, 2005.

Indole Sensing Mechanisms that Control Growth Phase-dependent Expression of Xenobiotic Exporter Genes (Poster), *H. Hirakawa, A. Kobayashi, T. Hirata and A. Yamaguchi, American Society of Microbiology, 105th General Meeting, Atlanta, Georgia, June 5-9, 2005.

Contributions to International Conferences and Journals

A. Yamaguchi International Symposium on Biological Membrane Transport 2005
(Conference Chair)

Publications in Domestic Meetings

79 th Japanese Society for Bacteriology	4 papers
The 8 th Japan-Korea International Symposium on Microbiology	1 paper
126 th The Pharmaceutical Society of Japan	4 papers
21st Century COE nano-bio group symposium	5 papers
31 th Japanese Bioenergetics Group	4 papers
28 th The Molecular Biology Society of Japan	7 papers
National Project on Protein Structural and Functional Analyses ” Brain and	1 paper

Nervous System” 4 th Workshop	
27 th Membrane-Drug Interaction Symposium	4 papers
9 th Spring-8 Symposium	1 paper
Sakigake Live 2004	2 papers
78 th The Japanese Biochemical Society	11 papers
17 th Symposium on Microbial Sciences	2 papers
5 th Protein Science Society of Japan	2 papers
2 nd 21st Century research conference on <i>Escherichia coli</i>	1 paper
4 th BIO EXPO JAPAN	1 paper
78 th Japanese Society for Bacteriology	4 papers

Academic Degrees

Doctor Degree of Pharmaceutical Sciences

N. Kobayashi	Identification of secretion mechanism of bioactive lipid, sphingosine 1-phosphate
H. Hirakawa	Studies on regulation mechanisms of drug resistance and pathogenicity of bacteria controlled by signal transduction

Master Degree of Pharmaceutical Sciences

T. Masaki	Studies on the regulation mechanism of the expression of AcrD and MdtABC multidrug transporters in <i>Escherichia coli</i> , and its physiological significance
A. Iwata	Molecular design of AcrB conferring super carbenicillin resistance
M. Ohigashi	Functional analysis of mouse ABCA5
A. Kobayashi	Investigation of the transcriptional regulation on xenobiotic exporter genes mediated through the sense-and-response system for environmental changes in <i>Escherichia coli</i>
S. Shibata	Functional analysis of the ABCA7 expressed in mouse platelets

Bachelor Degree of Pharmaceutical Sciences

A. Kishi	Construction of stable transfectant for exhaustive functional analysis of ABC-transporter
E. Nikaido	Analysis of sensing mechanism for indole signal
Li-Yuan WANG	Isolation and analysis of <i>E. coli</i> mutants with lower biofilm-forming ability

Sponsorship

Grant-in-Aid for Scientific Research on the Priority Area (B)

A. Yamaguchi	Studies on the Nano-structure and Transport Mechanism of Antiport-type Efflux Transporter for Organic Compounds.	¥28,500,000
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Grant-in-Aid for Scientific Research (S)

A. Yamaguchi	Post-genome Analysis of Bacterial Xenobiotic Exporter	¥15,200,000
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and Studies on the Novel Resistance Mechanism.

Grant-in-Aid for Young Scientists (B)

S. Murakami	Identification of Intrinsic Substrates of Multidrug transporters	¥1,500,000
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Grant-in-Aid for JSPS Fellows

N. Kobayashi	Structure and Functional Analysis of the first ABC-type Drug-Exporter of Gram-negative Bacteria, MacB.	¥900,000
H. Hirakawa	Studies on the Transcriptional Networks of Xenobiotic Transporters Regulated by the Sense-and-Response System for Environmental Changes in Bacteria.	¥900,000

Entrusted Research

A. Yamaguchi	Japan Science and Technology Agency (CREST)	Investigation of the Structure and Function for Xenobiotics Transporters and Clarification of Multidrug Resistance Mechanism.	¥10,400,000
S. Murakami	Japan Science and Technology Agency (Sakigake 21)	Structural Analysis of Drug Recognition Mechanism in Multidrug Efflux Transporter for Drug Resistance.	¥650,000
T. Hirata	National Agriculture and Bio-oriented Research Organization	Molecular Mechanism and Regulation for the Acquisition of Drug Resistance in <i>Escherichia coli</i> .	¥3,200,000
S. Murakami	Ministry of Education, Culture, Sports, Science and Technology, Protein 3000 Project	Research programs at Universities (Brain and Nervous System)	¥1,000,000
S. Murakami	SOSHO Inc.	Evaluation of protein crystals	¥500,000
S. Murakami	Japan Science and Technology Agency (CREST)	Creation of perfect protein crystals	¥4,030,000
(Other Allocations)			
A. Yamaguchi	COE fund	Crystallographic analysis of bacterial xenobiotic exporter	¥3,506,673
S. Murakami	COE fund	Visualization of transport activity of multidrug efflux transporter using single-molecule imaging techniques	¥1,000,000

H. Hirakawa	COE fund	Studies on drug resistance and posttranscriptional regulation of xenobiotic efflux nano-machine in <i>Escherichia coli</i>	¥500,000
A. Yamaguchi	The Program of Founding Research Centers for Emerging and Reemerging Infectious Diseases	Exhaustive, systematic analysis of bacterial pathogenicity and transcriptional regulation of multidrug transporters, and new strategy for drug design	¥300,000
Other Research Fund			
A. Yamaguchi	Japan Science and Technology Agency (CREST)	Investigation of the Structure and Function for Xenobiotics Transporters and Clarification of Multidrug Resistance Mechanism.	¥38,416,000
S. Murakami	Japan Science and Technology Agency (Sakigake 21)	Structural Analysis of Drug Recognition Mechanism in Multidrug Efflux Transporter for Drug Resistance.	¥8,350,000

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

- Intensity fluctuations of an electron beam accelerated with the L-band linac in the transient mode, which is most frequently used for users experiments, are reduced to one tenth of a previous value before remodeling through study for improving performance of the linac.
- As part of studies to produce and measure highly brilliant electron beams, developed are a measurement system of electron beam characteristics based on the quadrupole scanning method, which makes the measurement in a few minutes or one tenth of a past value possible, and a wire scanner, with which beam sizes can be precisely measured.
- A strong focusing wiggler is fabricated based on the edge focusing wiggler and the FODO lattice in the study of development of a new wiggler of higher performance.

- As strong SASE is generated as the intensity observed before remodeling the L-band linac in experiments with the newly developed strong focusing wiggler.
- First comprehensive and quantitative studies on charge carriers and reactive intermediates of conjugated polymers /organic molecules by pulse radiolysis and microwave techniques.
- Drastic improvements in the S/N ratio of the subpico-, pico-, and nano-second pulse radiolysis system.
- Success in analysis of reaction mechanisms of high sensitive resists for nanoelectronics.
- Formation of size-controlled nano-wires along particle trajectories in polymeric materials.
- Pulse radiolysis studies on biological systems including DNA, active oxygen, and NO.
- Application of slow positron beams to polymer science and technology as the probes for nano-sized space in the materials.

Department of Accelerator Science

Professor:	Goro ISOYAMA
Associate Professor:	Ryukou KATO
Research Associates:	Toshiji IKEDA, Shigeru KASHIWAGI
Graduate Students:	Tetsuya IGO, Takanori NODA, Shuto UMEZONO, Yuki Yoshi KON
Research Student:	Daisuke KASAMA

Outlines

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 Programs

1. Remodeling of the L-band linac

We began extensive and routine operation of the L-band linac for users experiments in 2005, for the first time after the large-scale remodeling of the L-band linac started in 2002. Since stability and reproducibility of operation are significantly improved, the linac can be used for pulse radiolysis experiments in the second measurement room without any fine-tuning following the morning startup in the transient mode, which is the most usual operation mode. We measured intensities of an electron beam in this operation mode over more than one hour and found that the standard deviation of the intensity variation was reduced to 0.27 % at the exit of the linac, which is one tenth of a value measured before remodeling.

It was one of the objectives of the large-scale upgrade of the L-band linac to improve the flatness of the square pulse on the top produced with a klystron modulator. It was not possible to reduce it less than a 0.1 % variation over 8 μ s pulse duration, which is the design target, with a 16 stage pulse forming network (PFN) designed and fabricated initially, so that the PFN was increased to 20 stages by adding 4, resulting in a 0.12 % variation over 8 μ s and the target has been practically achieved. Another problem with the klystron modulator was that a lifetime of a thyatron for switching the PFN circuit was shorter than one year. By consulting with manufacturers of the thyatron and the klystron modulator, it turned out that the choice of the model was not appropriate, so that the thyatron was replaced with another model with larger capacity. Since characteristics of the PFN circuit have been changed due to this replacement and now we are reviewing measures against the change.

2. Production and Measurement of Highly Brilliant Electron Beams

It is a basis for production of quantum beams to improve performance of the L-band electron linac and to adjust a beam line to most suitable conditions by measuring and evaluating characteristics of electron beams accelerated with it. The quadrupole scanning method is used to measure the emittance and Twiss parameters of an electron beam, in which beam sizes are measured with a measurement system consisting of a fluorescent screen, a video camera, and an image processing system as a function of the excitation current of a quadrupole magnet placed upstream of the measurement system. An automatic measurement system based on a personal computer has been newly developed, which enables characterization of the electron beam in a few minutes, which is one tenth of the previously necessary time in the manual measurement.

The beam size measurement with a fluorescent screen might lead to inaccurate results due to blurring of a fluorescent image. In order to solve this problem, we have fabricated a wire scan monitor, with which the beam size can be precisely measured, with the support of the High Energy Accelerator Research Organization (KEK) and have installed it in a beam line of the L-band linac.

3. Development of a High Performance Wiggler for SASE

We are developing a new type of wiggler to be used for SASE, which squeezes the electron beam small so that gain of SASE is enhanced, in collaboration with the insertion device group of KEK. It is a Halbach type wiggler with an edge angle for focusing and named the edge-focusing wiggler. Following trial manufacturing of a model wiggler with 5 periods, we have fabricated a strong focusing wiggler for FEL and SASE at ISIR, Osaka University, based on the edge focusing wiggler and the FODO lattice. Since there is no change with the mechanical frame of the wiggler, we have adopted the same basic parameters of the wiggler; a 6 cm period length and 32 wiggler periods. The strong focusing wiggler is made of four FODO cells, which are composed of every three normal wiggler periods alternatively inserted with one period of the edge focusing wiggler with edge angles of $\pm 5^\circ$. The magnetic field of the newly made wiggler was measured at KEK and then it was installed on the mechanical frame of the wiggler at Osaka University.

4. Basic Study on SASE in the Far-Infrared Region

SASE is a process that spontaneous light emitted by high-energy electrons in a wiggler is amplified exponentially to high-power coherent light by an FEL amplifier. Because no mirrors are necessary for the optical resonator, it is expected to be a promising candidate for realizing X-ray lasers. We are conducting basic study on SASE in the infrared region using the existing FEL system and a high-intensity single-bunch beam accelerated with the L-band linac. We have resumed SASE experiments with the newly introduced strong focusing wiggler. When the strong focusing wiggler is used, the electron beam optics in the beam line has to be smoothly matched to that of the wiggler in order to show its distinguished characteristic that electron beam is strongly focused to a small beam size. We have adjusted the beam line optics for FEL and SASE using the newly developed system for measuring electron beam characteristics and have succeeded in producing SASE as strong as the maximum intensity observed before remodeling of the linac.

Publications

Original Papers

Compact soft x-ray source using Thomson scattering, S. Kashiwagi, R. Kuroda, T. Oshima, F. Nagasawa, T. Kobuki, D. Ueyama, Y. Hama, M. Washio, K. Ushida, H. Hayano and J. Urakawa: J. Appl. Phys., 98 (2005) 123302/1-6.

Synchronization of femtosecond UV-IR laser with electron beam for pulse radiolysis, A. Saeki, T. Kozawa, S. Kashiwagi, K. Okamoto, G. Isoyama, Y. Yoshida and S. Tagawa: Nucl. Instr. Meth. A, 546 (2005) 627-633.

Development of compact picosecond pulse radiolysis system, M. Kawaguchi, K. Ushida, S. Kashiwagi, R. Kuroda, T. Kuribayashi, M. Kobayashi, Y. Hama and M. Washio: Nucl. Instr. Meth. B, 236 (2005) 425-431.

Review Papers

Full Account of the Siam Photon Project, G. Isoyama: Journal of the Particle Accelerator Society of Japan, 2 (2005) 523-535 (in Japanese).

International Conferences

Analysis of Intensity Fluctuations of SASE using the AR Model, (Poster) *R. Kato, S. Kashiwagi, S. Isaka, C. Okamoto, T. Yamamoto, S. Suemine, G. Isoyama, H. Sakaki, Proc. of the 26th International Free Electron Laser Conference and the 11th FEL Users Workshop, Trieste, Italy, August 29 - September 3, 2004, Comitato Conferenze Elettra 2005, pp.167-170 (MOPOS26).

First Model of the Edge-Focusing Wiggler for SASE, (Poster) *S. Kashiwagi, K. Kobayashi, T. Noda, R. Kato, G. Isoyama, S. Yamamoto and K. Tsuchiya, Proc. of the 26th International Free Electron Laser Conference and the 11th FEL Users Workshop, Trieste, Italy, August 29 - September 3, 2004, Comitato Conferenze Elettra 2005, pp.458-461 (TUPOS25).

Upgrade of the L-band Linac at ISIR, Osaka University for a Far-infrared FEL, (Poster) * R. Kato, S. Kashiwagi, T. Yamamoto, S. Suemine, G. Isoyama, Proc. of the 26th International Free Electron Laser Conference and the 11th FEL Users Workshop, Trieste, Italy, August 29 - September 3, 2004, Comitato Conferenze Elettra 2005, pp.462-465 (TUPOS26).

Study of Electron Beam Dynamics in the Strong Focus Wiggler for SASE, (Poster) * S. Umezono, G. Isoyama, R. Kato, S. Kashiwagi, T. Noda, Proc. of 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, November 18-19, 2005, Mie, Japan, p.111.

Advanced Beam Measurement System and Its Application to Development of a Highly Brilliant Electron Beam for Nanoscience Accelerated with the Linac, (Poster) * T. Igo, R. Kato, S. Kashiwagi, T. Noda, S. Umezono, Y. Kon, D. Kasama, G. Isoyama, Proc. of

4th 21th Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, November 18-19, 2005, Mie, Japan, pp.112-113.

Strong Focusing Wiggler for SASE and FEL in the Far-infrared Region at ISIR, Osaka University, (Poster) * S. Kashiwagi, T. Noda, R. Kato, G. Isoyama, S. Yamamoto and K. Tsuchiya, Proc. of 4th 21th Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, November 18-19, 2005, Mie, Japan, pp.115-116.

Publications in Domestic Meetings

The 2nd Annual Meeting of Particle Accelerator Society of Japan and the 30th Linear Accelerator Meeting in Japan, July 20-22, 2005, Tosu, Japan 9 papers

The 4th Scientific Meeting of the Japanese Society of Radiation Safety Management, November 23-25, 2005, Kyoto University, Kyoto, Japan 1 paper

Academic Degrees

Master Degree of Science

S. Umezono Numerical Analysis of SASE Dynamics in the Far-Infrared Region by Use of the Strong-Focusing Wiggler.

Sponsorship

Grant-in-Aid for Young Scientists (B)

S. Kashiwagi Basic study of SASE using the edge-focusing wiggler in the far-infrared region. ¥2,900,000

Cooperative Research

G. Isoyama KEK Cooperative R&D Generation of SASE by use of the Edge Focusing Undulator and Investigation of SASE Dynamics in the High Power Region. ¥1,000,000

Other Research Fund

G. Isoyama KEK Accelerator Supporting Project Technology Development on SASE-FEL in the Long Wavelength Region and Generation of SASE by use of the Edge Focusing Undulator and Investigation of SASE Dynamics in the High Power Region. ¥4,000,000

S. Kashiwagi The REIMEI Research Resources of Japan Energy Agency Study of high intensity polarized X-ray generation using inverse Compton scattering between SASE-FEL light and electron beam. ¥1,000,000

Department of Beam Materials Science

Professor:	Seiichi TAGAWA
Associate Professor:	Shuhei SEKI (from February 1, 2006)
Research Associates:	Kazuo KOBAYASHI, Akinori SAEKI
Graduate Students:	Atsuro NAKANO, Satoshi TSUKUDA, Hiroki YAMAMOTO, Yoshiko KOIZUMI, Yusuke DOI, Ryuhei YAMAGAMI, Takumi SHIGAKI Yuko OHNISHI, Kenichiro NATSUDA
Under Graduate Students:	Shingo SAKAMOTO, Naoto YAMAMOTO
Post Doctoral Fellow:	Anjali ACHARYA (until October, 2005)
Support Staff:	Kaoru KOJIMA
Guest Professor:	Kazuyuki HORIE (from January, 2006)
Research Technical Expert:	Shinichi FUJITA

Outlines

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, γ -rays, and lasers).

Current Research Programs

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. 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

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, EUV, and laser beams to design newly developed lithography technique in the present program. We focused on the time evolutions of spatial distribution of chemical intermediates such as proton, radical cation, electrons, and counter anion, which were measured by picosecond pulse radiolysis technique.

5. Electrodeless measurement of conductivity in organic semiconductors by microwave technique

For the sake of elucidation of charge carriers dynamics and mechanism of their generations, and measurement of intrinsic mobility in organic semiconductors such as σ and π conjugated polymers, we have developed in-situ measurement system of time-resolved microwave conductivity and transient optical spectroscopy. Using this system, electrodeless measurement of charge carrier mobility in regioregular polythiophene-tetracyanoethelene films, demonstrating the mobility was increased with the content of tetracyanoethelene. Other conjugated polymers like polysilane and polygermane were also investigated.

6. Ionizing Radiation Induced Damage in DNA

Clustered DNA damage sites, in which two or more lesions are formed within a few helical turns of DNA after passage of a single radiation track, are suspects as critical lesions producing lethal and mutagenic effects of ionizing radiation. Closed-circular plasmid DNA (pUC19) were irradiated to determine the yields of single- and double-strand breaks as well as base lesions, which are converted into detectable single-strand break by the base excision repair enzymes endonuclease III (Nth) and formamidopyrimidine-DNA (Fpg). The G value of total clustered damage is in the range 0.04 to 0.06.

Time-resolved microwave conductivity (TRMC) technique allows measurement of the conductivity of photo-generated charge carriers on an isolated molecular chain without an attached electrode. This method was applied to the charge transport of DNA. A novel DNA-lipid complex, which was prepared by mixing DNA with cationic amphiphilic lipids, was confirmed to form double strands even in organic solvents, and was employed as a sample. Upon laser exposure of anthraquinone-bound the DNA-lipid complex, the TRMC signals from charge carriers from charge carriers and transient absorption were measured. We calculated the mobility of holes in DNA as $5 \times 10^{-3} \text{ cm}^2/\text{Vs}$. This is comparable to the values for conjugated polymers (1.0×10^{-3} to $1.0 \text{ cm}^2/\text{Vs}$).

Publications

Original Papers

Requirements for Laser-Induced Desorption/Ionization on Submicrometer Structures, S. Okuno, R. Arakawa, K. Okamoto, Y. Matsui, S. Seki, T. Kozawa, S. Tagawa, Y. Wada: *Anal. Chem.*, 77 (2005) 5364.

Effect of Ion Beam Energy and Polymer Weight on the Thickness of Nanowires Produced by Ion Bombardment of Polystyrene Thin Films, S. Tsukuda, S. Seki, S. Tagawa, M. Sugimoto: *Appl. Phys. Lett.*, 87 (2005) 233119.

Transient Formation of a Neutral Ubisemiquinone Radical and Subsequent Intramolecular Electron Transfer to Pyrroloquinoline Quinone in the *E. coli* Membrane-Integrated Glucose Dehydrogenase, K. Kobayashi, G. Mustafa, S. Tagawa, M. Yamada: *Biochemistry*, 44 (2005) 13567.

Mobilities of Charge Carriers in Dendrite and Linear Oligogermanes by Flash Photolysis Time-resolved Microwave Conductivity Technique, S. Seki, A. Acharya, Y. Koizumi, A. Saeki, S. Tagawa, K. Mochida: *Chem. Lett.*, 34 (2005) 1690.

The Intramolecular Electron Transfer between the Type 1 Cu and the Type 2 Cu in a Mutant of *Hyphomicrobium* Nitrite Reductase, S. Suzuki, T. Maetani, K. Yamaguchi, K. Kobayashi, S. Tagawa: *Chem. Lett.*, 34 (2005) 36.

Study of Transport Properties in Fullerene-Doped Polysilane Films Using Flash Photolysis Time-Resolved Microwave Technique, A. Acharya, S. Seki, A. Saeki, Y. Koizumi, S. Tagawa: *Chem. Phys. Lett.*, 404 (2005) 356.

Control of Nano-Step Structures on Sapphire Wafer Surface by Focused Ion Beam Processing, A. Takeuchi, T. Kotaki, K. Koyama, K. Sunakawa, Y. Yaguchi, Y. Matsui, S. Seki, S. Tagawa, W. Hara, M. Yoshimoto: *J. Ceram. Soc. Jpn.*, 113 (2005) 478.

Effect of Substituents on Charge Carrier Dynamics in Thiophene Oligomers, A. Acharya, Y. Koizumi, S. Seki, A. Saeki, S. Tagawa, Y. Ie and Y. Aso: *J. Photochem. Photobiol A*, 173 (2005) 161.

Correlation between Edge Roughness of NanoStructures and Backbone Configuration of Polymer, S. Seki, S. Tsukuda, S. Tagawa, M. Sugimoto: *J. Photopolymer Sci. Technol.*, 18 (2005) 449.

Basic Aspects of Acid Generation Processes in Chemically Amplified Electron Beam Resist, T. Kozawa, S. Tagawa: *J. Photopolym. Sci. Technol.*, 18 (2005) 471.

Etching Efficiency of Polymethacrylates for Monochromatic Low Energy Ion Beams, S. Seki, S. Kawachi, S. Tagawa, A. Egami, K. Kurihara, M. Nakamura, H. Itoh: *J.*

Photopolym. Sci. Technol., 18 (2005) 255.

Fluoropolymer Outgassing in Focused Ion Beam Micromachining, Y. Matsui, S. Seki, S. Tagawa: J. Photopolym. Sci. Technol., 18 (2005) 501.

Increase of Mobility of Photogenerated Positive Charge Carriers in Polythiophene, A. Saeki, S. Seki, Y. Koizumi, T. Sunagawa, K. Ushida, S. Tagawa: J. Phys. Chem. B, 109 (2005) 10015.

Photogeneration of Charge Carriers and Their Transport Properties in Poly[bis(p-n-butylphenyl)silane], A. Acharya, S. Seki, Y. Koizumi, A. Saeki, S. Tagawa: J. Phys. Chem. B, 109 (2005) 20174.

Study on Acid Generation from Polymer, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato, H. Komano: J. Vac. Sci. Technol. B, 23 (2005) 2728.

Proton and Anion Distribution and Line Edge Roughness of Chemically Amplified Electron Beam Resist, T. Kozawa, H. Yamamoto, A. Saeki, S. Tagawa: J. Vac. Sci. Technol. B, 23 (2005) 2716.

Nanopatterning of Polyfluorene Derivative Using Electron-Beam Lithography, Y. Doi, A. Saeki, Y. Koizumi, S. Seki, K. Okamoto, T. Kozawa, S. Tagawa: J. Vac. Sci. Technol. B, 23 (2005) 2051

Experimental Studies of Transverse and Longitudinal Beam Dynamics in Photoinjector, J. Yang, T. Kondoh, Y. Yoshida and S. Tagawa: Jpn. J. Appl. Phys., 44 (2005) 8702.

Effects of Dielectric Constant on Acid Generation in Chemically Amplified Resists for Post-Optical Lithography, T. Kozawa, K. Okamoto, A. Saeki, S. Tagawa: Jpn. J. Appl. Phys., 44 (2005) 3908.

Resist Thickness Effect on Acid Concentration Generated in Poly(4-hydroxystyrene) Film upon Exposure to 75 keV Electron Beam, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto, S. Tagawa: Jpn. J. Appl. Phys., 44 Part2 (2005) L1298.

Reaction Mechanism of Brominated Chemically Amplified Resists, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato, H. Komano: Jpn. J. Appl. Phys., 44 (2005) L842.

Formation of Nanowires Based on π -Conjugated Polymers by High-Energy Ion Beam Irradiation, S. Tsukuda, S. Seki, M. Sugimoto, S. Tagawa: Jpn. J. Appl. Phys., 44 (2005) 5839.

Potential Cause of Inhomogeneous Acid Distribution in Chemically Amplified Resists for Post Optical Lithography, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S.

Tagawa, T. Ando, M. Sato, H. Komano: Jpn. J. Appl. Phys., 44 (2005) 5836.

Dependence of Acid Yield on Acid Generator in Chemically Amplified Resist for Post-Optical Lithography, A. Nakano, K. Okamoto, Y. Yamamoto, T. Kozawa, S. Tagawa, T. Kai, H. Nemoto, Jpn. J. Appl. Phys., 44 (2005) 5832.

Effects of Backbone Configuration of Polysilanes on Nanoscale Structures Formed by Single-Particle Nanofabrication Technique, S. Seki, S. Tsukuda, K. Maeda, S. Tagawa, H. Shibata, M. Sugimoto, K. Jimbo, I. Hashitomi, A. Kohyama, Macromolecules, 38 (2005) 10164.

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"Subpicosecond Pulse Radiolysis Study on Geminant Ion Recombination Process in n-Dodecane", Y. Yoshida, A. Saeki, T. Kozawa, J. Yang, S. Tagawa: Ultrafast Phenomena 14 (2005) 479.

"Relation between Resolution, Sensitivity and Reaction Mechanism in Chemically Amplified Resists" T. Kozawa and S. Tagawa: Silicontechnology 72 (2005) 39.

"Sensor Protein in Response to Oxidative Stress", Kazuo Kobayashi: Kagaku to Kyoiku 53 (2005) 124.

"Formation of Nanowire using Ion Beam Irradiation" S. Seki, S. Tsukuda, and S. Tagawa: Radiation and Industry 105 (2005) 19.

"Recent Topics of Lithography-toward Nanolithography": T. Kozawa and S. Tagawa: Radiationchemistry 79 (2005) 3.

"Deprotonation Mechanism of Poly(4-hydroxystyrene) and its Derivative", A. Nakano, K. Okamoto, Y. Yamamoto, T. Kozawa, S. Tagawa, T. Kai, H. Nemoto and T. Shimokawa, Proc. SPIE 22 (2005) 1034.

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Matrix-Free Laser Desorption/Ionization of Peptides on Sub-Micrometer Structures: Grooves on Silicon and Metal-Coated Porous Alumina, S. Okuno, R. Arakawa, K. Okamoto, Y. Matsui, S. Seki, T. Kozawa, S. Tagawa, Y. Wada, ASMS conference on

mass spectrometry, June, 2005

Cross-Linked Silicon Based Polymer Nanowire Formation by High Energy Charged Particles, S. Seki, S. Tsukuda, S. Tagawa, M. Sugimoto, 14th International Conference on Surface Modification of materials by Ion Beams, September, 2005

Femtosecond Pulse Radiolysis Study on Primary Process of Radiation Chemistry of Polymer, Y. Yoshida, J. Yang, T. Kondo, A. Yoshida, T. Kozawa, S. Tagawa, Pacifichem2005, December 15, 2005

Formation Mechanism and Characteristics of Polymer Nanowires by Single Ion Event, S. Tsukuda, S. Seki, M. Sugimoto, S. Tagawa, Pacifichem2005, December 15, 2005

Mobility and Dynamics of Charge Carriers in Polythiophene- Tetracyanoethylene Blend Films Studied by Microwave Technique, A. Saeki, S. Seki, Y. Koizumi, T. Sunagawa, K. Ushida, and S. Tagawa, Pacifichem2005, December 15, 2005

Charge Carrier Mobility on Isolated Si Chains by Pulse-Radiolysis and Flash-Photolysis Time-Resolved Microwave Conductivity and Transient Absorption Spectroscopy Measurement, S. Seki, K. Okamoto, A. Saeki, A. Acharya, S. Tagawa, F. C. Grozema, L. P. Candeias, J. M. Warman, L. D.A. Siebbeles, Pacifichem2005, December 15, 2005

Nanowire Formation by Non-Homogeneous Crosslinking in Ion Tracks, S. Seki, S. Tsukuda, K. Maeda, A. Saeki, S. Tagawa, H. Shibata, M. Sugimoto, K. Jimbo, I. Hashitomi, A. Kohyama, Pacifichem2005, December 15, 2005

Study on Acid Generation from Base Polymer, H. Yamamoto, A. Nakano, K. Okamoto, T. Kozawa, S. Tagawa, T. Ando, M. Sato, H. Komano, EIPBN, May, 2005

Nanowires with Freely Controlled Sizes Formed by Single Ion Track Reactions in Polymers, S. Tsukuda, S. Seki, M. Sugimoto, S. Tagawa, 14th International Conference on Surface Modification of Materials by Ion Beams, September, 2005

Photoinduced Charge Transfer of DNA in Organic Solvent by Time-Resolved Microwave Conductivity, R. Yamagami, K. Kobayashi, A. Saeki, S. Seki, S. Tagawa, Miller Conference, September, 2005

Nanopatterning of Polyfluorene Derivative using Electron-Beam Lithography, Y. Doi, A. Saeki, Y. Koizumi, S. Seki, K. Okamoto, T. Kozawa, S. Tagawa, Pacifichem2005, December 15, 2005

Acid Generation Process in Aromatic Polymers for Chemically Amplified Electron Beam Lithography, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato H. Komano: Pacifichem2005, December 15, 2005

Delocalization of Charge Carriers on Oligofluorene Backbone, Y. Koizumi, S. Seki, A. Saeki, S. Tagawa, Pacifichem2005, December 15, 2005.

Photoinduced Charge Transfer of DNA in Organic Solvent by Time-Resolved Microwave Conductivity, R. Yamagami, K. Kobayashi, A. Saeki, S. Seki, S. Tagawa, Pacifichem2005, December 15, 2005

Nanospace and Picosecond Reactions of Resists for EUV and Electron Beam Lithographies, S. Tagawa, K. Kozawa, Pcifichem2005, December 15, 2005

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	9 papers
Atomic Energy Society of Japan	4 papers
The Japan Society of Applied Physics:	10 papers
Society of Polymer Science, Japan	2 papers
The Japanese Biochemical Society	1 paper

Academic Degrees

Doctor Degree of Engineering

A. Nakano	Radiation Chemical Studies on Acid Generation in Irradiated Polymer Matrces
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Master Degree of Engineering

T. Shigaki	Study on Acid Generation and Energy Deposition in Chemically Amplified Electron Beam Resist
Y. Doi	High-sensitive Nanofabrication of Polyfluorene Based on Chemical Amplification and its Emission Property
R. Yamagami	Photogenerated Hole Mobility in DNA Measured by Time-Resolved Conductivity

Sponsorship

Grant-in-Aid for Scientific Research (S)

S. Tagawa	Femtosecond Pulse Radiolysis Study on Time Profile of Radiation-Induced Processes in Nanoscopic Region ¥23,900,000
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Grant-in-Aid for Young Scientists (A)

S. Seki	Formation Processes and Characterization of Nanowires Produced by Single Particle Nanofabrication Technique ¥12,870,000
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Grant-in-Aid for Young Scientists (B)

A. Saeki	Charge Carrier Mobility in Isolated Polymer Chain and Functionalization of Electric Property of Polymer Studied by Electron Accelerator ¥1,100,000
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Grant-in-Aid for Exploratory Research

S. Seki	Development of Plateless Conductivity Measurement in Isolated Nanostructure and Molecular Element	¥500,000
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Grant-in-Aid for JSPS Fellows

S. Tsukuda	Formation and Characterization of Polymer Nanostructure by Single Ion Event	¥900,000
Anjali ACHARYA	Electronic Conductivity of Charge Carriers on Isolated Biomedical Conjugated Polymer Chains.	¥400,000

Entrusted Research

S. Tagawa	Japan Nuclear Energy Safety Organization	Development of Color Film Dosimeter Based on Advanced Radiation Chemistry
S. Tagawa	Advanced Semiconductor Engineering and Technology	Reaction Mechanism in Chemically Amplified Resist Materials
S. Tagawa	Semiconductor Leading Edge Technology Inc., Tokyo Ohka Kogyo	Study on Development of High Sensitive EPL Resist
S. Tagawa	Semiconductor Leading Edge Technology Inc.	Study on Solvent for Immersion Lithography
S. Tagawa	Mitsubishi Gas Chemical Company, Inc.	Fundamental Research on ArF Resist
S. Tagawa	Intel	Nanoscale Distribution of Acids Generated in Chemically Amplified EUV Resists

Activities of Centers

Nanoscience and Nanotechnology Center

Director Professor: Katsuaki SUGANUMA

Support Staff: Aya KOMOTO

Outlines

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

Outlines

The main purpose of this department 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 department is 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.

Design and syntheses of supramolecules such as artificial DNA, proteins, photosynthetic molecules, and nanoparticles having more efficient and selective functions than those of single molecules have been investigated towards constructions of organized supramolecular systems such as artificial living cells and nanodevices exhibiting multifunctions, complex properties, and conjugated functions.

Proteins and their complex 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.

Achievements

- 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.
- Control of nano-scale interface among organic, inorganic, and metal materials.
- Development of bottom up nano technology system.
- Creation of super-five senses sensor and brain type memory.
- Programmed self-assembly and self-organization for molecular device.
- Selective nano-fabrication by chemical surface modifications.
- Electronic properties of single molecule connected to metals or semiconductors.
- Novel techniques on scanning probe microscopy and scanning electron microscopy for molecular devices.
- Construction of DNA Nanostructures Producing Charge-Separated State
- Biological Effects of Charge Transfer in DNA
- Preparation of nanoparticles by self-assembly.
- Preparation of molecular devices by synthesis and assembly of functionalized polymers.
- Structural and functional studies of nano bio devices.
- Characterization of nano machines acting as a drug efflux transporter.

Department of Artificial Nanomaterials for Bio-Information Systems

Professor:	Hitoshi TABATA
Research Associate:	Hiromasa SAEKI
Associate Professor:	Michael HERRMANN
Research Associate:	Hiroaki MATSUI
Post Doctoral Fellow:	Kimihiko NORIZAWA
Graduate Student:	Atsuhiko DOI, Eriko MIZUNO, Koji TSURUTA
Under Graduate Student:	Takushi KOIDE, Kazuya TAMEKUNI, Hiroyasu YAMAHARA
Supporting Staff:	Megumi IKEDA

Outlines

In our group, we are studying about frontier materials such as strongly collated compounds and/or artificial super lattices formed by a laser MBE technique, which enables us to control the crystal structure with atomic scale accuracy. Oxide electrics have been studied, for example, low dimensional physics in oxide magnetic materials, fluctuation in spin glass or relaxor ferroelectrics, multi ferrotronics in ferromagnetic-ferroelectrics, spintronics in wide band gap semiconductors and photo induced magnetic materials.

Furthermore, the research about bio sensor/memory devices, which are constructed by self organizing system such as DNA and bio, related molecules are discussed. Observation in the nano-scale region is also performed by scanning probe microscopy.

A new method based on THz-spectroscopy is also constructing for direct detecting of hydrogen bond of base pairs in DNA double helix and/or that of protein-DNA molecules.

Current Research Programs

Development of spintronics with wide gap oxide semiconductor (ZnO)

The degree of freedom for spin is added to the semiconductor which work by using only the conduction career, and it is widely researched from a basic and applied viewpoint in recent years. In this research, it aims at making clarification and the heterostructure of a basic character of ZnO that adds transition metal (Co), and doing the magnetic conduction control. It reports on the main result at current year.

It is understood that a ferromagnetism characteristic appears by doping doing Co to ZnO. Typical samples show ferromagnetic hysteresis which is observed around 300K neighborhood. It is important for academic and applying it to investigate the origin of magnetic behavior.

Firstly, the transport character depends on magnetism like this can become the circumstantial evidence of the career generated ferromagnetism. Because the career and magnetism are strongly related, use as the tunnel magnet resistive element can be expected of a genuine quality.

TMR structure is constructed on the atomically flat ZnO substrate. Non-doped and

Co-doped ZnO layers were deposited on the substrate firstly. Next, insulating layer (alumina) and metallic magnetic layer (Fe) were deposited as a cap layer. 200 μ m processed this columnar, the electric conduction characteristic was measured.

The result of the electric conduction character show the typical TMR hysteresis shape. The applied voltage -0.5V and the measurements were done by 10K. In 0Oe neighborhood A magnetic reversing happened at Fe layer, and next, reversing of Co-ZnO magnetization has happened in addition of 150Oe neighborhood. As a result, it is thought that the effect of TMR of making the alumina layer a tunnel barrier has happened. The coercive force of 35Oe for Fe layer and 150 Oe for Co-ZnO is observed by SQUID measurement.

As for the magnetism of Co-ZnO, it strongly relates to the conduction career, and it has been understood to expect it as a material candidate of spin FET besides the TMR element from these results.

Self-organization of on-dimensional nanostripe arrays and pronounced anisotropy of low temperature electron transport

Employment of self-organized growth towards the fabrication of surface nanostructures provides advantages to nanoscale engineering and a basic technology for the production of quantum effects utilized low-dimensional nano-space. Recently, it was found that highly anisotropic surface morphology with self-organized nanostripe arrays along the [0001] direction was formed during homoepitaxial growth of ZnO (10-10). The formation of nanostripe structure was caused by a conversion from two-dimensional (2D) to three-dimensional (3D) growth mode with a critical thickness of 10 nm. In lattice-matched homoepitaxial growth, the conversion from 2D to 3D growth mode is related to a step-faceting mechanism based on Schwoebel barrier effect. Cross-section transmission electron microscopy revealed that the nanostripe arrays was consisted of side facets with the (4-1-30) and (31-40) equivalent planes being misoriented by 13.9° along the [1-210] and [-12-10] directions, respectively, from the (10-10) surface.

Electrical conductivity parallel ($\sigma_{[0001]}$) and perpendicular ($\sigma_{[11-20]}$) to the nanostripe arrays was measured using a four-probe Hall bar configuration. $\sigma_{[0001]}$ along the nanostripe arrays showed band conductivity in high-temperature ranges from 300 to 150 K, and low-temperature regions (10-150 K) was dominated by hopping conductivity. On the other hand, in $\sigma_{[11-20]}$ along the [11-20] direction, the high-temperature regions displayed variable range hopping (VRH) conductivity obeyed with $\sigma \propto T^{-1/4}$, furthermore, Hall mobility ($\mu_{H[11-20]}$) was controlled by grain boundary scattering with a barrier potential of 85 meV. This indicated that grain boundary was formed between nanostripes. Besides, in-plane electrical transport in $\text{Mg}_{0.12}\text{Zn}_{0.88}\text{O}/\text{ZnO}$ multi-quantum wells structure was evaluated at low temperatures below 100 K. Ionized impurity scattering is screened at the low temperatures since electrons confined to quantum wells possessed 2D property. $\mu_{H[11-20]}$ along the nanostripe arrays was higher than $\mu_{H[0001]}$ perpendicular to the arrays. A roughening at a heterointerface between $\text{Mg}_{0.12}\text{Zn}_{0.88}\text{O}$ barrier and ZnO well caused an interface scattering of 2D electrons along the [11-20] direction. Hereafter, high-resolution XRD and TEM analyzes will be requested. The above results showed that it is expected to be promising for fabrications of field-effect transistor devises combined with surface nanostructures and one-

dimensional varistor conductivity.

Terahertz spectroscopy and imaging of DNA-related biomaterials

THz spectroscopy is useful for biological molecules. The vibration modes of hydrogen bonds and intermolecular vibration appear in the THz (far-infrared) range compared to the intramolecular vibration modes in the mid-infrared range. In particular, biomolecules show a unique fingerprint spectrum in THz region. Additionally the DNA hybridization was recognized by THz spectrum. This is because the hydrogen-bond vibration mode of $-NH_2$ structure between complementary DNA. We demonstrate the use of THz time-domain spectroscopy (THz-TDS) for recording DNA-related base molecules toward the DNA-chips for hybridization recognition without fluorescent probes.

We have a typical THz-TDS and imaging system. A photoconductive dipole antennas (LT-GaAs) were used as the both of THz emitter and receiver, but ZnTe crystal was sometimes used as the emitter. The observed THz pulse had a frequency component of 0.1 to 3 THz. The DNA-related base molecule samples were adenine (A), thymine (T), guanine (G), cytosine (C), deoxyadenosine monophosphate (dAMP), deoxyguanosine monophosphate (dGMP) and deoxyadenosine triphosphate (dATP). All the samples were powdered in a mortar and sandwiched between scotch tapes and then the time-domain pulse shape was obtained. The frequency-domain spectrum was obtained from FFT calculation.

The result of basic and theoretical analysis in this work should be applied to the future development of THz imaging and sensing for DNA-chips and other biochips.

Publications

Original Papers

Characterization of Magnetic Components in the Diluted Magnetic Semiconductor $Zn_{1-x}Co_xO$ by X-ray Magnetic Circular Dichroism, M. Kobayashi, Y. Ishida, J.I. Hwang, T. Mizokawa, A. Fujimori, K. Mamiya, J. Okamoto, Y. Takeda, T. Okane, Y. Saitoh, Y. Muramatsu, A. Tanaka, H. Saeki, H. Tabata, and T. Kawai : Phys. Rev. B, 72 (2005) 201201(R) (4 pages)

Self-organized Nanostripe Arrays on ZnO (10-10) Surfaces Formed During Laser Molecular-beam-epitaxy Growth, H. Matsui, H. Tabata : Appl. Phys. Lett., 87 (2005) 143109(3pages)

SEM Observation of Collagen Fibrils Secreted from the Body Surface of Osteoblasts on a CO_3 apatite-collagen Sponge, I. Hirata, Y. Nomura, H. Tabata, Y. Miake, T. Yanagisawa and M. Okazaki : Dent. Mater. J., 24 (2005) 460-464.

Epitaxial Growth and Characteristics of N-doped Anatase TiO_2 Films Grown Using a Free-radical Nitrogen Oxide Source, H. Matsui, H. Tabata, N. Hasuike, H. Harima and B. Mizobuchi : J. Appl. Phys., 97 (2005) 123511(8pages)

DNA Patterning by Nano-imprinting Technique and Its Application for Bio-chips, H.

Tabata, T. Uno, T. Ohtake and T. Kawai : J. Photopolym. Sci. Technol., 18 (2005) 519-522.

Photoemission Study of Poly(dA)-poly(dT) DNA: Experimental and Theoretical Approach to the Electronic Density of States, H. Wadati, K. Okazaki, Y. Niimi, A. Fujimori, H. Tabata, J. Pikus and J.P. Lewis : Appl. Phys. Lett., 86 (2005) 023901(3pages)

Self-assembly ZnO Nanorods by Pulsed Laser Deposition Under Argon Atmosphere, S. Choojun, H. Tabata and T. Kawai : J. Cryst. Growth, 274 (2005) 167-172.

High-temperature Cluster Glass State and Photomagnetism in Zn- and Ti-substituted NiFe_2O_4 Films, M. Seki, A.K.M. Akther Hossain, T. Kawai and H. Tabata : J. Appl. Phys., 97 (2005) 083541(6pages)

Photocontrol of Magnetization in Al-substituted Fe_3O_4 Thin Films, M. Seki, Akther A.K.M. Hossain, H. Tabata, T. Kawai : Solid State Commun., 133 (2005) 791-796.

Review Papers

Fusion between DNA and Semiconducting Nano-technology, H. Tabata : Bio Clinica, 20[1] (2005) 47-52.

DNA Nanotechnology/Fusion Technology between Top Down Nanotechnology in Semiconductors and Self Organizing Bottom Up One, H. Tabata : Hyomengijutsu, 56(12) (2005) 892-896.

THz Spectroscopy of Bio Related Materials, H. Tabata, M. Herrmann, K. Norizawa : Kogaku, 34(9) (2005) 475-477.

Relaxor Ferroelectrics -Bulks, Films and Superlattices-, H. Tabata, Y. Hotta, A. Doi, T. Kawai : Hyomenkagaku, 26(4) (2005) 200-207.

Book

Ferroelectric Thin Films, H. Tabata : Springer Verlag, (2005) 161-173.

Patents

Ferroelectric Memory and Its Manufacturing Method, T. Kawai, H. Kobayashi, H. Tabata, E. Rokuta, Patent No.3663436

Measuring Method in Which Biomolecule Configuration and Information are Detected Using IS-FET and System Therefore, T. Ohtake, T. Uno, C. Hamai, H. Tabata, T. Kawai, WO 2005/090961 A1

Patterning Method for Self Organizing Materials, the Nano-patterned Substrates Formed by this Technique, and Mask-less Photo Mask by Using Self Organized Pattern of Bio Molecules, T. Ohtake, H. Tabata, T. Kawai, S. Matsui, K. Nakamatsu, PCT/JP2005/017930

International Conferences

Spintronics Based on High-Tc DMSs of (Zn,Co)O:Cobalt Substituted Zinc Oxides(Invited), *H. Tabata, H. Saeki and H. Matsui, Wide Band Gap Ferromagnetic Semiconductors Workshop, Edinburgh, UK, May 15-19, 2005

High Temperature Photoinduced Magnetization in Spinel and Garnet Ferrite Thin Films, *M. Seki, K. Tsuruta, T. Kawai, and H. Tabata, The 8th International Symposium on Sputtering & Plasma Processes (ISSP 2005), Kanazawa, Japan, Jun. 8-10, 2005

Spin-glass and Dipole-glass(Relaxor) Behaviors in Oxide Superlattices (Invited), *H. Tabata, Y. Hotta, A. Doi, M. Seki and T. Kawai, ICE-2005(International Conference on Electroceramics 2005), Seoul, Korea, Jun. 12-16, 2005

DNA Patterning by Nano-Imprinting Technique and Its Application for Bio-chips (Invited), *H. Tabata, T. Uno, T. Ohtake and T. Kawai, The 22nd International Photopolymer Conference, Chiba, Japan, Jun. 21-24, 2005

Magnetic and Optical Properties of Transition Metal Doped ZnO Films (Invited), H. Saeki, H. Matsui, T. Kawai and *H. Tabata, 3rd International Conference on Materials for Advanced Technologies 2005(ICMAT-2005), Singapore, Jul. 3-8, 2005

Terahertz Time-domain Spectroscopy and Imaging of DNA, *M. Herrmann, H. Tabata, T. Kawai, International Quantum Electronics Conference 2005 and the Pacific Rim Conference on Lasers and Electro-optics 2005 (IQEC/CLEO-PR 2005), Tokyo, Japan, Jul. 11-15, 2005

Formation of Multiple-quantum Wells (MQWs) Based on Polar Controlled ZnO Homoepitaxial Systems(poster), *H. Matsui, N. Hasuike, H. Harima and H. Tabata, The 23rd International Conference on Defects in Semiconductors (ICDS-23), Awaji, Japan, Jul. 24-29, 2005

Biometric Bottom-up Nanotechnology for Advanced Device Fabrication(Invited), *H. Tabata, Seminar on Nano Material Fabrication Technologies, Chiang Mai, Thailand, Jul. 28-29, 2005

Growth Mode Mapping of Polarity-controlled $\text{Co}_x\text{Zn}_{1-x}\text{O}$ Heteroepitaxy towards Heterostructures(Poster), *H. Matsui, H. Saeki and H. Tabata, The 3rd International School and Conference on Spintronics and Quantum Information Technology (Spintech III), Awaji, Japan, Aug. 1-5, 2005

Magnetic and Transport Properties of Co-doped ZnO(Poster), *H. Saeki, H. Matsui, H. Tabata, The 3rd International School and Conference on Spintronics and Quantum Information Technology (Spintech III), Awaji, Japan, Aug. 1-5, 2005

Spintronics Based on ZnO Thin Films(Invited), *H. Tabata, H. Saeki and H. Matsui, 2005 International Conference on Solid State Devices and Materials (SSDM 2005), Kobe, Japan, Sep. 12-15, 2005

THz Time-domain Spectroscopy and Vibration Analysis of DNA-related Base Molecules(Invited), *K. Norizawa, M. Herrmann, H. Tabata, T. Kawai, The Joint 30th International Conference on Infrared and Millimeter Waves and 13th International Conference on Terahertz Electronics (IRMMW-THz 2005), Williamsburg, USA, Sep. 19-23, 2005

THz Time-domain Spectroscopy of Natural and Artificial DNA(Invited), M. Herrmann, *K. Norizawa, H. Tabata, T. Kawai, The Joint 30th International Conference on Infrared and Millimeter Waves and 13th International Conference on Terahertz Electronics (IRMMW-THz 2005), Williamsburg, USA, Sep. 19-23, 2005

Magnetic and Transport Properties of (Zn,Co)O Thin Films(Poster), *H. Saeki, H. Matsui and H. Tabata, The 12th International Workshop on Oxide Electronics(WOE12), Chatham, USA, Oct. 2-5, 2005

Photocontrol of Cluster-glass States in Spinel and Garnet Ferrite Thin Films (Poster), *M. Seki, K. Tsuruta, H. Tabata, T. Kawai, The 12th International Workshop on Oxide Electronics(WOE12), Chatham, USA, Oct. 2-5, 2005

Dielectric Properties and Crystal Structures of Pb Free Ferroelectrics: $\text{Ba}(\text{Hf}_x\text{Ti}_{1-x})\text{O}_3$, $\text{Ba}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ (Poster), *A. Doi, S.J. Kim, Y. Kuroiwa, H. Tabata, The 12th International Workshop on Oxide Electronics(WOE12), Chatham, USA, Oct. 2-5, 2005

Introduction of Nanoscience and Nanotechnology Center. Nano-electronics and Nano-bio Science Based on Functionally Harmonized Materials (Invited), *H. Tabata, Osaka University and University of Groningen, Collaboration Symposium, Groningen, Netherlands, Oct. 24-26, 2005

Life Science on a Bio-chip ~DNA/Protein Transistors Based on Si-nanotechnology~(Invited), *H. Tabata, Seminar "Business Opportunities on Life Science in Osaka", Rotterdam, Netherlands, Oct. 28, 2005

THz Imaging of Thin Film DNA(Poster), *K. Norizawa, H. Tabata, T. Kawai, The International Workshop on Terahertz Technology 2005 (TeraTech '05), Osaka, Japan, Nov. 16-18, 2005

Spintronics Based on Oxide Wide-gap Semiconductors(Poster), *H. Tabata, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Mie, Japan, Nov. 18-19, 2005

Fusion Technology of Bio&Oxide Electronics (Bio nano electronics), *H. Tabata, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30- Feb. 1, 2006

Magnetic and Transport Properties of (Zn,Co)O Thin Film(Poster), *H. Saeki, H. Matsui, H. Tabata, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30- Feb. 1, 2006

THz Time-domain Spectroscopy and Vibration Analysis of DNA-related Base Molecules(Poster), *K. Norizawa, M. Herrmann, H. Tabata, T. Kawai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30- Feb. 1, 2006

Photo-control of Magnetization at Room Temperature in Spinel Ferrite Thin Films, *M. Seki, K. Tsuruta, and H. Tabata, International Symposium on Hybrid Nano Material Toward Future Industries (HNM 2006), Nagaoka, Japan, Feb. 3-5, 2006

Bottom-up Nanotechnology for Oxide and Bio-electronics, *H. Tabata, 1st Workshop on Nanoscience and Nanotechnology between Sanken and CNRS, Orsay, France, Feb. 12-13, 2006

Contributions to International Conferences and Journals

H. Tabata	International Conference on Solid State Devices and Materials 2005 (SSDM2005) (Steering Committee)
H. Tabata	International Conference on Solid State Devices and Materials 2005 (SSDM2005) (Publishing Committee)
H. Tabata	International Conference on Solid State Devices and Materials 2006 (SSDM2006) (Publishing Committee)
H. Tabata	12th International Workshop on Oxide Electronics (International Committee)
H. Tabata	Associate Editor of JJAP in special issue
H. Tabata	Chief aid of publication office in Japan Society of Applied Physics

Publications in Domestic Meetings

The Japan Society of Applied Physics	16 papers
The Society of Materials Science, Japan	2 papers
Others	2 papers

Sponsorship

Grants in aid for scientific research

Scientific Research in Priority Areas (2)

H. Tabata	Room Temperature Spintronics by Ultimate Control of Interface and Crystal Growth	¥2,400,000
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Fundamental Research (B)(2)

H. Tabata	Symmetry Broken Ferroelectric Relaxors Formed by Artificial Superlattices and Brain Mimetic Memories	¥9,100,000
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Exploratory Research

H. Tabata	Non Fluorescent Labeling DNA Transistor Formed by Self Organized Semiconductor	¥2,100,000
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Other Allocation**Scientific Research in Priority Areas (2)**

H. Tabata	Development and Application of Computational Nano-Materials Design Engine	¥1,500,000
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Cooperative Research

H. Tabata	Collaboration of Regional Entities for the Advancement of Technological Excellence(Wakayama Prefecture)	Development of Application Technology of Functional Materials by a Composite of Effective Agricultural Resources and Hydroxyl Apatite	¥500,000
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Other Research Fund

H. Tabata	Consortium R&D Projects for Regional Revitalization	Development of LIPS Method and its Application to the Future Model Touch Panel	¥1,008,000
H. Tabata	Sumitomo Seika Chemicals Co., Ltd.	Research for Visible Light Sensitive Photo Catalysis	¥4,200,000
H. Tabata	Kawasaki Heavy Industries, Ltd.	Research of Functional Materials	¥500,000
H. Tabata	Cluster Technology Co., Ltd.		¥300,000

Department of Single-Molecular Integrated Devices

Professor: Tomoji KAWAI
Associate Professor: Takuya MATSUMOTO
Research Associate: Masateru TANIGUCHI
Researcher: Akihiko TAKAGI, Pellegrino LUCA

Outlines

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 physical and chemical properties of single or several molecules.

Current Research Programs

Conductance Measurement of a DNA Network in Nanoscale by Point-Contact Current Imaging Atomic Force Microscopy

We measured the electrical conductivity of a DNA network as a spatially-resolved current-image using point-contact current imaging atomic force microscopy (PCI-AFM) under various humidity conditions. The simultaneous observation of topography and current image by PCI-AFM can provide information pertaining to the electrical properties of biological and/or soft materials in the nano-scale range. Under dry condition (0% humidity) no difference was observed for the electrical current both of the DNA network and mica surface, whereas the electrical current along the DNA network was larger than that of the mica surface by 20 pA at a bias voltage of 5 V under high humidity conditions of 60%.

Printing Electrode for Top-Contact Molecular Junction

We have developed a fabrication method of electrodes for molecular electronics based on nanotransfer printing lithography using a release agent layer and without any surface modification. A gold layer deposited on a release agent layer coating a mold can transfer to the nonmodified surfaces of SiO₂, sapphire, or organic layer. The printed electrode has a resistivity of $4 \times 10^{-6} \Omega\text{cm}$ which is close to the value of $2.1 \times 10^{-6} \Omega\text{cm}$ for bulk gold. The application of this process to top-contact type molecular junctions is demonstrated using carbon nanotubes and the electric potential distribution of the junctions is observed by Kelvin force microscopy.

Self-Organized Interconnect Method for Molecular Devices

We have developed an interconnect method to program three kinds of component molecules (interface control molecule, orientation control molecule, and function control molecule) with their own functions, and to wire a molecular device between nano-scale electrodes in a self-organized manner. By using the interconnect method we developed, we produced conductive wires and optical switching devices and have demonstrated their device functions. Combining these three control molecules allows us to produce molecular wires with various device properties that can be controlled. In applying our approach to molecular devices, we will be able to develop highly

integrated single-molecule transistors or other highly integrated single-molecule devices.

Electrical Conductance Spectroscopy of Chemical Reactions on Nano-Space

We theoretically investigated the electrical conductivity of a molecule during the progress of the chemical reaction, using the standard method of quantum chemistry and equilibrium Green's function formalism. As a result, the current-voltage profile corresponded to the energy profile along the chemical reaction path. Furthermore, we found that the changes to the current value that could be detected experimentally were in the order of micro amperes. Our results indicate possibilities to track and detect chemical reactions using electrical conduction measurements of molecules, and suggest a new principle of chemical analysis.

Publications

Original Papers

Directly Meso-Meso Linked Porphyrin Rings: Synthesis, Characterization, and Efficient Excitation Energy Hopping, Y. Nakamura, in-Wook Hwang, N. Aratani, Tae Kyu Ahn, Dah Mee Ko, A. Takagi, T. Kawai, T. Matsumoto, Dongho Kim, and A. Osuka : J. Am. Chem. Soc., 127 (2005), 236-246.

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Books

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Takuya Matsumoto, Tomoji Kawai: Analysis of Organic and Biological Molecules, in Scanning Probe Spectroscopy for Nanoscale Science and Technology, ed. By H. Shigekawa, M. Yoshimura, M. Sakata, A. Kawazu (Shokabo, Tokyo 2005)

Patents

Production method of microelectrode and microelectrode made by the same, T. Matsumoto, S. Matsui, K. Nakamatsu, K. Ojima, T. Kawai PCT/JP2005/005584

Probe device, T. Matsumoto, T. Kawai, PCT/JP2005/005583

Bipolar Organic Thin-Film Field-Effect Transistor and Making Method, K. Kawai, M. Taniguchi, E. Mizuno, I. Fukui, JP-2005-088914.

International Conferences

Construction of Protein Biosynthesis Chip using Ribosome, *T. Matsuura, Hiro. Tanaka, T. Matsumoto and T. Kawai, The 8th International Conference on Atomically Controlled Surfaces, Interfaces & Nanostructures / 13th International Congress on Thin Films, Stockholm International Fairs, Stockholm, Sweden, Jun. 19-23, 2005.

Tunneling Spectra for Single Molecules of HEX-Fluorescent Dye Attached to DNA Adsorbed on Cu (111) Surfaces, *T. Kawahara, T. Takahashi, N. Kubo, Hiro. Tanaka, M. Taniguchi, T. Kawai, The 8th International Conference on Atomically Controlled Surfaces, Interfaces & Nanostructures / 13th International Congress on Thin Films, Stockholm International Fairs, Stockholm, Sweden, Jun. 19-23, 2005.

Chirality Inversion and Electric Conduction of Porphyrin/DNA Complex, *C. Takatoh, T. Matsumoto, T. Kawai, T. Saitoh and K. Takada, The Eleventh International Conference on Organized Molecular Films, Sapporo, Japan, Jun. 26-30, 2005.

Self-assembly of Cysteine-modified Peptide Nucleic Acid on Gold Surfaces, *T. Matsuura, K. Ojima, Hiro. Tanaka, T. Matsumoto and T. Kawai, The 11th International Conference on Organized Molecular Films, Sapporo, Japan, Jun. 26-30, 2005.

Tunneling Conduction of Cytochrome c Molecules, *T. Matsumoto, M. Kataoka and T. Kawai, The Eleventh International Conference on Organized Molecular Films, Sapporo, Japan, Jun. 26-30, 2005.

AFM Imaging of Ribosomes Lined on mRNA at Translation State, *E. Mikamo, C. Takamori, H. Tanaka, T. Matsumoto and T. Kawai, 13th International Conference on

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Conductance Measurement of a DNA Network in Nanoscale by Point Contact Current Imaging Atomic Force Microscopy, *T. Matsumoto, A. Terawaki, Y. Otsuka, H. Y. Lee, Hide. Tanaka and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

Conduction Through Cytochrome c Molecules, *T. Matsumoto, M. Kataoka and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

Kinetic and Thermodynamic Control by Chemical Bond Rearrangement on a Si(001) Surface, C. Hamai, *A. Takagi, M. Taniguchi, T. Matsumoto and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

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Nanopatterning of Transition Metal Oxides by the Voltage-Biased Tip of an Atomic Force Microscope, *L. Pellegrino, E. Bellingeri, I. Pallecchi, G. Canu, A.S. Siri, D. Marré M. Hirooka, Y. Yanagisawa, M. Ishikawa, Hide. Tanaka, T. Matsumoto, A. Takagi and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

Observation of Various Porphynoids Adsorbed on a Substrate by Using AFM/STM, *A. Takagi, N. Aratani, T. Matsumoto, A. Osuka and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

Potential Mapping of Top-contacted Junctions: Molecules and Nanotransfer Printing Electrode, *K. Ojima, K. Nakamatsu, Y. Otsuka, T. Matsumoto, S. Matsui and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

Structure and Electrical Property of DNA Molecules Immobilized on Patterned Hydrophobic / Hydrophilic Surface, *Y. Otsuka, K. Ojima, T. Matsumoto, H. Tabata and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques in Conjunction with 13th International Colloquium on Scanning Probe Microscopy, Sapporo, Japan, Jul. 3-8, 2005.

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Surface Potential and Capacitance Image of Molecules on Insulating Substrates, *T. Matsumoto, F. Yamada and T. Kawai, 8th International Conference on Non-Contact Atomic Force Microscopy, Bad Essen, Germany, Aug.15-18, 2005.

Conductivity Measurement of Single/Small Number of DNA (Invited), *T. Matsumoto, Nanoelectronics and Dynamics of DNA, Hawaii, U.S.A., Aug. 28-31, 2005.

Electron-Molecular-Vibration Coupling for Small Polarons in Poly(dA)·Poly(dT) and Poly(dG)·Poly(dC), *M. Taniguchi and T. Kawai, Nanoelectronics and Dynamics of DNA, Honolulu, Hawaii, Aug. 28-31, 2005.

Printing Electrode for Top-Contact Molecular Junction, *K. Ojima, K. Nakamura, Y. Otsuka, T. Matsumoto, S. Matsui and T. Kawai, Nanoelectronics and Dynamics of DNA, Hawaii, U.S.A, Aug. 28-31,2005.

Conduction in Single/Small Number of Molecules Including DNA and Cytochrome c (Invited), *T. Matsumoto and T. Kawai, The54th Fujihara Seminar, Tomakomai, Japan, Aug. 31- Sep.4, 2005.

Visualization of Nano-Scale Magnetic Structures of Magnetoresistive (La,Ba)MnO₃ and Granular Fe/ Al₂O₃ by Frequency-Modulation Magnetic Force Microscopy (Invited), *T. Matsumoto and T. Kawai, 6th Pacific Rim Conference on Ceramic and Glass Technology, Maui, Hawaii, U.S.A., Sep. 11-16, 2005.

Fabrication of Mn-Doped Fe₃O₄ Nano-Channel Structures by AFM Lithography and Applications to Nano FET Devices, *L. Pellegrino, Y. Yanagisawa, M. Ishikawa, T.

Yanagida, T. Matsumoto, Hide. Tanaka and T. Kawai, 12th International Workshop on Oxide Electronics, Boston, U.S.A., Oct. 2-5, 2005.

Conduction Through Cytochrome c Molecules, *T. Matsumoto, M. Kataoka and T. Kawai, AVS 52nd International Symposium and Exhibition, Boston MA, U.S.A., Oct. 30-Nov. 4, 2005.

Potential Difference Mapping of Molecules and Particles on Insulating Substrate, *F. Yamada, T. Matsumoto, H. Tanaka and T. Kawai, AVS 52nd International Symposium and Exhibition, Boston MA, U.S.A., Oct. 30-Nov. 4, 2005.

Surface Potential Mapping of DNA-protein Complex at Molecular Level, *E. Mikamo, F. Yamada, T. Matsumoto and T. Kawai, AVS 52nd International Symposium and Exhibition, Boston MA, U.S.A., Oct. 30-Nov. 4, 2005.

Top-Contact Junctions for Molecules Electronics: Nano-Transfer Printing, *K. Ojima, K. Nakamatsu, Y. Otsuka, T. Matsumoto, S. Matsui and T. Kawai, AVS 52nd International Symposium and Exhibition, Boston MA, U.S.A., Oct. 30-Nov. 4, 2005.

Electrical Detection of Chemical Reactions on Nano-Space, *K. Yokota, M. Taniguchi and T. Kawai, International Symposium on Surface Science and Nanotechnology, Omiya, Japan, Nov. 14-17, 2005.

Fabrication of DNA Nanofibers by Electrospinning, *T. Takahashi, M. Taniguchi and T. Kawai, International Symposium on Surface Science and Nanotechnology, Omiya, Japan, Nov. 14-17, 2005.

Immobilization of DNA Molecules on The Patterned Self-Assembled Monolayers and Electrical Properties of DNA Molecules by Top-Contacted Nanogap Electrodes, *Y. Otsuka, T. Matsumoto, H. Tabata and T. Kawai, International Symposium on Surface Science and Nanotechnology (ISSS-4), Saitama (Omiya), Japan, Nov. 14-17, 2005.

Surface Potential and Capacitance Measurement of Molecules on Insulating Substrates Molecular Electronics, *F. Yamada, A. Takagi, T. Matsumoto and T. Kawai, International Symposium on Surface Science and Nanotechnology (ISSS-4), Saitama (Omiya), Japan, Nov. 14-17, 2005.

Ambipolar Organic Field-Effect Transistors Using Gate Insulator Hysteresis, *M. Taniguchi, E. Mizuno and T. Kawai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Fourth International Symposium, Mie, Japan, Nov. 18-19, 2005.

Approach to Electrical Conductance Spectroscopy of Chemical Reaction on Nano-Space, *K. Yokota, M. Taniguchi and T. Kawai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Fourth International Symposium, Mie, Japan, Nov. 18-19, 2005.

Fabrication of DNA Nanofibers by Electrospinning, *T. Takahashi, M. Taniguchi and T. Kawai, 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” Fourth International Symposium, Mie, Japan, Nov. 18-19, 2005.

Fabrication of Mn-doped Fe₃O₄ Nano-Channel Structures by AFM Lithography and Applications to Nano FET Devices. *L. Pellegrino, Y. Yanagisawa, M. Ishikawa, T. Yanagida, T. Matsumoto, Hide. Tanaka and T. Kawai, 4th 21st Century COE International Symposium, Toba, Japan, Nov. 18-19, 2005

Fabrication of Mn-Doped Fe₃O₄ Nanochannel Structures and Application to Nano FET Devices by AFM Lithography. *Hide. Tanaka, L. Pellegrino, Y. Yanagisawa, M. Ishikawa, T. Matsumoto and T. Kawai, 2005 MRS(Materials Research Society) Fall Meeting, Boston, USA, Nov. 28 – Dec. 2, 2005

Molecular Electronic Using Biological Materials (Invited), *T. Matsumoto and T. Kawai, International Symposium on Molecular Scale Electronics (In conjunction with 6th Molecular Scale Electronics Workshop in Japan), Tsukuba, Japan, Dec. 5-6, 2005.

Contributions to International Conferences and Journals

- | | |
|--------------|---|
| T. Matsumoto | Program Committee
International Symposium on Surface Science and Nanotechnology (ISSS-4) |
| T. Matsumoto | Program Committee
The 13 th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (STM'05)/ The 13 th International Colloquium on Scanning Probe Microscopy (ICSPM13). |
| T. Matsumoto | Organization Committee
International Symposium on Molecular Scale Electronics |

Publications in Domestic Meetings

- | | |
|--------------------------------------|----------|
| The Japan Society of Applied Physics | 12papers |
| The Surface Science Society of Japan | 2papers |
| Others | 9papers |

Academic Degrees

Master Degree of Engineering Science

- | | |
|--------------|---|
| T. Takahashi | Development of stretch-and-positioning method for DNA and electrical conductivity of DNA |
| E. Mizuno | Study on Ambipolar Organic Field Effect Transistors Using High-K Insulating Polymer (CyEPL) |

Master Degree of Science

- | | |
|-----------|---|
| Y. Nojima | Fabrication of photoswitching molecular device and electrical |
|-----------|---|

conductance spectroscopy of photochemical isomerization

Doctor Degree of Science

C. Takatho	Studies on DNA-templated porphyrin arrays and their molecular-scale electrical properties
Y. Otsuka	Study on charge transport properties through DNA by nanoscale electrical measurements

Sponsorship

Grant-in-Aid for Scientific Research (B)

T. Matsumoto	Stroboscopic Scanning Probe Microscopy and Time-Resolved Molecular-Scale Imaging of Photoexcited Carriers	¥5,300,000
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Exploratory Research

T. Matsumoto	Imaging of Transient Photoexcited Carrier Formation by Time-Resolved Force Measurement	¥1,300,000
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Grant-in-Aid for Young Scientists (B)

M. Taniguchi	Synthesis of Programmed Molecular Wires and Electrical Measurements of Them Using Nano-Gap Electrodes	¥800,000
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Entrusted research

T. Matsumoto	Japan Science and Technology Corporation	Mesoscopic Devices of Huge Porphyrin Arrays	¥1,100,000
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Other Research Funds

T. Matsumoto	Japan Science and Technology Corporation	Mesoscopic Devices of Huge Porphyrin Arrays	¥11,000,000
M. Taniguchi	Shin-Etsu Chemical Co., Ltd	Development of FET	¥2,000,000
M. Taniguchi	Kansai Research Foundation from Technology Promotion	Development of high-mobility FET Based on Polymers Using Inkjet Process	¥900,000

Department of Supramolecular Chemistry

Professor: Hiroaki SASAI
Associate Professor: Kiyohiko KAWAI
Research Associate: Shinobu TAKIZAWA

Outlines

Towards the construction of organized supramolecular systems with multifunctionality, the design and syntheses of supramolecules such as spherical nanoparticles, artificial DNA, peptides, photosynthetic molecules, and metal-bridged polymers having more efficient and selective functions than those of single molecules have been investigated.

Current Research Programs

1. Metal-bridged Polymers as Enantioselective Catalysts

The general immobilization of enantioselective catalysts involves the random introduction of chiral ligands onto polymer backbone. However, this method is less effective for multicomponent asymmetric catalysts, composed of plural ligands and metals, due to the haphazard of ligands and functional units on the polymer support. To further the development of immobilization method for the catalysts, metal-bridged polymers have been prepared from (*R,R*)-bi(BINOL) linking at each the 6-position and LiAlH_4 . Al-bridged polymers promoted asymmetric Michael reaction with high enantioselectivity. The Al-bridged polymer also can be reused. In this time, novel chiral linking ligands (*S*)-BINOL-(*S*)-BINAP and (*S*)-BINOL-(*S*)-MeO-MOP have been synthesized. The different coordination ability to transition metals on the ligands would efficiently foremed metal-bridged polymers with a several kind of metals. In fact, Al-Pd-bridged polymer as insoluble catalyst was prepared from (*S*)-BINOL-(*S*)-MeO-MOP in THF and LiAlH_4 followed by the addition of $\text{Pd}(\text{OAc})_2$.

2. Spherical Nanoparticles as Asymmetric Catalysts

Taking advantage of the facile adsorption of thiols to the surface of gold cluster, the disulfide bearing (*R*)-BINOL moieties at each terminal position has been successfully introduced on monolayer-protected metal cluster (MPC). Treatment of the metal cluster with $\text{Ti}(\text{O-}i\text{-Pr})_4$ afforded an insoluble Ti-BINOLate complex with high catalyst activity in the asymmetric alkylation of aldehyde with dialkylzinc. As an alternate approach, dendrimer-like catalyst was synthesized by immobilization of (*R*)-BINOL derivative on the polymer obtained by micellar polymerization system. The polymer-supported Ti-BINOLate complex generated with this polymer also exhibited high catalytic activity. Further applications of functional particles to new asymmetric reactions are in progress.

3. Construction of DNA Nanostructures Producing Charge-Separated State

The development of macromolecular chemical systems that are capable of generating a long-lived charge-separated state is of particular interest for technological advances in solar energy conversion and molecular devices. Recently, we found that hole transfer

between adenines in DNA proceeds rapidly and can be utilized to generate a photo-induced charge-separated state in DNA. By refining the photosensitizer to diphenylacetylene, we successfully produced a long-lived charge-separated state with a quantum yield of up to 26%.

4. Biological Effects of Charge Transfer in DNA

Based on the direct spectroscopic measurements of the hole transfer in DNA and quantification of the yield of the DNA oxidative damage, consecutive adenine sequences were found to be a good launching site for the photosensitizers to inject a hole in DNA, where the following rapid hole transfer between adenines causes a long-lived charge-separated state leading to DNA oxidative damage. According to the results, the essential requisites for the efficient and/or harmful photosensitizer are determined as follows: be able to oxidize adenine to trigger hole transfer between adenines, and react rapidly with molecular oxygen following its reduction avoiding the charge recombination and making the reaction irreversible. These results will greatly help us to classify photosensitizers harmful to human health, and to design an improved photosensitizer for biochemical applications.

Publications

Original Papers

Spiro Crown Ethers Bearing (S)-1,1'-Spirobiindanes as Chiral Backbones, K. Yonezawa, M. L. Patil, H. Sasai, and S. Takizawa, *Heterocycles*, 66 [1] (2005) 639-644.

Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman Reaction, K. Matsui, S. Takizawa, and H. Sasai, *J. Am. Chem. Soc.*, 127 [11] (2005), 3680-3681.

Micelle-Derived Polymer Supports for Enantioselective Catalysts, S. Takizawa, M. L. Patil, F. Yonezawa, K. Marubayashi, H. Tanaka, T. Kawai, and H. Sasai, *Tetrahedron Lett.*, 46 [7] (2005) 1193-1197.

Enantioselective Morita-Baylis-Hillman (MBH) Reaction Promoted by a Heterobimetallic Complex with a Lewis Base, K. Matsui, S. Takizawa, and H. Sasai, *Tetrahedron Lett.*, 46 [11] (2005) 1943-1946.

Fragmentation of Tertiary Cyclopropanol Systems Catalyzed by Vanadyl Acetylacetonate, M. Kiriara, M. Ichinose, Y. Ochiai, S. Takizawa, K. Okubo, R. Takizawa, H. Kakuda, and M. Shiro, *Tetrahedron*, 61 [20] (2005) 4831-4839.

Selective Guanine Oxidation by UVB-Irradiation in Telomeric DNA, K. Kawai, M. Fujitsuka, T. Majima : *Chem. Commun.* [11] (2005) 1476-1477.

Recognition of Substituted Cytosine Derivatives by the Base Pairing with Guanine Connected to Pyrene, T. Kawai, M. Ikegami, K. Kawai, T. Majima, Y. Nishimura, T.

Arai : Chem. Phys. Lett. 407 [1-3] (2005) 58-62.

Contributions of the Distance-Dependent Reorganization Energy and Proton Transfer Process to Hole Transfer in DNA, T. Takada, K. Kawai, M. Fujitsuka, T. Majima : Chem. Eur. J. 11 [13] (2005) 3835-3843.

Synthesis and Properties of Terthiophene Modified Oligodeoxynucleotides, K. Kawai, A. Sugimoto, H. Yoshida, S. Tojo, M. Fujitsuka, T. Majima : Bioorg. Med. Chem. Lett. 15 [20] (2005) 4547-4549.

Consecutive Adenine Sequences are Potential Targets in Photosensitized DNA Damage, K. Kawai, Y. Osakada, M. Fujitsuka, T. Majima : Chem. Biol. 12 [9] (2005) 1049-1054.

Kinetics of Transient End-to-End Contact of Single-Stranded DNAs, K. Kawai, H. Yoshida, A. Sugimoto, M. Fujitsuka, T. Majima : J. Am. Chem. Soc. 127 [38] (2005) 13232-13237.

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Review Papers

Photosensitized One-Electron Oxidation of DNA, K. Kawai, T. Majima : Pure Appl. Chem. 77 [6] (2005) 963-975.

Mechanism of photosensitized oxidation damage of DNA. Understanding and application to medicine (In Japanese): K. Kawai : Kagaku to Kogyo, 58 [2] (2005) 125-128.

Book

Spectroscopic Investigation of Oxidative Hole Transfer via Adenine Hopping in DNA, K. Kawai, T. Majima, In *Charge Transfer in DNA*, H.-A. Wagenknecht, Eds., Wiley-VCH, Weinheim, (2005) 117-132.

Patents

Preparation of Optically Active Spirobis(isoxazoline) Derivatives and their Transition Metal Complexes as Asymmetric Catalysts, H. Sasai, K. Wakita, T. Kato, M. A. Arai, T. Shinohara, and S. Takizawa, JP2006076939 (2006).

Preparation of Optical Active Spirobis(isoxazole) Derivatives and their Transition Metal Complexes as Asymmetric Catalysts, H. Sasai, K. Wakita, T. Kato, M. A. Arai, T. Shinohara, and S. Takizawa, JP2006076915 (2006).

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Takizawa, and H. Sasai, JP2006076911 (2006).

Preparation of Spiro Imidazoliums and their Salts as Ionic Fluids, M.L. Patil, C. V. L. Rao, S. Takizawa, and H. Sasai, JP2006076887 (2006).

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Process of Manufacture of Catalyst for Asymmetric Synthesis, M. Shibasaki, H. Sasai, and Y. Tahara, JP2005028363 (2005).

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Dinuclear Vanadium Complexes with Dual Activation: Enantioselective Homolytic Coupling Reaction of 2-Naphthols (Poster), *H. Sasai, H. Somei, Y. Asano, T. Yoshida, T. Katayama, S. Takizawa, The 13th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS13), Geneva, Switzerland, Jul. 17-21, 2005.

Development of Novel Chiral Ligands Bearing Spiro Skeleton (Oral), P. S. Koranne, T. Tsujihara, T. Shinohara, S. Takizawa, *H. Sasai, Palermo, Italy, the 20th International Congress of Heterocyclic Chemistry, Jul. 31-Aug. 5, 2005.

Novel Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman (aza-MBH) Reaction (Poster), *K. Matsui, S. Takizawa, H. Sasai, The 3rd International Symposium on Integrated Synthesis 2005 (ISIS-3), Osaka, Japan, Sep. 30-Oct. 1, 2005.

Rational Design and Synthesis of Novel Chiral Spiro Type Ligands (Poster), *P. S. Koranne, T. Tsujihara, J. Yogo, S. Takizawa, H. Sasai, The 3rd International Symposium on Integrated Synthesis 2005 (ISIS-3), Osaka, Japan, Sep. 30-Oct. 1, 2005.

Multifunctional Asymmetric Organocatalyst (Invited), *H. Sasai, The 10th International Chemical Conference in Taipei (ICCT10), Hsinchu, Taiwan. Oct. 28-30, 2005.

Development of Enantioselective Intramolecular Aminocarbonylation Catalyzed by Pd-SPRIX (Poster), *T. Tsujihara, P. S. Koranne, J. Yogo, K. Wakita, T. Shinohara, M. A. Arai, T. Arai, S. Takizawa, K. Onitsuka, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Design and Synthesis of Novel Chiral Ionic Liquids with Spiro Skeleton (Poster), *C. V. L. Rao, M. L. Patil, K. Yonezawa, S. Takizawa, K. Onitsuka, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Synthesis of Dendric Copper(I) Complex and its Reactivity Towards Dioxygen (Poster), *R N. Nadaf, D. Jayaprakash, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

A Rational Approach Toward the Development of Spiro Ligands (Poster), *P. S. Koranne, T. Tsujihara, J. Yogo, S. Takizawa, H. Sasai, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Development of Functionalized Nanoparticles Towards Targeted Drug Delivery Systems (Poster), *S. Takizawa, K. Tatematsu, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Mie, Japan, Nov. 18-19, 2005.

Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman (aza-MBH) Reaction (Invited), K. Matsui, K. Tanaka, S. Takizawa, *H. Sasai, PACIFICHEM 2005, Hawaii, USA, Dec. 15-20, 2005.

Development of Novel Chiral Spiro-Type Ligands Bearing Isoxazoline/Isoxazole Rings (Invited), P. S. Koranne, T. Tsujihara, J. Yogo, M. A. Arai, S. Takizawa, *H. Sasai, PACIFICHEM 2005, Hawaii, USA, Dec. 15-20, 2005.

New Concepts for Immobilization of Asymmetric Catalysts (Invited), *H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Development and Applications of Metal-Bridged Polymers as Asymmetric Catalysts (Poster), S. Takizawa, *N. Inoue, H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Development of Effective Enzyme Mimics Utilizing Dendrimers (Poster), *D. Jayaprakash, R. N. Nadaf, H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Kinetics of End-to-End Contact of Single-Stranded DNA (Poster), *K. Kawai, M. Fujitsuka, T. Majima, Fourth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Mie, Japan, Nov.18-19. 2005.

Charge Transfer in DNA and Photosensitized DNA Damage (Poster), *K. Kawai, Y. Osakada, M. Fujitsuka, T. Majima, Fourth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Mie, Japan, Nov.18-19. 2005.

Fluorescence Properties of 2-Aminopurine in Telomeric DNA (Poster), T. Kimura, *K. Kawai, M. Fujitsuka, T. Majima, Fourth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Mie, Japan, Nov.18-19. 2005.

Effects of Reorganization Energy and Proton Transfer on Hole Transfer in DNA (poster), *T. Takada, K. Kawai, M. Fujitsuka, T. Majima, Fourth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Mie, Japan, Nov.18-19. 2005.

Efficient Charge Separation in Diphenylacetylene-Modified DNA *T. Takada, K. Kawai, M. Fujitsuka, T. Majima, Fourth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Mie, Japan, Nov.18-19. 2005.

Kinetics of end-to-end contact of single-stranded DNAs (Poster), *K. Kawai, H. Yoshida, A. Sugimoto, M. Fujitsuka, T. Majima, International Chemical Congress of Pacific Basin Societies (Pacifichem), Hawaii, USA, Dec.15-20. 2005.

Hole transfer in DNA and photosensitized DNA damage, *K. Kawai, Y. Osakada, M. Fujitsuka, T. Majima, International Chemical Congress of Pacific Basin Societies (Pacifichem), Hawaii, USA, Dec.15-20. 2005.

2-Aminopurine as a probe for DNA conformational transition (Poster), *K. Kawai, T. Kimura, T. Majima, International Chemical Congress of Pacific Basin Societies (Pacifichem), Hawaii, USA, Dec.15-20. 2005.

Publications in Domestic Meetings

The 4th Symposium on Reaction Control of Dynamic Complexes	1 paper
National Meeting of Chemical Society of Japan	19 papers
The 1st Symposium on Ionic Liquid	1 paper
Symposium on Organometallic Chemistry	2 papers
Symposium on Combinational Chemistry	1 paper
Congress of Heterocyclic Chemistry	2 papers
Symposium on Progress in Organic Reactions and Syntheses	1 paper
Symposium on Organic Synthesis	1 paper
The 1st Symposium on Creation of Biologically Functional Molecules	1 paper
Symposium on Photochemistry	4 papers

Sponsorship

Grant-in-Aid for Scientific Research (2)

H. Sasai	Development of Enantioselective Cascade Reaction	¥2,900,000
H. Sasai	Development of Artificial Enzyme with Synergistic Multicooperation in Active Sites	¥2,000,000

Grant-in-Aid for JSPS Fellows

H. Sasai	Development and Application of Novel Asymmetric Spiro Catalyst	¥1,500,000
H. Sasai	Polymer-Supported Artificial Enzyme with Dendritic Systems	¥800,000

Other Research Fund

H. Sasai	Yamada Science Foundation	Development of Enzyme-like Asymmetric Bifunctional Organocatalyst	¥2,000,000
S. Takizawa	The Uehara Memorial Foundation	Development and Application of Cascade Ring-formation	¥3,400,000
S. Takizawa	21 st Century COE Program for Young Scientists	Development of Functionalized Nanoparticles towards Targeted Drug Delivery Systems	¥2,000,000
K. Kawai	21st Century COE Program for Young Scientists	Regulation of Photoinduced Charge Transfer Processes using DNA Nano Structure	¥600,000

Japan Science and Technology Corporation

S. Takizawa	Preparation of Functionalized Nanoparticles by Self-assembly	¥19,390,000
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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 Programs

1. Active-site structure of copper amine oxidase probed by three hydrazine derivatives reactive with the TPQ cofactor.

Since potent irreversible inhibitors, hydrazine compounds, have a nitrogen atom at the position corresponding to the α -carbon of substrate, the α -proton is prevented from being abstracted and a stable adduct is formed with the TPQ cofactor. To elucidate the cofactor environment within the hydrophobic substrate-binding pocket, the structure of the complex between CAO from *Arthrobacter globiformis* (AGAO) and three hydrazine derivatives, phenylhydrazine (PHZ), benzylhydrazine (BHZ), and 4-hydroxybenzylhydrazine (4-OH-BHZ), were determined by X-ray crystallography. The refined complex structures showed that the hydrazone form, an analogue to substrate SSB intermediate, was predominant in tautomerization of hydrazine adduct. Therefore, the distance from the catalytic base (Asp298) to the N2 nitrogen atom of hydrazone corresponds to that to the C α atoms of SSB formed with amine substrates. In the refined complex structures, the distance in the PHZ complex was longer by approximately two folds than those of the BHZ and 4-OH-BHZ complexes, which is consistent with the low catalytic efficiency of AGAO for benzylamine, relating to PHZ, in the proton abstraction step. Moreover, the formation of hydrazones was monitored by rapid-scan stopped-flow spectroscopy. Global analysis of the UV/vis spectral changes in the reaction with BHZ and 4-OH-BHZ provided the spectra of carbinolamine intermediate with the rate constants of each reaction step. The spectrum of each carbinolamine intermediate was observed for the first time for all copper amine oxidases.

2. 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-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. In 2002, we reported the high resolution crystalline structure of the xenobiotic exporter AcrB. This is the first case for the crystal structure determination of multidrug transporters. In this year, we have succeeded to determine the crystal structure of the substrate-bound form of the xenobiotic efflux transporter AcrB. The substrate-bound AcrB was an asymmetric trimer. Only one substrate bound to one of the three protomers, which represents the

binding form. The other two protomers corresponded to the two other transport steps, access and release. One trimer crystal contained all snap shots of the three transport steps. Therefore, this crystal structure clearly indicates that AcrB mediates drug export by means of the completely novel functionally rotating binding change mechanism.

Publications

Original Papers

PKCepsilon-PKD1 Signaling Complex at Z-discs Plays a Pivotal Role in the Cardiac Hypertrophy Induced by G-protein Coupling Receptor Agonists, M. Iwata, A. Maturana, M. Hoshijima, K. Tatematsu, T. Okajima, J. R. Vandenheede, J. Van Lint, K. Tanizawa, and S. Kuroda: *Biochem. Biophys. Res. Commun.*, 327 (2005) 105–113.

Nuclear-cytoplasmic Shuttling of a RING-IBR Protein RBCK1 and Its Functional Interaction with Nuclear Body Proteins, K. Tatematsu, N. Yoshimoto, T. Koyanagi, C. Tokunaga, T. Tachibana, Y. Yoneda, M. Yoshida, T. Okajima, K. Tanizawa, and S. Kuroda: *J. Biol. Chem.*, 280 (2005) 22937–22944.

Preparation and Characterization of Ca^{2+} -free Methanol Dehydrogenase from *Hyphomicrobium denitrificans* A3151, M. Nojiri, D. Hira, K. Yamaguchi, T. Okajima, K. Tanizawa, and S. Suzuki: *Chem. Lett.*, 34 (2005) 1036–1037.

Cytoplasmic Tethering of a RING Protein RBCK1 by Its Splice Variant Lacking the RING Domain, N. Yoshimoto, K. Tatematsu, T. Koyanagi, T. Okajima, K. Tanizawa, and S. Kuroda: *Biochem. Biophys. Res. Commun.*, 335 (2005) 550–557.

Re-investigation of Metal Ion Specificity for Quinone Cofactor Biogenesis in Bacterial Copper Amine Oxidase, T. Okajima, S. Kishishita, Y.-C. Chiu, T. Murakawa, M. Kim, H. Yamaguchi, S. Hirota, S. Kuroda, and K. Tanizawa: *Biochemistry*, 44 (2005) 12041–12048.

The Specific Delivery of Proteins to Human Liver Cells by Engineered Bio-Nanocapsules, D. Yu, C. Amano, T. Fukuda, T. Yamada, S. Kuroda, K. Tanizawa, A. Kondo, M. Ueda, H. Yamada, H. Tada, and M. Seno: *FEBS J.*, 2005, 272, 3651–3660.

Spatial Learning of Mice Lacking a Neuron-specific EGF Family Protein, NELL2, S. Matsuyama, N. Doe, N. Kurihara, K. Tanizawa, S. Kuroda, H. Iso, and M. Horie: *J. Pharmacol. Sci.*, 98 (2005) 239–243.

Review Papers

Development of Pinpoint Drug Delivery System by Bio-Nanoparticles (in Japanese), A. Kondo, S. Kuroda, K. Tanizawa, M. Seno, and M. Ueda: *Chemical Engineering*, 28 (2005) 351–356.

Innovative nanocarrier: Pinpoint Drug Delivery System by Bio-Nanoparticles (in Japanese), A. Kondo, S. Kuroda, K. Tanizawa, M. Seno, and M. Ueda: *Bio Industry*, 22 (2005) 22–27.

Bio-nano capsules allowing cell- and tissue-specific gene delivery (in Japanese), T. Yamada, M. Seno, M. Ueda, A. Kondo, K. Tanizawa, and S. Kuroda: *Seibutsukougakkaishi*, 83 (2005) 380–383.

Books

Protein Self-processing (in Japanese), T. Okajima and K. Tanizawa: *in* Protein Science—Structure, Property, Function, eds Y. Goto, K. Kuwajima, and K. Tanizawa, Kagaku-Dojin, Kyoto, (2005) 351–362.

Patents

“Drugs for the Treatment of Cancer and Their Production” M. Seno, H. Tada, T. Fukuda, S. Kuroda, K. Tanizawa, A. Kondo, M. Ueda, and H. Hamada: JP2005-84438.

International Conferences

Active-site Structure of Copper Amine Oxidase Probed by Three Hydrazine Derivatives Reactive with the TPQ Cofactor (Oral), *T. Murakawa, T. Okajima, M. Taki, Y. Yamamoto, S. Kuroda, H. Hayashi, and T. Tanizawa, International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Awaji, Hyogo, Japan, November 6–11, 2005.

Reaction Mechanism of Bacterial Copper Amine Oxidase: X-ray Crystal Structures of Catalytic Intermediates with Reduced Forms of the TPQ Cofactor (Poster), *T. Okajima, T. Murakawa, S. Kuroda, and K. Tanizawa, International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Awaji, Hyogo, Japan, November 6–11, 2005.

Involvement of a Hypothetical [Fe-S]-binding Protein in the Biogenesis of Quinohemoprotein Amine Dehydrogenase (Poster), *K. Ono, M. Tani, T. Okajima, D. Sun, V. L. Davidson, S. Kuroda, and K. Tanizawa, International Interdisciplinary Conference on Vitamins, Coenzymes, and Biofactors, Awaji, Hyogo, Japan, November 6–11, 2005.

Involvement of a [Fe-S]-binding Protein in the Biogenesis of Quinohemoprotein Amine Dehydrogenase (Poster), *T. Okajima, K. Ono, M. Tani, S. Kuroda, and K. Tanizawa, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Mitochondrial Transport is Regulated by FEZ1 in Neurites of NGF-differentiated PC12 Cells (Poster), *J. Ikuta, A. Maturana, T. Fujita, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Nano-scale Structure of Copper Amine Oxidase Probed by Three Hydrazine Derivatives Reactive with the TPQ Cofactor (Poster), *T. Murakawa, T. Okajima, M. Taki, Y.

Yamamoto, S. Kuroda, H. Hayashi, and K. Tanizawa, Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Hepatitis B Virus Envelope pre-S Peptide as a Useful Human Liver-specific Homing Peptide (Poster), *T. Kasuya, A. Ueda, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Cell Signaling Machineries of Novel Differentiation Factors for Neural Crest-derived Cells, NELL1 and NELL2 (Poster), *N. Bokui, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Pinpoint Drug and Gene Delivery System Using ZZ-displaying BIO-nanocapsule and Targeting Molecular-fused IgG Fc Protein (Poster), *H. Tono, H. Tada, A. Ueda, T. Kasuya, K. Tatematsu, T. Okajima, A. Kondo, M. Senno, M. Ueda, K. Tanizawa, and S. Kuroda, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18–19, 2005.

Involvement of a Hypothetical [Fe-S]-binding Protein in the Biosynthesis of Quinolacton Amine Dehydrogenase (Invited), *K. Tanizawa, Gordon Research Conference on Protein Derived Cofactors, Radicals and Quinones, Ventura, California, U.S.A., January 22–27, 2006.

Active-site Structure of Copper Amine Oxidase Probed by Three Hydrazine Derivatives Reactive with the TPQ Cofactor (Poster), *T. Murakawa, T. Okajima, M. Taki, Y. Yamamoto, S. Kuroda, H. Hayashi, and K. Tanizawa, Gordon Research Conference on Protein Derived Cofactors, Radicals and Quinones, Ventura, California, U.S.A., January 22–27, 2006.

Involvement of a Hypothetical [Fe-S]-binding Protein in the Biosynthesis of Quinolacton Amine Dehydrogenase (Poster), *K. Ono, M. Tani, T. Okajima, D. Sun, V. L. Davidson, S. Kuroda, and K. Tanizawa, Gordon Research Conference on Protein Derived Cofactors, Radicals and Quinones, Ventura, California, U.S.A., January 22–27, 2006.

Reaction mechanism of bacterial copper amine oxidase: X-ray crystal structures of catalytic intermediates with reduced forms of the TPQ cofactor (Poster), *T. Okajima, T. Murakawa, S. Kuroda, and K. Tanizawa, Handai Nanoscience and Nanotechnology International Symposium, Suita, Osaka, Japan, January 30–February 1, 2006.

Publications in National Meetings

Japanese Biochemical Society	3 papers
SPring8 symposium	1 paper
The Molecular Biology Society of Japan	1 paper
Annual Meeting of Nanotechnology Center	1 paper
Bimonthly Meeting of Vitamin B Committee	2 papers

Sponsorship**Entrusted Research**

K. Tanizawa	Japan Society for the Promotion of Science	Survey and Research on the Academic Trends in Biological Sciences	¥3,500,000
K. Tanizawa	Mitsubishi Electric Company, Ltd. (NEDO)	Analysis of Intracellular Signal Networks for Industrial Application of Genomics	¥4,200,000
K. Tanizawa	Japan Science and Technology Agency (CREST)	Creation of Functional Materials/ System that Utilize Nano Biotechnology for Realizing a Noninvasive Medical Treatment System: Novel Cell-selective Gene Delivery System Using Intracellular Signal-responsive Molecular System	¥11,950,000
K. Tanizawa	Bio-oriented Technology Research Advancement Institution (BRAIN)	Development of Innovative and Hypersensitive Bio-sensing Technology Using Yeast-derived Bio-nanocapsule	¥21,805,000

Other Research Funds

K. Tanizawa	Vitamin B Committee	Research on Built-in Cofactors	¥250,000
K. Tanizawa	Applied Enzyme Association of Japan	Biogenesis and Catalytic Function of Peptide Built-in Quinone Cofactors	¥1,000,000

Department of Nanosystem Design

Guest Professor: Ryusuke NISHITANI (2005. 4.-6)

Outlines

The local optical and electronic analysis of materials on a nanometer scale is an indispensable research for the development of nanometer electronics. The STM based spectroscopy enables us its analysis by combination of spectroscopic apparatus with STM technology. In this study, we have developed a system of STM-induced luminescence measurement, and carried out spectroscopic measurements of molecular luminescence on the metal surfaces.

Achievements

1. The STM-induced luminescence on a nanometer scale has been obtained in air by combining the STM in air and the spectrograph instruments.
2. The molecular luminescence of porphyrin film on a nanometer region has been observed in air for the first time. The spectra excited by tunneling electron injected from STM shows peaks which are nearly identical to photo luminescence peaks.
3. The enhancement of STM luminescence is observed for the porphyrin molecules on the substrates of noble metals, Au and Ag, but not on the Graphite and ITO.
4. The mechanism of molecular luminescence and its enhancement on noble metals can be explained in terms of the local plasmon induced luminescence and the plasmon enhanced molecular luminescence.
5. The molecular luminescence by STM can be analyzed by a model of the interaction of molecules with electromagnetic fields in a cavity, surrounded by the STM tip and the metal substrate, which is originated from the plasmon polarization created by tunneling electron from STM. The polarization of molecular luminescence should be resonated with the plasmon field to enhance the molecular luminescence resulted from plasmon field on noble metals.

Publication

Original Papers

Scanning Tunneling Microscope (STM)-Excited Molecular Fluorescence from Porphyrin Thin Films, Hongwen LIU, Ryusuke Nishitani, Yutaka Ie, Tatsuo Yoshinobu, Yoshio Aso and Hiroshi Iwasaki, Jpn. J. Appl. Phys., 44 (2005) L566-L569.

International Conference

Study of Porphyrin Molecules Adsorbed on Conductive Substrates by STL (Poster), *H. W. Liu, R. Nishitani, Y. Ie, T. Yoshinobu, Y. Aso and H. Iwasaki, third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium (ISCOE-2005), Shiga, March. 9-10, 2005

Plasmon-enhanced molecular fluorescence by using a STM, *H. W. Liu, R. Nishitani, Y. Ie, M. Nowicki, T. Yoshinobu, K. Sudoh, Y. Aso, H. Iwasaki, Scanning Probe Microscopy, Sensors, and Nanotechnology, Cancun, Mexico, Jun. 5-8, 2005

Fluorescence of Porphyrin Thin Films on Conductive Substrates by STL, *H. W. Liu, R. Nishitani, T. Yoshinobu, K. Sudoh, H. Iwasaki, Y. Ie and Y. Aso, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (STM'05), Sapporo, July. 3-8, 2005

Alternate current of STM for organic molecules adsorbed metal in terms of equivalent circuit of STM, *R. Nishitani, F. Begum and H. Iwasaki, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (STM'05), Sapporo, July. 3-8, 2005

Department of Nanosystem Design

Guest Associate Professor: Ryuji Nagaishi(2005.4.～2005.6.)

Outlines

Room-temperature ionic liquids, which are nonvolatile and nonflammable, have been proposed as solvents for green processing. The ionic liquids are also expected for design of new materials in nanoscience and nanotechnology. In this department, the chemical kinetics or reactions of ionic liquid were studied by using a pulse radiolysis technique to open new applications of ionic liquids.

Achievements

The spectrum and kinetic behavior of solvated electron were investigated in a hydrophobic ionic liquid (IL) of diethylmethyl(2-methoxy)ammonium (demma) – bis (trifluoromethanesulfonyl)imide (tfsi) salt by using pulse radiolysis technique. The absorption peak of the electron, corresponding to the potential well of the electron in IL, was blue-shifted from 1050 to 780 nm with increasing water content of 0 to 1.4 wt%, i.e., changing the dehydrated IL to the water-saturated IL. It indicates that the solvation structure of electron varied in an IL at a constant temperature, from that of electron solvated with demma cations to that of electron hydrated with water molecules. The structure variation affects the kinetic behavior of the electron. The self-decay constant decreased with increasing the water content. The reactions of the solvated electron with electron scavengers, such as acetone and trivalent ion of europium (III), were also investigated in the presence and absence of water. The solvation process of the electron in IL was firstly observed by using picosecond pulse radiolysis.

Department of Nanosystem Design

Guest Professor: Ken-ichiro SUETSUGU (2005.7. - 2005.9.)

Outlines

Development of novel lead-free solders for realizing highly reliable electronics packaging technology was performed. From the viewpoint of practical applications, various types of solder alloys, including low temperature and high temperature solders, are required to be developed. However, the theoretical methodologies for designing multiple-element alloys have never been established sufficiently. In the present project, the thermodynamic analysis based on the two-component eutectic mixing model was applied to the alloy design for novel lead-free solder alloys.

Achievements

The academic basis of two-component eutectic mixing model for multiple component alloys was examined by thermodynamic consideration of a model alloy system. The liquidus temperature of the multiple component alloys that can be expressed using the two-component eutectic mixing model was clarified to be a sum rule of $\sum W_i T_{\text{eu-}i}$, where W_i and $T_{\text{eu-}i}$ indicate the content and eutectic temperature of the constitutional eutectics. The liquidus temperature of various lead-free solder alloys can be predicted using this rule. Several candidate alloys for low temperature and high temperature solders were proposed in the present research project.

Department of Nanosystem Design

Guest Associate Professor: Makio UWAHA (2005.7-9.)

Outlines

Since crystal growth technology has been used at various situations in nano-technology, physical understanding of crystal growth becomes increasingly important. In order to utilize bottom-up processes in fabrication of future devices composed of nano-scale structures, understanding of self-organization phenomena including crystal growth is important. On these issues, in particular, step dynamics on crystal surfaces, and thermal relaxation of nano-scale structures, theoretical investigations have been performed.

Achievements

Thermal relaxation and coarsening of the surface morphology of $\text{SrTiO}_3(001)$ observed by scanning tunneling microscopy (STM) have been analyzed. Performing Monte Carlo simulations based on the solid-on-solid model, fundamental understanding on surface evolution of $\text{SrTiO}_3(001)$ surfaces was obtained.

A series of lectures on fundamental physics of crystal growth has been given for young researchers. The subjects covered in the lectures were as follows; (1) Dynamics of the first order phase transition (Review of thermodynamics), (2) Crystal surface structures and roughening transition, (3) Nucleation, (4) Crystal growth mechanism, (5) Morphogenesis in diffusion field, and (6) Mesoscopic pattern formations on the surfaces.

Department of Nanosystem Design

Guest Professor: Shozo Tero-Kubota (2005.10. – 2005.12.)

Outlines

Much attention has been paid to double-strand DNA because of its potential application as molecular devices. The dynamics of hole transfer have also been extensively investigated. Several hole transfer mechanisms, such as a super-exchange mechanism, hopping mechanism, and polaron mechanism, have been proposed. However, the hole transfer mechanism is still unclear

Using time-resolved EPR (TR-EPR) spectroscopy, we have studied the electronic state and dynamics of radical pairs generated by laser photolysis of the DNA conjugated with naphthalimide as the electron acceptor molecule. The double-strand DNA were synthesized in Majima Laboratory. The TR-EPR spectra observed were assigned to spin correlated radical pairs of the naphthalimide anion and DNA base cation radicals.

Achievements

We have successfully observed the TR-EPR spectra due to the spin correlated radical pairs in the double-strand DNA conjugated with naphthalimide by selective excitation of the electron acceptor with a Nd:YAG laser. The TR-EPR signals showed the E/A/E/A type spin polarization, where A is absorption and E is emission of microwave, respectively. The transient EPR signals were assigned to the radical pairs of the naphthalimide anion radical and the base cation radical generated from the singlet excited state of naphthalimide. The signals due to the hole showed short relaxation time compared with that of the anion radical site, indicating high mobility of the hole on the bases in the DNA strand. The recombination reaction rates were determined based on the analysis of the transient EPR spectra. The recombination rate depends on the oxidation potential of the substituted base.

The collaboration works were presented in the following symposiums:

- 1) S.Nakajima, K.Akiyama, K.Kawai, T.Takada, T.Ikoma, S.Tero-Kubota, T. Majima, Time-resolved EPR Study of Photoinduced Radical Ion Pairs in Double Strand DNA, 2005 Korea-Japan Symposium on Frontier Photoscience (2005, 10, 7-11, Busan, Korea).
- 2) K. Akiyama, K. Kawai, T. Takada, T. Ikoma, T. Majima, S. Tero-Kubota, Transient Radical Pair in the Photoinduced Electron Transfer Mediated by the Double Strand DNA, XXIst IUPAC Symposium on Photochemistry (2006, 4, 2-7, Kyoto, Japan).
- 3) S.Nakajima, K.Akiyama, K.Kawai, T.Takada, T.Ikoma, T. Majima, S. Tero-Kubota, Time-resolved EPR measurements of radical ion pairs in DNA 86th Spring Meeting of Chemical Society of Japan (2006, 3, 27-30, Chiba).

Department of Nanosystem Design

Guest Associate Professor: Ryoichi Hajima (2005.10.~2005.12.)

Outlines

Femtosecond pulse radiolysis is a powerful tool for the studies of quantum-beam-induced reactions in a femtosecond time region and in nano-space. In order to achieve the femtosecond time resolution in pulse radiolysis, a sub-100-femtosecond electron bunch generation in the photocathode RF linear accelerator was studied. A technique of equivalent velocity spectroscopy was constructed by using the ultrashort electron bunch.

Achievements

Bunch length growth due to space-charge effect and higher-order effect in the magnetic bunch compressor, especially the higher-order effect, should be considered and reduced to generate a sub-100-femtosecond electron bunch. For example, to compress a 3ps-long electron bunch, a energy spread of 1% is required. The increase of the bunch length due to the second-order effect is 180 fs. To reduce the nonlinear effects, we used the curvature of the rf waveform in the linac. By re-phasing the linac away from the zero-crossing of the rf (i.e. away from the linear slope), a nonlinear energy correlation along the bunch length can be introduced. The correlation can offset the effects of the nonlinear path length in the magnetic compression by optimizing the magnetic fields of four quadrupole magnets. In the simulation, a 70-fs-long electron bunch is expected to generate in the photocathode RF linac with the magnetic compressor, and the bunch length is shortened to be 45 fs by reducing the third order effect with a slit at the midplane of the compressor.

Department of Nanosystem Design

Guest Professor: Koichi KUGIMIYA (2006.1. - 2006.3.)

Outlines

The materials and devices developed using nanotechnology are assessed from the viewpoint of the environmental and health problems.

Achievements

Excessive expectations on Nanotech and Nano-particles have contributed to the very fast development of technologies but left environmental and health problems, which may exceed Asbestos' behind. Multinational efforts among governmental, private institutes and individual researchers are made to create common knowledge banks registering hazard reports on Nano-particles which effects on humans are still not known. The researchers are required to make sincere efforts to protect their surroundings, and to observe the potential hazards studied on Asbestos and heavy metals.

Department of Nanosystem Design

Guest Professor: Yoshihiro Kuroiwa (2006.1.–3.)

Outlines

Ferroelectric relaxor material is very attractive as a functional material. Recently, the environmental problem makes the Pb-free relaxor to be more important. In order to reveal the microscopic origin of homo-valence, Pb-free ferroelectric relaxor, we have performed the structural study of $\text{BaZr}_x\text{Ti}_{1-x}\text{O}_3$ (BZT) at the electron charge density level by analyzing synchrotron radiation powder diffraction data (BL02B2 in SPring-8) using the MEM/Rietveld method.

Achievements

The thermal parameter variations of each atom are carefully measured in the cubic perovskite phase at 473 K associated with the relaxor behavior. A clear discontinuity of the thermal parameters around $x = 0.5$ is found, where BZT shows a relaxor property. The charge density at the mid point in the Zr(Ti)-O covalent bond also shows a maximum around $x = 0.5$. The structural characteristics conflicting at this concentration are related to the appearance of relaxor behavior in BZT system.

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 quantum beam science.

Achievements

- Development of laser photocathode RF linear accelerator
- Generation of femtosecond electron beam
- 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
- Improvement of L-band linear accelerator for nanoscience
- 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
- Generation of ultrashort electron beam with laser-plasma

Department of Beam Science for Nanofabrication

Professor: Yoichi YOSHIDA
Assistant Professor: Jinfeng YANG
Assistant Professor: Takafumi KONDOH
Graduate Students: Kouji TAKEYA, Kouichi KAN, Youichi KURODA,
Susumu TAKEMOTO
Research Students: Masayoshi HIROSE, Akira ASANO, Shiya IZAWA
Support Staff: Mie TERASHITA

Outline

Elucidation 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. A technique of femtosecond pulse radiolysis based a femtosecond electron beam and a femtosecond laser light is a powerful tool for the studies of quantum-beam-induced reactions in a femtosecond time region and in nano-space. It is also expected for the development of quantum-beam fabrication process for nanotechnology.

In 2005, the bunch length growth due to space-charge effect and higher-order effect in the magnetic bunch compressor was studied to generate a sub-100-femtosecond electron bunch in the photocathode RF linear accelerator (linac). Moreover, to improve the time resolution of pulse radiolysis into femtosecond time region, a new technique of equivalent velocity spectroscopy (EVS) was constructed to avoid degradation of time resolution due to the velocity difference between light and electron in sample. In EVS, the electron bunch should be rotated into an angle as same as the injection angle between the electron beam and the analyzing light. In order to rotate the electron bunch, the nonlinear modulation of the longitudinal bunch phase space in the linac was studied. The technique of rotating the nonlinear bunch phase space in magnetic field was developed.

Furthermore, a double-decker electron beam accelerator based on the photocathode RF gun was developed successfully to reduce the time jitter between the electron beam and the analyzing light. It allows us open the next pulse radiolysis for studying the quantum-beam-induced reactions on femtosecond/attosecond time scale in the next ultimate fabrication.

Current Research Programs

1. Sub-100-femtosecond electron bunch generation in photocathode linac

Recently, a femtosecond pulse radiolysis system with time resolution of <100fs is developed in Osaka University. In order to achieve such time resolution, a laser-driven photocathode RF gun based linear accelerator (linac) was constructed to produce a low-emittance femtosecond electron beam, such as <3 mm-mrad and < 100 fs. In 2004, a 98-femtosecond electron single bunch with normalized transverse emittance of 3.8 mm-mrad at bunch charge of 0.2 nC was obtained by using the photocathode RF linear accelerator (linac) and a magnetic bunch compressor. However, the bunch length growth

due to space-charge effect and higher-order effect in the magnetic bunch compressor, especially the higher-order effect, should be considered and reduced to generate a sub-100-femtosecond electron bunch. For example, to compress a 3 ps-long electron bunch, an energy spread of 1% is required. The increase of the bunch length due to the second-order effect is 180 fs.

To reduce the nonlinear effects, we used the curvature of the rf waveform in the linac. By re-phasing the linac away from the zero-crossing of the rf (i.e. away from the linear slope), a nonlinear energy correlation along the bunch length can be introduced. The correlation can offset the effects of the nonlinear path length in the magnetic compression by optimizing the magnetic fields of four quadrupole magnets. In the simulation, a 70-fs-long electron bunch is expected to generate in the photocathode RF linac with the magnetic compressor, and the bunch length is shortened to be 45 fs by reducing the third order effect with a slit at the middle-plane of the compressor.

2. Equivalent velocity spectroscopy pulse radiolysis study

The pulse radiolysis is a powerful method for ultrafast reaction/phenomena studies. A femtosecond pulse radiolysis system is developed in ISIR by using the photocathode RF gun linac. The time resolution of the pulse radiolysis is not only decided on pulse length of both the electron beam and analyzing light, and time jitter between the electron beam and the analyzing light, but also limited on degradation of time resolution due to the velocity difference between light and electron in sample. To avoid degradation of time resolution due to the velocity difference between light and electron in sample, a new technique of equivalent velocity spectroscopy (EVS) was developed. In EVS, the electron beam and the laser light were injected with an angle of θ in sample. The angle (θ) was adjusted as $\theta = \arccos(1/n)$, where n is the refractive index of sample. Furthermore, the shape of electron beam bunch is also rotated with the same angle to overlap on the light pulse. Therefore, the degradation of time resolution due to the velocity difference between light and electron in sample can be avoided in the system.

In order to rotate the electron bunch, we used the curvature of the rf waveform in the linac to produce an oblique shape of the bunch in longitudinal phase space. The bunch is passed through the magnetic bunch compressor and rotated the shape of the energy-phase correlation by optimized the magnetic fields of four quadrupole magnets in the compressor.

3. Double-decker electron accelerator and attosecond science

An attosecond pulse radiolysis is considered for the future time-space reaction analysis into attosecond time region. To achieve the attosecond time resolution, a double-decker electron accelerator system based on the photocathode RF gun linac was developed. The double-decker electron beams with time interval of 1.4 ns and maximum bunch charge of 2 nC were generated successfully in the photocathode RF linac. The double electron beams were compressed into femtosecond with the magnetic compressor. The beam transverse normalized emittance of 3~4 mm-mrad was observed for both beams at an electron charge of 0.5 nC/pulse. The beam energy was 31 MeV. The compressed bunch length was 400-500 fs. In next step, the double-decker electron beams are utilized for studies of ultrafast reactions by means of pulse radiolysis.

Publications

Original Papers

Experimental Studies of Transverse and Longitudinal Beam Dynamics in Photoinjector, J. Yang, T. Kondoh, Y. Yoshida and S. Tagawa: Japn. J. Appl. Phys., 44 (2005), 8702-8707.

Synchronization of femtosecond UV-IR laser with electron beam for pulse radiolysis studies, A. Saeki, T. Kozawa, S. Kashiwagi, K. Okamoto, G. Isoyama, Y. Yoshida and S. Tagawa: Nucl. Instrum. Meth. A, 546 (2005) 627-633.

Femtosecond single electron bunch generation by rotating longitudinal bunch phase space in magnetic field, J. Yang, T. Kondoh, K. Kan, T. Kozawa, Y. Yoshida, and S. Tagawa: Nucl. Instrum. Meth. A, 556(2005), 52-56.

Subpicosecond Pulse Radiolysis Study on Geminate Ion Recombination Process in n-Dodecane, Y. Yoshida, A. Saeki, T. Kozawa, J. Yang and S. Tagawa: Ultrafast Phenomena XIV, (Springer, Berlin, 2005) 479-481.

International Conferences

Ultra-low emittance and ultrashort bunch electron sources (Invited), *J. Yang, 36th ICFA Advanced Beam Dynamics Workshop, Uji Campus, Kyoto University, Japan, Oct. 17-21, 2005.

Development of Femtosecond and Atto-second Pulse Radiolysis by Using Laser Photocathode RF Gun S-Band Electron Linac, *Y. Yoshida, J. Yang, and T. Kondoh, 2005 Particle Accelerator Conference, Knoxville, Tennessee, USA, May 16-20, 2005.

Experimental observation of a 100-femtosecond single electron bunch in photocathode linac with longitudinal emittance compensation technique, *J. Yang, K. Kan, T. Kondoh, T. Kozawa, Y. Yoshida, and S. Tagawa, 2005 Particle Accelerator Conference, Knoxville, Tennessee, USA, May 16-20, 2005.

Generation of double-decker femtosecond electron beams in a photoinjector, *J. Yang, Y. Kuroda, K. Kan, T. Kondoh, T. Kozawa, Y. Yoshida, and S. Tagawa, 2005 Particle Accelerator Conference, Knoxville, Tennessee, USA, May 16-20, 2005.

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Femtosecond pulse radiolysis study on primary process of radiation chemistry of polymer, Y. Yoshida, J. Yang, T. Kondoh, A. Yoshida, T. Kozawa, S. Tagawa, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Study of spectrum and kinetic behavior of solvated electron in hydrophobic ionic liquid

with controlling water content by pulse radiolysis, *J. Yang, R. Nagaishi, T. Kondoh, Y. Yoshida, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Selective polymerization of 5,7-dodecadiyne-1,12-diol bis[phenylcarbamate] (TCDU) crystals and concentration of the B-phase chain in TCDU-1 crystals using the electron beam excitation, *T. Kondoh, C. Itoh, J. Yang, Y. Yoshida, K. Tanimura, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005.

Experimental observation of 98-femtosecond single electron bunch in photocathode linear accelerator, *J. Yang, K. Kan, T. Kondoh, A. Yoshida, T. Kozawa, Y. Yoshida and S. Tagawa, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Toba, Mie, Japan, November 18-19, 2005.

Generation of a gradation electron beam pulse by a photo cathode RF gun LINAC for single shot pulse radiolysis measurement, *T. Kondoh, J. Yang, K. Kan, Y. Kuroda, S. Takemoto, A. Asano, A. Yoshida, T. Yamamoto, T. Kozawa, Y. Yoshida, and S. Tagawa, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Toba, Mie, Japan, November 18-19, 2005.

Femto-Second Bunch Length Measurement Using Spectral Broadening of Undulator Radiation, *T. Kondoh, J. Yang, A. Yoshida, Y. Yoshida and a. Ogata, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Toba, Mie, Japan, November 18-19, 2005.

Theoretical Description of Higher Order Effect Compensation in Magnetic Bunch Compressor for Femtosecond Electron Bunch Generation, *K. Kan, J. Yang, T. Kondoh, A. Yoshida and Y. Yoshida, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Toba, Mie, Japan, November 18-19, 2005.

Generation of double-decker electron beams for pulse radiolysis, *Y. Kuroda, J. Yang, T. Kondoh, A. Yoshida and Y. Yoshida, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Toba, Mie, Japan, November 18-19, 2005.

Measurement System of Femtosecond Pulse Radiolysis based on femtosecond electron beam and femtosecond laser light, *S. Takemoto, J. Yang, T. Kondoh, A. Yoshida and Y. Yoshida, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Toba, Mie, Japan, November 18-19, 2005.

Generation of femtosecond electron beam for ultrafast reaction analysis in nanofabrication, *J. Yang, K. Kan, T. Kondoh, A. Yoshida, T. Kozawa, Y. Yoshida and S. Tagawa, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan.30-Feb.1, 2006.

Generation of 98-femtosecond single electron bunch in photocathode linear accelerator, *Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

Femtosecond electron beam and ultrafast reaction analysis in nano-space, *J. Yang, K. Kan, T. Kondoh, A. Yoshida, T. Kozawa, Y. Yoshida and S. Tagawa, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

Generation of a gradation electron beam pulse toward the intensity modified radiation therapy (IMRT), *T. Kondoh, J. Yang, A. Yoshida, T. Yamamoto, Y. Yoshida and S. Tagawa, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

Study of beam dynamics in photocathode RF Linac and magnetic bunch compressor for femtosecond electron bunch generation, *K. Kan, J. Yang, T. Kondoh, A. Yoshida, Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

A new picosecond pulse radiolysis based on a photocathode Linear accelerator, *A. Asano, J. Yang, T. Kondoh, A. Yoshida and Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

A concept of double-decker electron beam accelerator for atto/femtosecond reaction analysis, *Y. Kuroda, J. Yang, T. Kondoh, A. Yoshida, Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

Publications in Domestic Meetings

Symposium on Advanced Radiation Chemistry	2 papers
The Japan Society of Radiation Chemistry	7 papers
The Particle Accelerator Society of Japan	6 papers
Atomic Energy Society of Japan	4 papers
Chemical Society of Japan	1 paper
Symposium on RF Electron Gun	7 papers
Symposium on TIARA	2 papers

Academic Degrees

Master Degree of Engineering

Kouichi Kan Study on femtosecond/attosecond electron bunch generation

Sponsorship

Grant-in-Aid for Scientific Research (A)

Y. Yoshida	Basic Research on Subfemtosecond and Attosecond Pulse Radiolysis	¥5,900,000
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Grant-in-Aid for Scientific Research (C)

J. Yang	Basic Research on Heavy Ion Pulse Radiolysis	¥1,500,000
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Cooperative Researches

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
	Sumitomo Heavy Industries, Ltd.	Research on photocathode RF gun and high brightness electron beam
	National Institute of Radiological Science	Beam control technique on the intensity modified radiation therapy
	Tokyo Univ.	Study on beam monitor

Department of Quantum Beams for Nanotechnology

Professor: Goro ISOYAMA
Associate Professor: Yoshihide HONDA
Research Associate: Norio KIMURA

Outlines

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 Programs

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. When a new electron linac called an RF gun linac was additionally installed in 2002 in the same room, which has a common RF power transmitter with the S-band linac, power supplies for the S-band linac were modified to improve their performance and then moved to a new place. Since then, we have been commissioning the S-band linac. In this year, we had several troubles such as faults of output voltage and frequent blows of fuses in a high voltage power supply for one of the two original klystron modulators as well as electric discharges in waveguides and leakage of the insulation gas from silver brazed parts in a directional coupler of the waveguides. The troubles in the DC high voltage power supply were mainly caused by electric noises coming into a feedback circuit for voltage regulation, so that we did wiring for grounding again from scratch, improved a noise-cut filter in the DC power supply including re-adjustment of a time constant. As a result, the DC power supply can be operated stably without blowing fuses, but the measures against the noise problem are not sufficient and we plan to improve the total grounding system of the klystron modulator again. As for the troubles with the waveguides, we fixed the gas leakage from the directional coupler with glue as

in last year and coped with the discharge problem by gradually increasing the high voltage in startup.

2. Design of a New Moderator for Positron Diffraction Experiment

The positron beam is currently produced with a large moderator to obtain as many positrons as possible and it is guided to a room for positron experiment through a magnetic transport system. In order to conduct diffraction experiments, a highly bright positron beam is necessary in the non-magnetic region. The positron beam is extracted from the magnetic transport system and then its brightness is enhanced using a special technique utilizing the reemission process of positrons from matter called as a remoderator. When low energy positrons are injected into a remoderator, some of the positrons are reemitted perpendicularly from the surface of the remoderator irrespective of their incident angles. If a low energy positron beam is injected and focused to a small beam size onto the remoderator, the emittance of the positron beam, which is approximately given by a product of the beam size and the angular spread, is reduced when it comes out from the surface due to reduction in the angular spread. Even if the intensity is reduced due to annihilation in the remoderator, the brightness can be enhanced by reducing the emittance further. We carried out an experiment to enhance brightness of the positron beam formerly, but it was not successful because the intensity decreased too much to conduct a diffraction experiment. This is mainly because the emittance of the positron beam was so large that the positron beam was not extracted efficiently from the magnetic transport system. In this year, we studied the moderator for producing slow positrons and the magnetic transport system again to reduce the emittance of the positron beam.

In order to suppress divergence of the positron beam at the extraction point from the magnetic field and to focus the positron beam effectively on the remodulator, the magnetic field around the modulator should be as weak as possible and at the same time positrons should have as small momenta in the azimuthal direction as possible, because the canonical angular momentum is conserved on the way from the moderator to the remoderator. Thus, preferable conditions are that the moderator is placed in a weak cusp magnetic field and many tungsten foils composing the moderator are coaxially stacked. When the magnetic field is weak, on the other hand, it is anticipated that the number of positrons reflected back by a magnetic mirror will increase. The higher voltage should be applied to the moderator to extract positrons against the mirror field. In order to extract positrons from the magnetic transport system and to focus them onto the remoderator using electrostatic lenses, on the other hand, the lower extraction voltage is preferable, since the focusing power in the electrostatic lens depends on the voltage ratio of an incoming electrode to an outgoing electrode. We conducted a simulation study to design a new moderator consisting of several tungsten foil layers in a cusp magnetic field under such conflicting requirements by optimizing parameters such as the number of layers, a space between layers, a tilt angle of the foils, and the strength and a distribution of the magnetic field. It is found that the loss of positrons due to the magnetic mirror field is serious, so that in order to avoid such a loss the average magnetic field in the transport system should be reduced as small as possible and the moderator should be placed at an optimum position with respect to magnetic lines.

3. Study on Electrolyte Membranes for Fuel Cells using Positron Annihilation

Spectroscopy

A Polymer Electrolyte Membrane used in Fuel Cells (PEMFC) is required to have such characteristics as high proton conductivity, high corrosion and deterioration resistance, high mechanical strength, and a low cost. Nafion[®] produced by DuPont is, at present, a good and well-balanced material at a high level for the membrane; nevertheless problems are that the cost is high and a working temperature is limited, so that many efforts have been devoted to find new materials surpassing Nafion[®]. Characterization of materials is indispensable for developing new functional materials. We plan in this study to analyze the structure of PEMFC in the vicinity of acid in the side chain and its degradation mechanism using positron annihilation spectroscopy. In the conventional analysis of space sizes near sulfonic acid groups by means of positron annihilation lifetime spectroscopy (PALS), positrons are assumed to annihilate in isotropic and uniform spaces and effects of functional groups on the positronium lifetime have not been considered yet. Since base polymers have the perfluorinated structure and sulfonic acid groups in the side chain, these functional groups may affect annihilation processes of positron and positroniums, so that the annihilation site may be localized in the vicinity of the acid. In order to investigate such effects, not only the lifetime of positrons but also momenta of annihilated electrons have to be measured. It is also necessary to investigate a correlation between positron or positronium lifetimes and the amount of water involved in the membrane, and a relation between the space size in the membrane and mobility of protons, a water-molecule content, and molecular motion.

4. Influence of Functional Groups on Positronium Formation in Polymers

The reductive cleavage of the carbon-halogen bond in alkyl halides upon addition of one electron is a simplest example of dissociative electron-transfer reactions. An important mechanistic and practical issue is whether the reaction is concerted or stepwise. Recent theoretical studies show that electron attachment and bond dissociation are completed within a few hundred femto-seconds (fs). The application of fs technique to study the dissociative electron attachment reaction has, to my knowledge, not been attempted so far.

We examined the effect of chloride functional group on positronium (Ps) formation was studied by measuring the ortho-Ps yield in poly(vinylbenzyl chloride), poly(4-chlorostyrene), and poly(vinyl chloride). According to the spur model, Ps formation process competes with other spur reactions, such as electron-cation recombination and electron and positron scavenging. It was found that the benzyl chloride group captures all the thermalized electrons, indicating that the dissociative electron attachment reaction takes place more rapidly than the Ps formation reaction (few ps). It can therefore be presumed that the positron annihilation method is useful to investigate the radiation chemistry at the early stage.

Publications

International Conferences

Study of annihilation processes of positrons in polystyrene related polymers, Y. Honda, T. Shimada, M. Tashiro, N. Kimura, Y. Yoshida, G. Isoyama, S. Tagawa, 8th International

Workshop on Positron and Positronium Chemistry, September 5-10, 2005, Coimbra, Portugal.

Study of Annihilation Processes of Positrons in Polymers, Y. Honda, N. Kimura, G. Isoyama, S. Tagawa, S. Nishijima, S. Takeda, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium. November 18-19, 2005, Toba, Japan

Contributions to International Conferences and Journals

Publications in Domestic Meetings

Linear Accelerator Meeting

2 papers

Department of Beam Science for Nanotechnology

Professor: Seiichi TAGAWA

Associate Professor: Shu SEKI (untill January 31, 2006)

Associate Professor: Takahiro KOZAWA

Outlines

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 an 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 Programs

1. Electronic Structure and Physical Properties of Molecular Nano-wires

Polysilanes and polygermanes containing only silicon and germanium in the backbone attracted 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 an improvement the physical properties of the conjugated polymers.

2. 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.

3. 1-D Nanostructure Formation by Charged Particle

High density energy deposition by charged particles causes non-homogeneous crosslinking reaction of polysilane derivatives within a nano-sized cylindrical area along an ion trajectory, and gives β -SiC based nano-wires of which sizes (length, thickness) and number densities are completely under control by changing the parameters of incident ion beams and molecular sizes of target polymers.

4. Gas Evolution from Nanoelectronic Materials

Gas evolved from resists deposits on optical system during lithographic exposure, leading to serious optical contamination. This is therefore one of the most grave issues in next generation optical lithography. Dependence of gas evolution on resist structure was investigated by using quadrupole mass spectrometer in order to obtain information on design of contamination-free resist.

5. 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 a spatial resolution and reaction mechanisms was investigated by a subpicosecond pulse radiolysis.

6. Radiation-Induced Reactions in Aromatics

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.

Publications

Original Papers

Proton and anion distribution and line edge roughness of chemically amplified electron beam resist, Takahiro Kozawa, Hiroki Yamamoto, Akinori Saeki and Seiichi Tagawa: J. Vac. Sci. Technol. B, 23(2005) 2716-2720.

Study on acid generation from polymer, Hiroki Yamamoto, Takahiro Kozawa, Atsuro Nakano, Kazumasa Okamoto, Seiichi Tagawa, Tomoyuki Ando, Mitsuru Sato and Hiroji Komano: J. Vac. Sci. Technol. B, 23 (2005) 2728-2732.

Resist Thickness Effect on Acid Concentration Generated in Poly(4-hydroxystyrene) Film upon Exposure to 75 keV Electron Beam, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto and S. Tagawa: Jpn. J. Appl. Phys., 44 (2005) L1298-L1300.

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Nanowires with Freely Controlled Sizes Formed by Single Ion Track Reactions in Polymers S. Seki, S. Tagawa, M. Sugimoto, 14th International Conference on Surface Modification of materials by Ion Beams, Kusadasi, Turkey, Sep. 4-10, 2005

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Contributions to International Conferences and Journals

(Conference Organizer)

T. Kozawa Microprocess and Nanolithograph Conference (Program Committee)

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	7 papers
Chemical Society of Japan	6 papers
Atomic Energy Society of Japan	5 papers
The Japan Society of Applied Physics:	6 papers
Society of Polymer Science, Japan	4 papers

Sponsorship

Grant-in-Aid for Scientific Research (S)

S. Tagawa	Femtosecond Pulse Radiolysis Study on Nano Spatial-temporal Reactions	¥23,900,000
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Grant-in-Aid for Exploratory Research

S. Seki	Development of Plateless Conductivity Measurement in Isolated Nanostructure and Molecular Element	¥500,000
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Grant-in-Aid for Scientific Research, Encouragement of Young Scientist (A)(2)

S. Seki	Formation and Property of Nanostructure using Chemical Reaction Induced by Single Particle	¥12,870,000
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Grant-in-Aid for Scientific Research, Encouragement of Young Scientist (B)(2)

T. Kozawa	Creation of Ultimate Nano Process by Femtosecond Pulse Radiolysis	¥1,200,000
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Entrusted Research

S. Tagawa	Japan Nuclear Energy Safety Organization	Development of Color Film Dosimeter Based on Advanced Radiation Chemistry
S. Tagawa	Advanced Semiconductor Engineering and Technology	Reaction Mechanism in Chemically Amplified Resist Materials
S. Tagawa	Semiconductor Leading Edge Technology Inc., Tokyo Ohka Kogyo	Study on Development of High Sensitive EPL Resist

S. Tagawa	Semiconductor Leading Edge Technology Inc.	Study on Solvent for Immersion Lithography
S. Tagawa	Mitsubishi Gas Chemical Company, Inc.	Fundamental Research on ArF Resist
S. Tagawa	Intel	Nanoscale Distribution of Acids Generated in Chemically Amplified EUV Resists

Cooperative Research

S. Tagawa, S. Seki	Japan Atomic Energy Research Institute	Ion Beam Pulse Radiolysis in Condensed Matter
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Department of Ultrafast Spectroscopy of Nanostructures

Guest Associate Professor: Mohamed El-MAGHRABY (2005.7.–2006.3.)

Outlines

The properties of semiconductors (SC,s) are strongly dependent on their structures, from bulk to nano-scale. Wide band gap SC,s like ZnO are very important for its variety applications in industrial technology. One-dimensional structures are now in condense research because of the new functions that can perform as light emitting diodes, probes. Constructing an apparatus to prepare nano structures from single and compound oxides in principle as well as any ceramic target material was the task of the plan.

Achievements

Different proposals were discussed with the construction company in order to make Chemical vapor Deposition and Pulsed Laser Deposition with modifications suitable for deposition nanostructures. Ability, safety, suitable design and existing facilities were considered.

A Hot-Wall High-Temperature PLD system was built and experiments to examine, adjust was performed. The apparatus has the following characteristics:

- Deposition of both thin films as well as nano-structures.
- Working at low as well as high temperatures (from room temperature up to 1000°C).
- Deposition of single and multi layers of one or more targets on alternatively.

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

Department of Nanomaterials and Environmentally Conscious Technology (Suganuma Lab.)

- Solidification of Sn-Ag-Cu solder balls
- Reliability establishment of Sn-Zn solder in humid atmosphere
- TEM of Ni-P plating interfaces and identification of nano-structure
- Synthesis and characterization of calcium phosphate-AMP composite material
- HREM observation and simulation of BCN fullerene materials
- Development of advanced conductive adhesives for high density electronics packaging technology.
- Development of advanced touch sensor sheets using super-flexible wiring technology.

Department of Nano-Bio-Intelligent Systems Science (Mizoguchi Lab.)

- Development of function decomposition trees for material design of nanoparticles/films
- Revision of Cell Signaling Networks Ontology (CSNO), and reorganization of the related knowledge using CSNO
- Development of prototype system for supporting creative design of function and manufacturing process of nanomaterials at the functional level
- Development of contents management system based on nanotechnology ontology.

Department of Computational Nanomaterials Design (Katayama-Yoshida Lab.)

- Development of *ab initio* molecular dynamics simulation (OSAKA-2003-Nano)
- Electronic-excitation-induced nanostructure-process design (from graphite to nano-diamond)
- Development of the quantum simulation method for design of spintronics (Curie temperature, structure, doping, beyond LDA and electronic structure)
- Design of bottom-up nano-fabrication method using nano-scale spinodal decomposition and dimension control in the thermal non-equilibrium crystal

growth method.

- T_c -enhanced Co-doping and Nano-scale delta-doping method for diluted magnetic semiconductors.
- Materials design of high-efficiency thermo-electric nanomaterials.
- Design of nano-structure gettering center in silicon.
- Mechanism of CN-treatment of dangling-bond in amorphous silicon and high-efficiency photovoltaic solar cells.

Department of Nanomaterials and Environmentally Conscious Technology

Professor:	Katsuaki SUGANUMA
Associate Professor:	Takeo OKU
Research Associates:	Shunro YAMAGUCHI, Masahiro INOUE
Post Doctoral Fellow:	Junxiang JIANG
Research Promotion Staff:	Mariko HATAMURA
Graduate Students:	Jae-Ean LEE , Motoki KANENO, Toshiko NAKAGAWA, Kimihiro YAMANAKA, Seiji KUMAMOTO, Gorou IZUTA, Naruhiko KOI, Daisuke WAKUDA, Yuhi YORIKADO
Support Staff:	Yoshie SASAKI, Kozue IDE

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, the composite materials based on metals and intermetallic compounds, the structural characterization of BCN fullerenes, and the bio mimetic bone structures. We set our route towards contributions to our society in near future.

Current Research Programs

1. Environmentally Conscious Electronics Packaging

The development of environmentally conscious fine technologies for electronics packaging area, i.e., lead-free soldering and conductive adhesives, and the establishment of scientific basis required for those technologies are our goals. For lead-free soldering, we found that solidification phenomena become critical rather than the conventional leaded alloys. By using simulation and the in-situ observation method for soldering solidification, the mechanisms and the various factors influencing on CSP defect formation became clear. The suppression method of solidification defects was proposed. Sn-Zn alloy is one of the candidates as low temperature solder. The degradation mechanism of the joint under humid atmosphere was clarified. The composite mixture rules were adopted for understanding the properties of nanopaste and conductive adhesives and it was proved that the interface bonding nature has key role for understanding the practical conductive adhesives.

2. Atomic Structure Analysis and Electronic Properties of New BN/C Fullerene Materials

Synthesis and HREM structure analysis of the new BN/ C fullerenes, nanotubes and nanocapsules. Structural optimization, electronic state calculation and physical property prediction by *ab initio* molecular orbital and molecular dynamics calculation. Establishment of quantitative HREM of 3D atomic arrangement in nano scale region.

3. Biomimetic Approach to Artificial Joint

As an artificial joint model, a cultured cartilage fixed with porous apatite was fabricated. By incorporation of growth factor in the porous apatite, calcination inside of the porous apatite was promoted to afford tight fixation between the cultured cartilage and porous apatite.

4. Development of Bioactive Bone Cement

For bone cements the following characteristics were required. 1) biocompatibility, 2) mechanical strength, 3) shortening of hardening, 4) resorption of bone cement. As new bone cements satisfied with the requirement, we are developing a resorbable bone cement which consists of organic-calcium phosphate nanocomposite and nanocomposite-PMMA bone cement with self-repairing function.

5. Surface Functionalization of Metallic and Intermetallic Materials

Novel chemical processes for surface modification of metallic and intermetallic materials are developed in order to realize several functions including catalysis, biocompatibility and durability.

- 1) Fabrication of functional ceramic thin films by sol-gel electrophoresis process
- 2) Direct formation of graded functional ceramic layers by reactive plasma process
- 3) Surface modification of conductive fillers

Publications

Original Papers

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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	7 papers
Japan Institute of Metals	1 paper
Others	3 papers

Academic Degrees

Doctor Degree of Engineering

- | | |
|-----------|--|
| M. Nakata | Fabrication and Estimation of Ceramics/Metal Composite by a High Pressure Impregnation |
|-----------|--|

Master Degree of Engineering

N. Koi Synthesis, purification, structures and properties of BN nanomaterials

Sponsorship

Other Allocations

K. Suganuma 21st Century COE Program ¥4,000,000

Entrusted Research

K. Suganuma	Japan Society for the Investigation on academic Promotion of Science	research trends in the field of metallic material engineering.	¥3,500,000
K. Suganuma	NEC Corporation	Interconnect technology using conductive adhesives.	¥1,050,000
K. Suganuma	NEDO	Development of alternative technology of high temperature lead solders	¥76,090,000
K. Suganuma	Business Innovation Center Osaka	Development of super-flexible touch sensors	¥6,932,000
K. Suganuma	i Support	Promotion of capable people for digital information electronics industries	¥2,100,000

Cooperative Research

K. Suganuma	Osaka TLO	Development of electronics information media using low temperature sinterable metal nanoparticles	¥25,700,000
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Department of Computational Nanomaterials Design

Professor:	Hiroshi KATAYAMA-YOSHIDA
Associate Professor:	Koun SHIRAI
Research Associate:	Kazunori SATO
Post Doctoral Fellows:	Van An DINH, Hiroyuki NAKAYAMA, Ikutaro HAMADA, Susumu YANAGISAWA, Kyuhoo LEE, Kunihiko YAMAUCHI
Research Students:	Jon Bergmann MARONSSON
Graduate Students:	Naoki MITSUDA, Hiroki FUNASHIMA, Kazuhito MATSUKAWA, Hidetoshi KIZAKI, Masayuki TOYODA, Tetsuya FUKUSHIMA Akio OGURA, Takayuki NOGUCHI, Kousuke TAKEUCHI, Akihiro NAGOYA, Masaki HIRAMATSU, Haruhiko DEKURA, Hitoshi MINAI
Under Graduate Student:	Jun ISHISADA, Yosuke NAKANO, Kunihiko HARADA
Support Staff:	Mika ASADA

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 Programs

Development of Materials Design Engine and Materials Design for Semiconductor Spintronics

We have developed materials design engine and applied it to materials design for semiconductor spintronics. In general, dilute magnetic semiconductors (DMS) have solubility gap and in thermal equilibrium they are phase separated. In a quenching process for such systems, spinodal decomposition occurs, *i.e.*, local density fluctuations are amplified and finally lead to random patterns of high concentration regions which connect each other leading to high- T_C ferromagnetic phase. We have developed our materials design including such inhomogeneous impurity distribution.

Ab initio calculations for such inhomogeneous disordered systems are difficult and

no method has established. First, we calculate electronic structure of DMS from first-principles by using Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. Then, chemical pair interactions between magnetic impurities in effective CPA medium are estimated by using generalized perturbation method proposed by Ducastelle and Gautier. Magnetic exchange interactions are calculated by the Liechtenstein's formula. Next, spinodal decomposed phases are simulated by applying the Monte Carlo method for the Ising model which describes chemical interactions in dilute alloy. Curie temperatures of simulated spinodal phases are calculated within the random phase approximation with taking disorder into account. It is shown that T_C goes up in the decomposition process even in wide band gap DMS. However, this effect is remarkable only above the nearest neighbor percolation threshold concentration, because at low concentrations only small separated clusters are formed due to the spinodal decomposition.

In the above simulation, we suppose the spinodal decomposition occurs isotropic, however, in real experiment we use non-equilibrium crystal growth technique (such as MBE or MOCVD) and crystal growth proceeds layer-by-layer. We have introduced the layer-by-layer crystal growth condition in our simulation of spinodal decomposition. First, we put magnetic impurities in the 1st layer randomly and simulate phase separation in the layer. Due to the attractive interaction, magnetic impurities forms clusters in the layer. Then, we distribute impurities in the 2nd layer and simulate phase separation. The impurities in the 2nd layer feels attractive interactions from the clusters in the 1st layer and forms clusters just on the clusters in the 1st layer. By repeating this step, finally we find quasi-one-dimensional structures formed by the magnetic impurities. In (Ga, Cr)N and (Al, Cr)N, the quasi-one-dimensional structures are actually formed in the experiments by Newman et al. By introducing the layer-by-layer condition, rather large clusters can be formed at low concentration and super-paramagnetism of the ensemble of the clusters could explain the ferromagnetic behavior of wide gap DMS at high temperature.

We have developed our material design method to include self interaction correction (SIC) to the local density approximation. We employed the pseudo-SIC method proposed by Filippetti et al., and implemented the method into the MACHIKANAYAMA2002 KKR-CPA-LDA package. We applied the method to several DMS systems and calculated electronic structure, magnetic interactions and Curie temperatures of II-VI and III-V DMS. It is found that in (Ga, Mn)N, higher Curie temperatures are predicted than the LDA values, because in SIC-LDA unoccupied 3d states are predicted at higher energy resulting in the suppression of anti-ferromagnetic super exchange interaction. In (Ga, Mn)As, it is found that Mn 3d states are predicted at lower energy than the LDA and Curie temperature shows liner dependence on Mn concentration. This means that the p-d exchange is dominant magnetic interaction in (Ga, Mn)As.

We have proposed SiO₂-based dilute magnetic semiconductors. SiO₂ is one of the most important materials in Si-based electronics as insulating material. We have investigated the ferromagnetism in SiO₂-based dilute magnetic systems such as 3d-transition metal doped SiO₂ and C or N doped SiO₂. Total energy difference between ferromagnetic state and local magnetic disordered state is calculated to estimate the stability of the ferromagnetic state. It is found that in V-, Cr- and Mn-doped SiO₂ and N-doped SiO₂ the ferromagnetic states could be stable.

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 evaluation of spin polarization and generalized-gradient approximation. For molecular dynamic simulation, a technique of metadynamics has been implemented in order to accelerate the processes. This method is particularly suitable for simulation of diffusion.

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. The crystal stabilities of α - and β -borons are studied theoretically by Osaka2k. At zero temperature, it is found that α -boron is more stable than β -boron. The transition temperature is obtained to be 970 K, which is in qualitative agreement with the experimental value of 1400 K. At finite pressures, the stability of various polymorphs can be determined mainly using the atom density. For β -boron, an energetic consideration shows that the disorder in the atom arrangement is inherent. The present calculations reveal a small change in bond length for specific *intericosahedral* bonds, which is caused by an atomic disorder.

Mechanism of fast diffusion of Cu impurity in Si

A distinguishing property of copper impurities in silicon is their very fast diffusivity, which is clearly undesirable in silicon device processes. We have studied the fast diffusion of Cu by Osaka2k. It is shown that, even near room temperature, the amplitude of Cu vibrations is very large. The diffusion path is from an interstitial *T* site to the next *T* site through an *H* site. The Arrhenius plot of the calculated diffusion constants agrees with the experimental data on the intrinsic diffusion of Cu, which are currently most reliable data available.

Material Design for Cu Gettering in Crystal Si

In the silicon device process, there is a strong demand for eliminating copper contamination. Gettering of Cu by dopant atoms is a useful method for this purpose. The gettering of Cu by dopant atoms is studied by Osaka2k. We have assessed the efficiency of gettering through the evaluation of the binding energies between Cu and electronic dopants and the dissociation energies. The calculated dissociation energies well describe the efficiency of various dopants, which have been found experimentally. The present study provides the basis for further study of the gettering mechanism and for the design of efficient gettering centers.

Microscopic Roles of Hydrogen in Crystal Si

Hydrogen is an important impurity in Si devices and change its electronic role on the devices, depending of the situations. It is generally believed that a H is located at the bond-center site, and its vibration appears in the 2000-cm⁻¹ band in the IR spectrum. However, there is a problem of a large discrepancy in the frequency between the frozen-phonon calculation and MD simulation. This discrepancy has been studied.

Differently from the frozen-phonon calculation, in which a linear chain structure Si-H-Si is assumed, the bond Si-H-Si is actually bending at finite temperatures. The H is rotating around the bond axis.

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High-Pressure Control of Boron Crystals, *K. Shirai, H. Dekura and H. Katayama-Yoshida, 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

Microscopic Mechanism of Phosphorus Diffusion in Silicon, *H. Nakayama, K. Shirai and H. Katayama-Yoshida, 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

Self-interaction-corrected Calculations of Dilute Magnetic Semiconductors, *M. Toyoda, H. Akai, K. Sato and H. Katayama-Yoshida, 9th SANKEN International Symposium 2006(SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, Feb. 8-9, 2006

Computational Nano-materials Design for Semiconductor Nano-Spintronics and EU-Japan Research Training Network, *H. Katayama-Yoshida, 1st Symposium on Nanoscience and Nanotechnology between Sanken and CNRS, Paris, France, Feb. 12-13, 2006

First-principles Calculations of Exchange Interactions in CuAlO₂ Based Dilute Magnetic Semiconductors with Carrier Doping, *H. Kizaki, K. Sato and H. Katayama-Yoshida, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006

Spinodal Decomposition under Layer by Layer Growth Condition and High Curie Temperature Quasi-One-Dimensional Nano-Structure in Dilute Magnetic Semiconductor, *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006

Contributions to International Conferences and Journals

H. Katayama-Yoshida	23 rd International Conference on Defects in Semiconductors : ICDS23 (Conference Chair)
K. Shirai	23 rd International Conference on Defects in Semiconductors : ICDS23 (Organizing Committee)
H. Katayama-Yoshida	The third international school and conference on spintronics and quantum information technology: Spintech III (Conference Chair)
K. Sato	The third international school and conference on spintronics and quantum information technology: Spintech III (Organizing Committee)
H. Katayama-Yoshida	4 th International Conference on Physics and Application of Spin-related Phenomena in Semiconductors: PASPS-VI (International Advisory Committee and Program Committee)
H. Katayama-Yoshida	International Conference on Magnetism: ICM2006 (Organizing Committee)

Publications in Domestic Meetings

The Physical Society of Japan	9papers
The Japan Society of Applied Physics	11papers

Academic Degrees

Doctor Degree of Science

H. Funashima	Thermoelectric properties study of semiconductors with First Principles Calculation
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Sponsorship

Grant-in-Aid for Scientific Research on the Priority Area

K. Sato Development and application of computational nano- ¥13,300,000
materials design engine

Grant-in-Aid for Scientific Research for young researcher (B) (K. Sato)

K. Sato Ab initio calculation for electric transport properties ¥2,000,000
by non-local CPA method

Grant-in-Aid for Scientific Research on the Priority Area (M. Shirai)

K. Sato Design for Opto-spintronics and Spin Prove
H. Katayama-Yoshida

Entrusted Research

JSPS Core-to-Core Program –Integrated Action Initiative-

H. Katayama-Yoshida Computational Nano-Materials Design ¥18,000,000

Ministry of Education, Culture, Sports, Science and Technology

Grant-in-Aid for the Creation of Innovations through Business-Academic-Public Sector Cooperation

H. Katayama-Yoshida Research on selective and low-temperature impurity ¥12,350,000
diffusion in semiconductor by infra-red laser
excitation

Japan Science and Technology Corporation

H. Katayama-Yoshida Core Research for Evolutional Science and Technology
(H. Kobayashi)
Silicon Thin Film Solar Cells with New Chemical Bonds

New Energy and Industrial Technology Development Organization (NEDO)

H. Katayama-Yoshida Development of Method for Nano-materials Simulation
(H. Akai)

Cooperative Research

H. Katayama-Yoshida	Japan Science and Technology Corporation	Case study on advanced measurements and analysis	¥1,960,000
H. Katayama-Yoshida	Institute for Materials Research, Tohoku Univ.	Design and fabrication of transparent high-Tc spintronics materials	¥2,000,000
H. Katayama-Yoshida	SPRING8	Mechanism of New Materials Fabrication	

H. Katayama-Yoshida	International Institute of Advanced Study	Using Electronic Excitation New functionality of electronic systems
H. Katayama-Yoshida	Jülich Institute (Germany)	Computational Materials and Devices Design for Nanospintronics
K. Sato	Juelich Research Center (Germany)	Electronic structure and magnetism of dilute magnetic semiconductors by KKR-CPA-LDA+U method (JSPS Bilateral program)

Department of Nano-Bio Intelligent Systems Science

Professor: Riichiro MIZOHUCHI

Research Associate: Kouji KOZAKI

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.

Current Research Projects

1. Development of Content Management System base on Nanotechnology Ontology

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.

2. Development of a System for Supporting Creative Design of Nanomaterials

Aiming at bridging required functions stated by engineers in industries and basic functions(or quality) and at facilitating the creative design, systematization of function achievement ways in a particular domain and development of a support system of functional design of materials are currently conducted in parallel.

In general, a function is achieved by performing multiple sub-functions. The achievement is supported by a physical principle and/or structure of the device or materials which is conceptualized as *Function achievement way*. The decomposition is continued concerning each sub-function to eventually form a function decomposition tree for each device/material. There exist multiple ways of functional decomposition so that the computer can help device/material designers to help their design process by giving possible alternative ways stored in a function achievement way server.

We have conducted the cross-over collaboration between us and Niihara & Kawai Labs. The concrete results on this collaboration include development of functional

decomposition trees of Nano-film and nano-particle together with a prototype system of creative design support system using a function achievement way server we developed. In addition we described function achievement ways by using Hozo system which we have developed, and we stored them in the server system. And we developed a prototype of the system for supporting creative design of nanomaterials.

3. 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.

Publications

Original Papers

A Framework for Organizing Role Concepts Based on their Dependencies on Contexts (In Japanese), E. Sunagawa, K. Kozaki, Y. Kitamura and R. Mizoguchi, Transactions of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 461-472.

An Integrative Model for Representation of Signaling Pathways on the Basis of Device Ontology (In Japanese), T. Takai-Igarashi and R. Mizoguchi, Transactions of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 406-416.

Reviewed Paper

A Present State of Ontology Development Tools (In Japanese), K. Kozaki and R. Mizoguchi, Journal of the Japanese Society for Artificial Intelligence, 20 [6] (2005) 407-714.

International Conferences

Developing Ontology-based Applications using Hozo, *K. Kozaki, Y. Kitamura and R.

Mizoguchi, The Fourth IASTED International Conference on Computational Intelligence (CI2005), Calgary, Canada, July 4-6, 2005.

A Framework for Organizing Role Concepts in Ontology Development Tool: Hozo, *E. Sunagawa, K. Kozaki, Y. Kitamura, and R. Mizoguchi, Roles, an Interdisciplinary Perspective: Ontologies, Programming Languages, and Multiagent Systems, The AAAI Fall Symposium, Arlington, Virginia, USA, Nov. 4-6, 2005.

Hozo: an Ontology Development Environment -Treatment of “Role Concept” and Dependency Management - (Poster), *K. Kozaki, E. Sunagawa, Y. Kitamura, and R. Mizoguchi, The 4th International Semantic Web Conference (ISWC2005), Galway, Ireland, Nov. 6-10, 2005.

Development of Ontology-based Knowledge Integration and Management System for Nanotechnology (Poster), *K. Kozaki, Y. Kitamura and R. Mizoguchi, Handai Nanoscience and Nanotechnology International Symposium, Icho Kaikan, Osaka University, Japan, Jan. 30 - Feb. 1, 2006.

Contributions to International Conferences and Journals

Riichiro Mizoguchi	European Project on SEKT (Steering committee member)
Riichiro Mizoguchi	Semantic Web Science Association (Vice-president)
Riichiro Mizoguchi	The 2 nd European Semantic Web Conference (ESWC2005) (PC member)
Riichiro Mizoguchi	The 2005 IFIP International Conference on Intelligence in Communication Systems (INTELLCOMM 05) (PC member)
Riichiro Mizoguchi	Second IFIP Conference on Artificial Intelligence Applications and Innovations, AIAI2005 (PC member)
Riichiro Mizoguchi	Third International Conference on Knowledge Capture (K-CAP 2005) (PC member)
Riichiro Mizoguchi	LORNET Conference I2LOR 2005 (PC member)
Riichiro Mizoguchi	Third IEEE International Workshop on Wireless and Mobile Technologies in Education (WMTE 2005) (PC member)
Riichiro Mizoguchi	Fourth international semantic web conference (Posters and demo chair)
Riichiro Mizoguchi	The 5th IEEE International Conference on Advanced Learning Technologies (PC member)
Riichiro Mizoguchi	The 14th International World Wide Web Conference Educational track (Vice chair)
Riichiro Mizoguchi	The 13th International Conference on Computers in Education (ICCE2005) (PC member)
Riichiro Mizoguchi	International Artificial Intelligence in Education Society (Executive Committee member)

Riichiro Mizoguchi	Asia-Pacific Society for Computer in Education (APSCE) (Board member)
Riichiro Mizoguchi	International Journal of Applied Ontology (Editorial board)
Riichiro Mizoguchi	International Journal of Artificial Intelligence in Education (Editorial board)
Riichiro Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
Riichiro Mizoguchi	International Journal of Web Semantics (Editorial board)
Riichiro Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	4 papers
The society of chemical engineers, Japan	1 paper

Sponsorship

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

R. Mizoguchi	Development of a Theory-Aware Authoring Workbench	¥9,600,000
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Grant-in-Aid for Encouragement of Young Scientists (B)

K. Kozaki	Development of Web Contents Management System based on Ontology and its Application to Nanotechnology	¥1,100,000
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Entrusted Research

R. Mizoguchi	Galaxy Express Corporation	MEXT IT Program e-Science Project Building a support system for operating a large-scale system using advanced IT	¥1,050,000
R. Mizoguchi	The Society of Chemical Engineers, Japan	Surveillance Study for Development of Structured Knowledge Platform for Nano-Materials and Products of Nano-particle and Nano-carbon (1) Brush up of Basic Systems and Information Gathering about Nano-particle and Nano-carbon to expand the Contents	¥2,100,000

Department of Nanotechnology Transfer

Guest Associate Professor: Mohamed El-MAGHRABY (2005.4.–2005.6.)

Outlines

The properties of semiconductors (SC,s) are strongly dependent on their structures; from bulk to nano-scale. Wide band gap SC,s like ZnO are very important for its variety applications in industrial technology. One-dimensional structures are now in condense research because of the new functions that can perform as light emitting diodes, probes. Searching the most suitable technique to prepare ZnO nanorods was the task of the plan.

Achievements

I have searched the most suitable technique to prepare ZnO nano rods. Two ideas; Chemical Vapor Deposition and Pulsed Laser Deposition ablation techniques are considered in order to construct nanorods deposition apparatus. Ability, structure and existing facilities were considered.

Department of Nanotechnology Transfer

Guest Professor: Chien-Tien CHEN (2005.7.1. - 2005.8.29.)

Outlines

The aim of this department is to transfer research results to the industry, and to create new industrial field.

Achievements

In order to develop novel organic light emitting display and reagent for chemoselective and stereoselective reaction, the following research topics have been discussed.

1. Vanadyl complex-mediated asymmetric catalysis in acylation, oxidative couplings of 2-naphthols, Mukaiyama aldol additions, and site-specific DNA photocleavage.
2. Chiral triarylcarbenium ions in asymmetric catalysis.
3. Dibenzosuberane-based helicenes as LC optical switches and potential optoelectronic templates in OLED.
4. Dibenzazapine-based triarylamine as hole-transporting materials in OLED.

Publications

Original Papers

Direct Atom-efficient Esterification between Carboxylic Acids and Alcohols Catalyzed by Amphoteric, Water-Tolerant $\text{TiO}(\text{acac})_2$, C.-T. Chen, S. Y. Munot, J. Org. Chem., 70 [21] (2005), 8625-8627.

Doubly Ortho-linked Quinoxaline/Triarylamine Hybrid as a Bifunctional, Dipolar Electroluminescent Template for Optoelectronic Applications, C.-T. Chen, J.-S. Lin, V. R. K. M. Moturu, Y.-W. Lin, W. Yi, Y.-T. Tao, C. H. Chien, Chem. Commun., [31] (2005), 3980-3982.

Stripping off Water at Ambient Temperature: Direct Atom-Efficient Acetal Formation between Aldehydes and Diols Catalyzed by Water-Tolerant and Recoverable Vanadyl Triflate, C.-T. Chen, S.-S. Weng, J.-Q. Kao, C.-C. Lin, M.-D. Jan, Org. Lett., 7 [15] (2005), 3343-3346.

Diethylene Glycol Ether-linked 3,4,5-Trihydroxybenzamides as Triply Branched Dendritic Anchors to CdSe/ZnS Core/Shell Type Nanoparticles: Potential Hydrophilic Fluorescent Probes, C.-T. Chen, V. D. Pawar, Y. S. Munot, C.-C. Chen, C.-J. Hsu, Chem. Commun., [19] (2005), 2483-2485.

Nucleophilic Acyl Substitutions of Anhydrides with Protic Nucleophiles Catalyzed by Amphoteric, Oxomolybdenum Species, C.-T. Chen, J.-H. Kuo, V. D. Pawar, Y. S. Munot, S.-S. Weng, C. -H. Ku, C. Y. Liu, J. Org. Chem., 70 [4] (2005), 1188-1197.

Synthesis of a Carboxyl Linker Containing Pk Trisaccharide, S.-Y. Hsieh, M.-D. Jan, L. N. Patkar, C.-T. Chen, C. C. Lin, Carbohydr. Res., 340 [1] (2005), 49-57.

Department of Nanotechnology Transfer

Guest Professor: Michael M. HALEY (2005.8. - 2005.9.)

Outlines

The purpose of this project is molecular structure design and synthetic route design of highly conjugated carbon-rich and planer compounds consisting of conjugated systems such as benzene, acetylene, and heteroaromatics. These compounds are expected to possess similar electronic structures to graphite. Their unique electronic properties and nonlinear optical characteristics have been investigated.

Achievements

Highly conjugated carbon-rich materials functionalized with electron donor and acceptor groups have attracted considerable interest. These materials often display reasonably large optical and nonlinear optical responses. We have studied the consequence of altering the substitution pattern of donor and acceptor groups conjugated in two dimensions across carbon-rich backbones. By locking the system into planarity to form macrocyclic aromatics, we have greatly increased the conjugation and further enhanced the optical properties. Also, as a result of the planarity of the conjugated systems and strong intermolecular interactions between the donor and acceptor groups, concentration-dependent self-association and polymerization readily occurs. The synthesis, self-association properties, and a systematic comparison of the optical and nonlinear optical data for a series conjugated systems as well as nonplanar mimics have been discussed.

The following two lectures have been also held.

"Dehydrobenzoannulene Chemistry: Carbon-rich π -Electronic Structures for Novel Applications", September 7, 2005.

"Chemistry of Metallabenzenes and Valence Isomers: New Ligands, New Metals, New Insights", September 29, 2005.

Department of Nanotechnology Transfer

Guest Associate Professor: Yury Nikolaevich MOLIN (2005.10. - 2005.11.)

Outlines

Investigation of structure, transformations and charge dynamics of alkane radical cations of and their Si and Ge- containing analogues in liquid solutions.

Combination of spin chemistry methods (Time Resolved Magnetic Field Effect, Optically Detected ESR, etc.) and pulse radiolysis technique will be used to get ESR parameters and optical absorption spectra of the radical cations in solutions, to measure mobility of radical cations and the rate of degenerate charge transfer, to determine the transformation routes and to measure the reaction rate constants for these radical cations.

Achievements

Radical cations with σ -bond delocalization of positive charge are known to play a crucial role in radiolysis, UV photolysis and many catalytic reactions involving organic molecules. The radical cations of σ -conjugated molecules (polysilanes and polygermanes) have also attracted recently a great interest as positive charge carriers in modern electronic devices. Therefore, a strong demand exists for investigations of electronic structure, chemical transformations and charge transfer ability of such radical cations. While the electronic structure of alkane radical cations was investigated in great details by ESR in low temperature matrices, little is known about the structure of their organo-element analogues and many problems are still open for investigations. It is not known, for example, if the spin and charge distribution is similar or different for alkane radical cations and their analogues or how the backbone branching and conformational variety affects the spin distribution and intramolecular or intermolecular charge dynamics. It is especially important to get information on σ -radical cations in solutions at ambient temperature where the structure and charge dynamics is not distorted by matrices interactions. This information is, however, unavailable in most cases due to instability of σ -radical cations. It is impossible, for example, to detect them by conventional ESR technique in liquid solutions at room temperature. On one hand, the classical pulse radiolysis technique, which is widely used to study short lived intermediates, will be employed. Recently, due to the improvement of time resolution of Osaka pulse radiolysis system, intermediates with picosecond and even sub-picosecond lifetime have become accessible for investigations. On the other hand, the spin chemistry methods developed by Novosibirsk group, such as Time Resolved Magnetic Field Effect (TR MFE) and Optically Detected ESR (OD ESR), as well as Time Resolved Electric Field Effect (TR EFE) will be used. It has been shown that these methods can be successfully applied to get information on ESR spectra of alkane radical cations in solutions at ambient temperature as well as on their mobility and reactions.

The following seminar was held on Oct 3, 2005.

“Alkane radical cations as studied by time resolved magnetic field effects and optically detected ESR techniques”

Department of Nanotechnology Transfer

Guest Professor: Ung Chan YOON (2005.12. - 2006.2.)

Outlines

Efficient light-energy conversion molecular devices are important in the field of the photofunctional supramolecules. The charge separation and recombination rates largely depend on the excitation energy, redox potentials, and distances between the donor and acceptor. From this point, effect of the linker was investigated systematically by using the picosecond time-resolved fluorescence spectra measurement and transient absorption spectroscopy.

Achievements

Naphthalimide and phenothiazine were employed as the acceptor and donor, respectively. As a linker, alkyl or polyether chain was employed to study the effect of the distance and oxygen in the linker. Formation of the charge separated state via singlet and triplet excited state of naphthalimide was confirmed by the transient absorption spectra. It was revealed that the charge separation efficiency decreased with the length of the linker. Furthermore, it was also revealed that the oxygen in the linker promotes the charge separation. In addition to these electron transfer processes, we found the formation of intramolecular exciplex between naphthalimide and phenothiazine. The formation process could be followed by the time-resolved fluorescence measurement.

This work has been published in *J. Phys. Chem. B* as follows:

1. "Intramolecular Exciplex and Intermolecular Excimer Formation of 1,8-Naphthalimide-linker-Phenothiazine Dyads"
D. W. Cho, M. Fujitsuka, K. H. Choi, M. J. Park, U. C. Yoon, and T. Majima
J. Phys. Chem.B **2006**, *110*(10), 4576-4582.
2. "Photoinduced Electron Transfer Processes in 1,8-Naphthalimide-linker-Phenothiazine Dyads"
D. W. Cho, M. Fujitsuka, A. Sugimoto, U. C. Yoon, P. S. Mriano, and T. Majima
J. Phys. Chem.B in press.

Division of Nanocharacterization

Outlines

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.

Achievements

- Atomistic structure analysis of metallic glasses using spherical-aberration-corrected transmission electron microscopy
- Local structure analysis of amorphous Fe-Si layers using high-resolution electron microscopy and nanobeam electron diffraction
- Establishment of nano-characterization of phase-change optical recording material using electron microscopy techniques.
- Establishment of the unified theory of photoinduced structural instability on semiconductor surfaces.
- Findings of surface phase transition from graphite to a new phase of diamond by femtosecond laser excitation.
- Elucidation of fundamental processes of structural instability on semiconductor surfaces induced by low-energy electron-beam irradiation.
- Nanocharacterization of ferromagnetic semiconductor nanostructures.
- Nanocharacterization of formation process of GaN nanorods.
- Visualization of 100nm MOSFET device nanostructures by STM.

Department of Advanced Nanostructural Characterization

Professor: Yoshihiko HIROTSU
Research Associate: 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 Programs

Development of structure analysis of amorphous materials using spherical-aberration-corrected transmission electron microscopy

The precise structure analyses of amorphous materials have been performed using a spherical-aberration-corrected high-resolution transmission electron microscopy. Nanoclusters with sizes of 1-2 nm embedded in a dense-randomly-packed amorphous matrix were clearly observed under an appropriate imaging condition. We demonstrated that sharp lattice images of crystalline nanoclusters can be clearly identified when the spherical aberration constant was close to zero and the defocus value was near the Gaussian focus.

Local atomic structures and crystallization behaviours in amorphous Fe-Si layer

We have investigated the local atomic structures and crystallization behaviors in amorphous Fe-Si thin layers using high-resolution electron microscopy and nanobeam electron diffraction. The amorphous Fe-Si thin layers were fabricated by high-dose Fe⁺ ion implantation into Si substrate at cryogenic temperature. Atomic pair-distribution functions extracted from electron diffraction patterns revealed that the nature of short-range order in the amorphous Fe-Si thin layer can be well described by the atomic arrangements of crystalline iron silicides. It was found that a continuous polycrystalline β -FeSi₂ layer was obtained and the most of the defects in the Si substrate were removed after annealing at 1073K for 2h.

Publications

Original Papers

Growth and Atomic Ordering of Hard Magnetic L1₀-FePt, FePd and CoPt Nanoparticles Studied by Electron Microscopy: Alloy System and Particle Size Dependence, Y. Hirotsu and K. Sato: J. Ceram. Proc. Res. 6 (2005) 236-244.

Two Dimensionally Dispersed Fe/FePd Nanocomposite Particles Synthesized by Electron Beam Deposition, Y. Hirotsu, K. Sato and J. Kawamura: Mater. Sci. Forum 502 (2005) 275-280.

Nanostructures of Binary and Ternary Fe-B Based Glasses Studied by HREM and Electron Diffraction, Y. Hirotsu, A. Hirata, T. Hanada and H. Mori: Archives Mater. Sci. 26 (2005) 25-29.

Identification of Soft Phonon Modes in Ge-Sb-Te using Electron Diffraction, M. Naito, M. Ishimaru, Y. Hirotsu and M. Takashima: J. Appl. Phys. 98 (2005) 034506(1)-034506(4).

Transmission Electron Microscopy Study on Ion-Beam Synthesized Amorphous Fe-Si Thin Films, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez and K. E. Sickafus: Appl. Phys. Lett. 87 (2005) 241905(1)-241905(3).

Review Papers

Structure Analysis of Amorphous Alloys using Electron Diffraction, T. Ohkubo and Y. Hirotsu: Materia Japan 44 (2005) 24-31 (in Japanese).

Books

Electron Microscopy Techniques, Y. Hirotsu: "Nano Materials (Vol. 2. Nano Metals)", Edited by A. Inoue, Fuji Technosystem, (2005) 314-327 (in Japanese).

International Conferences

Fabrication and Structural Analysis of Oriented L1₀-FePd Nanoparticles (Invited), *Y. Hirotsu and K. Sato, The 4th Academic Frontier Center International Symposium on "Future Data Storage Materials", Toyota Technological Institute Lecture Hall, April 9, 2005.

Local Structure Studies of Metallic Glasses Using High Resolution Electron Microscopy and Electron Diffraction (Invited), *Y. Hirotsu, A. Hirata, T. Ohkubo and T. G.Nieh, Bulk Metallic Glasses IV, Gatlinburg, Tennessee, USA, May 1-5, 2004.

Local Structure Studies of Metallic Glasses Using HREM and Electron Diffraction (Invited), *Y. Hirotsu, A. hirata and T. Ohkubo, The XII International Conference on Electron Microscopy of Solids (EM2005), kazimierz Dolny, Poland, June 5-9, 2005.

Nanocrystallization Process of Fe₈₄Nb₇B₉ Metallic Glass Studied by Electron Microscopy and X-ray Diffraction Techniques (Invited), *Y. Hirotsu, A. Hirata, E. Matsubara and A. Makino, 12th International Symposium on Metastable and Nano Materials (ISMANAM), Maison de la Chimie, Paris, France, July 3-7, 2005.

Fabrication and TEM Characterization of Hard Magnetic Ordered Alloy Nano-Particles (invited), *Y. Hirotsu and K. Sato, 4th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Int'l Symp., Toba, Nov.18-19, 2005.

Structure Analysis of Ion-Beam-Synthesized Amorphous Fe-Si Layers Using Transmission Electron Microscopy, *M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez, 13th International Conference on Radiation Effects in Insulators, Santa Fe, New Mexico,

USA, August 28 – September 2, 2005.

Contributions to International Conferences and Journals

Y. Hirotsu	5 th International Bulk Metallic Glasses Conference (Co-Chair)
Y. Hirotsu	16 th International Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Advisory Committee)
Y. Hirotsu	6 th Japan-Polish Joint Seminar on Materials Analysis (Organizing Committee)
Y. Hirotsu	International Conference on Magnetism 2006 (Organizing Committee)

Publications in Domestic Meetings

The Japan Institute of Metals	2 papers
The Japan Society of Applied Physics	2 papers

Sponsorship

Grant-in-Aid for Scientific Research on Priority Area (2)

Y. Hirotsu	In situ observation of atomistic structures in metallic liquid and metallic glass	¥20,300,000
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Grant-in-Aid for Scientific Research (S)

Y. Hirotsu	Fabrication and characterization of hard magnetic alloy nanoparticles produced by vapor quenching	¥22,600,000
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Entrusted Research

Y. Hirotsu	NEDO (Advanced Materials Technology Utilizing Glassy Metals for Commercial Uses)	Nano-structure Analysis for the Evaluation of Mechanical Properties in Glassy Metals	¥4,200,000
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Department of Advanced Characterization for Nano-Processing

Professor: Katsumi TANIMURA
Associate Professor: Jun'ichi KANASAKI

Outlines

Electronic excitations often induce structural instability on solid surfaces, such as structural changes, diffusion, and desorption of constituent atoms. The electronic excitations, which induce and promote atomic processes with site-sensitive rates, can be a promising method for creating novel surfaces and nano-scaled structures possessing new properties and functions that have been never achieved by conventional thermal processes. Our targets are to understand completely the fundamentals of underlying physics, and finally to establish advanced surface- and nano-processing technologies fully exploiting unique features of electronic-excitation effects.

Current Research Projects

Structural Instabilities of Semiconductor Surfaces Induced by Electronic Excitations

Semiconductor surfaces were excited by ns- and fs-laser beams, low energy electron beam, and injections of electrons and holes from metallic tips. Changes of surface structures induced by the excitations were directly probed by scanning tunneling microscopy (STM). The STM studies have demonstrated that the excitations induce bond breaking at intrinsic surface sites, resulting in formation of vacancies selectively on the outermost atomic layer. Recent results concerning the excitation-induced instabilities of semiconductor surfaces are summarized as follows.

- We have studied laser-induced structural instabilities of several semiconductor surfaces, Si(111)-(7x7), Si(111)-(2x1), Si(001)-(2x1), GaAs(110)-(1x1) and InP(110)-(1x1). The instabilities on the surfaces are commonly characterized by local bond breaking with efficiencies highly super-linear with respect to excitation intensity, together with significantly different features depending on properties of the surfaces. The results were systematically surveyed and we suggested non-linear localization of two holes at a surface atomic site is responsible for the excitation-induced bond breaking. We extended the two-hole localization model, originally formulated assuming successive localization of two surface-holes under thermal equilibrium condition, first to describe the role of non-equilibrium three-dimensional valence holes, and then to include synergistic effects between surface- and bulk-optical transitions. The extended model describes systematically and consistently the available experimental results through quantitative analysis of typical experimental results.

- Scanning tunnelling microscope is also suitable for manipulating surface atoms on surfaces by carrier injection. We observed structural changes of (110)-(1x1) surface of n-type InP sample upon injections of electrons or holes from STM-tips. The study has revealed that formation of vacancies at P and In sites is induced only by hole-injection, not by electron-injection. The efficiency of vacancy formation becomes significant

above tip-biases of +2.0V. We also successfully observed the sequential bond-breaking under hole-injection at atomic sites adjacent to pre-existing vacancies, leading to progressive growth of vacancies along the surface In-P chain direction.

- Structural instability of Si(111)-(7x7) surface induced by low-energy electron-beam was also studied by using STM, and we have shown that excitation with 15-50 eV electron beams removes adatoms from individual surface sites, resulting in the formation of vacancies. In contrast to the case of laser-induced bond breaking, the efficiency of vacancy formation is in proportion to the excitation intensity and the cross section of bond breaking shows a rapid decrease as the primary electron energy increases. Based on the results, we have suggested that surface plasmon generated by the excitation plays an important role in the structural instability and described the experimental results qualitatively using a semi-classical model.

Femtosecond-laser Induced Phase Transformation on Graphite Surfaces

Our group carried out STM observations of structural changes on Highly Oriented Pyrolytic Graphite (HOPG) surfaces induced by 80-fs laser pulses at a photon energy of 1.55eV. The scanning tunneling microscopy study has revealed that the excitation creates a new crystalline phase extending over 100 nm² on the surface. The laser-induced surface phase, which has never been reported, is characterized by downward relaxation of one-third of surface C atoms aligned along one third of $[1\bar{1}00]$ directions, together with outward relaxation of the other surface atoms along two third of the directions periodically. The atomic relaxation perpendicular to the surface is a clear indication of sp³-type bonding of carbon atoms between graphite layers, thus showing photo-induced bond-order transformation from sp²- to sp³-type. The phase transformation is induced by p-polarized lights, not by s-polarized lights, with an efficiency depending super-linearly with respect to the excitation intensity.

Publications

Original Papers

Structural instability of Si(111)-(7x7) induced by low-energy electron irradiation: Y. Sugita, H. Horiike, J. Kanasaki, and K. Tanimura: Surface Science 593(1-3) (2005) 168-172.

Time-resolved two-photon photoelectron spectroscopy of carrier dynamics on the Si(0 0 1)-(2 × 1) surface: S. Tanaka and K. Tanimura: Surface Science 593(1-3) (2005) 26-31.

Review Papers

Laser-Induced Structural Instability of Semiconductor Surfaces (in Japanese): J. Kanasaki and K. Tanimura: Journal of the Surface Science Society of Japan 26 (2005) 675-680.

International Conferences

Formation and clustering of surface vacancies under electronic excitation on semiconductor surfaces (Invited), *J. Kanasaki and K. Tanimura, The 23th International Conference on Defects in Semiconductors (ICDS-23), Awaji Island, Hyogo, Japan, July 24-29, 2005.

Photoinduced structural instability on semiconductor surfaces (Invited), *K. Tanimura, The 23th European Conference on Surface Science (ECOSS 23), Berlin, Germany, Sept. 4-9, 2005.

Laser-induced removal of fragmentary intact sheets and transformation into new structural phases on graphite (0001) surface, *J. Kanasaki and K. Tanimura, The 23th European Conference on Surface Science (ECOSS 23), Berlin, Germany, Sept. 4-9, 2005.

Differential STM image analyses of adatom-vacancies on Si(111)-(7x7) surfaces, *J. Kanasaki and K. Tanimura, The 23th European Conference on Surface Science (ECOSS 23), Berlin, Germany, Sept. 4-9, 2005.

Surface carrier dynamics on Si(001)-(2x1) studied by time-resolved two-photon photoelectron spectroscopy with tunable femtoseconds excitation lasers (Invited), *K. Tanimura and T. Ichibayashi, The 23th European Conference on Surface Science (ECOSS 23), Berlin, Germany, Sept. 4-9, 2005.

Laser-induced structural instabilities of Si surfaces, *J. Kanasaki, Workshop on Si Surfaces – Electronic Structure and Dynamics, Max-Born Institute, Berlin, Sept 10-11, 2005.

Photo-induced structural instability on silicon surfaces, *K. Tanimura, Workshop on Si Surfaces - Electronic Structure and Dynamics, Max-Born Institute, Berlin, Sept 10-11, 2005.

Voltage- and site-dependent changes in differential STM images of adatom-vacancies on Si(111)-(7x7) surface, *J. Kanasaki and K. Tanimura, International Symposium on Surface Science and Nanotechnology, Omiya, Saitama, Japan, Nov. 14-17, 2005.

Laser-induced structural instability of highly oriented pyrolytic Graphite (HOPG) surface, *J. Kanasaki and K. Tanimura, International Symposium on Surface Science and Nanotechnology, Omiya, Saitama, Japan, Nov. 14-17, 2005.

Spatially-differential STM image analyses of adatom-vacancies on Si(111)-(7x7) Surface, *J. Kanasaki and K. Tanimura, Handai Nanoscience and Nanotechnology International Symposium, Osaka University, Osaka, Japan, Jan 30 - Feb. 1, 2006

Photoexcitation of graphite creates a novel form of sp³-bonded carbon via structural-phase transition, K. Tanimura, Gordon Conference on Ultrafast Phenomena in Cooperative Systems, Santa Ynez Valley Marriott, Bueliton, CA, Feb. 5-10, 2006

Publications in National Meetings

The Physical Society of Japan	12 papers
The Japan Society of Applied Physics	1 paper
The Surface Science Society of Japan	3
papers	

Sponsorship**Grant-in-Aid for Scientific Research****(A)(2)**

K. Tanimura	Electronically Excited States on Quasi-two Dimensional Semiconductor Surfaces	¥22,880,000
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(C)(2)

J. Kanasaki	Structural Instabilities of Semiconductor Surface Induced by Low-Energy Electron Excitation	¥2,700,000
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Department of Quantum Materials and Devices Characterization

Professor: Hajime ASAH
Research Associate: Yi-Kai ZHOU

Outlines

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 Programs

1. Nano-Characterization of Diluted Magnetic Semiconductors

New diluted magnetic semiconductors, transition metal-doped and rare-earth metal-doped GaN, exhibit room temperature ferromagnetism and are gathering interest from the viewpoints of their physical properties as well as practical novel spintronics device applications. In 2005, we have characterized the functional properties of the GaN-based ferromagnetic semiconductor nanostructures grown by MBE. We have observed the magneto-optical effect in transmission MCD spectra. We also observed the increased magnetization from the GaGdN/GaN superlattice samples compared with those from the single layer GaGdN samples, which is attributed to the carrier-induced magnetization. We also conducted the AFM, XRD, TEM characterizations on the AlN and AlN/GaCrN samples to get the optimum growth conditions for the GaCrN/AlN heterostructures, which resulted to the realization of tunnel magnetoresistance behaviors in GaCrN/AlN/GaCrN trilayer diodes at 77 K for the first time for the all semiconductor spintronics devices.

2. Nano-Characterization of Structure and Functions of GaN Nanorods

GaN is expected to be promising to the application to the electric field emission electron sources because of a small electron affinity. We shown that the GaN grown on Si substrate with thin native SiO₂ layer has well-aligned nano-rod structures and exhibits excellent electric field emission characteristics. In 2005, to make clear the nano-rod formation process GaN/AlN superlattices were grown and conducted the TEM observation. We found that during the growth below 75 nm thick the surface is keeping flat, while during the growth of 90-165 nm thick the nano-rod structures are formed.

3. STM Characterization of 100nm MOSFET

According to the more and more downsizing of the Si-devices in Si-VLSI, the characterization with nanometer scale resolution becomes inevitably necessary, but it

becomes more and more difficult. STM-based technique is considered to be one of promising characterization methods. We have succeeded in the visualization of the device nano-structures for the 100 nm MOSFET samples with different cross section angle and position.

Publications

Original Papers

Magnetic, optical and transport properties of GaCrN-based ferromagnet/nonmagnet/ferromagnet trilayer structures, M.S. Kim, Y.K. Zhou, S. Kimura, S. Emura, S. Hasegawa and H. Asahi: J. Cryst. Growth 273 (2005) 675-679.

GaN-based diluted magnetic semiconductors for spintronics (Invited), H. Asahi, Y.K. Zhou, M.S. Kim, S. Emura, S. Shanthi, S. Kimura and S. Hasegawa, Inst. Phys. Conf. Ser.182 (2) (2005) 169-174.

Strongly localized exciton luminescence in Cr doped GaN, S. Shanthi, M. Hashimoto, Y.K. Zhou, S. Kimura, S. Emura, S. Hasegawa, N. Hasuike and H. Harima and H. Asahi, Appl. Phys. Lett. 86 (2005) 092102-1~3.

Magnetic and transport properties of ferromagnetic semiconductor GaDyN thin film, X.J. Li, Y.K. Zhou, M. Kim, S. Kimura, N. Teraguchi, S. Emura, S. Hasegawa and H. Asahi, Chinese Phys. Lett. 22(2) (2005) 463-465.

Polymorphism in the ferromagnetic GaCrN diluted magnetic semiconductor - Luminescence and structural investigations, S. Shanthi, M. Hashimoto, Y.K. Zhou, S. Kimura, M. S. Kim, S. Emura, N. Hasuike and H. Harima, S. Hasegawa, M. Ishimaru, Y. Hirotsu and H. Asahi, J. Appl. Phys. 98 (2005) 013526-1 ~ 013526-8

International Conferences

Photoluminescence investigations on the polymorphism observed in GaCrN, S. Shanthi, S. Kimura, M. S. Kim, Y.K. Zhou, S. Emura, N. Hasuike and H. Harima, S. Hasegawa, M. Ishimaru, Y. Hirotsu and H. Asahi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Shiga, Japan, March 9-10, 2005.

Growth and characterization of GaCrN-based heterostructures with an AlGaN barrier, M.S. Kim, Y.K. Zhou, S.W. Choi, S. Kimura, S. Kobayashi, S. Emura, S. Hasegawa and H. Asahi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Shiga, Japan, March 9-10, 2005.

Physical properties of AlN and GaN doped with rare-earth element (Gd), S. W. Choi, Y. K. Zhou, M. S. Kim, S. Kimura, S. Shanthi, S. Emura, S. Hasegawa, and H. Asahi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, March 9-10, 2005, Shiga, Japan.

Optical and magnetic properties of DyN/GaN superlattice and Dy-doped GaN, Y. K.

Zhou, M. S. Kim, S. W. Choi, S. Kimura, S. Kobayashi, S. Shanthi, S. Emura, S. Hasegawa and H. Asahi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, March 9-10, 2005, Shiga, Japan.

Growth and characterization of transition-metal-doped and rare-earth-doped III-Nitride based magnetic semiconductors, H. Asahi, Y.K. Zhou, M.S. Kim, S. Emura, S. Shanthi, S. Kimura and S. Hasegawa, Wide Band Gap Ferromagnetic Semiconductor Workshop, Edinburgh, UK, May 15-19, 2005.

Magnetic and optical properties of rare-earth-doped diluted magnetic semiconductors GaGdN and AlGdN, S. W. Choi, Y. K. Zhou, M. S. Kim, S. Kimura, S. Shanthi, S. Emura, S. Hasegawa, and H. Asahi, The third international school and conference on spintronics and quantum information technology, August 1-5, 2005, Awaji, Japan.

Optical and magnetic properties of DyN/GaN superlattice and Dy-doped GaN, Y. K. Zhou, S. W. Choi, M. S. Kim, S. Kimura, S. Kobayashi, S. Shanthi, S. Emura, S. Hasegawa and H. Asahi, The third international school and conference on spintronics and quantum information technology, August 1-5, 2005, Awaji, Japan.

Magnetic, optical and electrical properties of GaN and AlN doped with rare-earth element Gd, S. W. Choi, Y. K. Zhou, S. Emura, N. Teraguchi, A. Suzuki and H. Asahi, 6th International Conference on Nitride Semiconductors, Bremen, Germany, August 28 - September 2, 2005.

Studies on the nature of deep level defects in GaCrN diluted magnetic semiconductor, S. Shanthi, S. Kimura, M.S. Kim, S. Kobayashi, Y.K. Zhou, H. Hasegawa and H. Asahi, International Conference on Solid State Devices and Materials, Kobe, Japan, September 13-15, 2005.

Growth and characterization of GaCrN/AlGaIn/GaCrN Trilayer Structures, M.S. Kim, Y.K. Zhou, S. Emura, S. Hasegawa and H. Asahi, International Conference on Solid State Devices and Materials, Kobe, Japan, September 13-15, 2005.

Diluted magnetic semiconductors based on GaN in spintronics, S. Emura, Y.K. Zhou, S. Hasegawa and H. Asahi, CUP-2005, Seoul, Korea, October 14-15, 2005.

Epitaxial growth of ferromagnetic cubic GaCrN on MgO substrate, S. Kimura, S. Shanthi, Y.K. Zhou, M.S. Kim, S. Kobayashi, S. Emura, M. Ishimaru, Y. Hirotsu, S. Hasegawa and H. Asahi, Fourth International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Toba, Japan, November 18-19, 2005.

Growth and characterization of GaCrN/AlN/GaCrN trilayer structures, M.S. Kim, Y.K. Zhou, S. Matsuno, S. Emura, S. Hasegawa and H. Asahi, Fourth International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Toba, Japan, November 18-19, 2005.

Crystal growth and magnetic properties of Gd-doped GaN multiplayer, S.W. Choi, Y.K.

Zhou, M.S. Kim, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, Fourth International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Toba, Japan, November 18-19, 2005.

Contributions to International Conferences and Journals

H. Asahi	14th International Conference on Molecular Beam Epitaxy (Organizing Committee Vice-Chair, Program Committee Chair)
H. Asahi	17th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	The Third International School and Conference on Spintronics and Quantum Information Technology (Spintech III) (Organizing Committee member)
H. Asahi	13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (Publication Committee member)
H. Asahi	2005 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	15th International Conference on Ternary and Multinary Compounds (Program Committee member)
H. Asahi	Fourth International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" (Organizing Committee member)
H. Asahi	18th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	2006 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	Japan. J. Appl. Phys. (Editor)
H. Asahi	Journal of Crystal Growth (Editor)
H. Asahi	Current Applied Physics (Editor)
H. Asahi	J. of Materials Science: Materials in Electronics (Editor)
H. Asahi	e-Journal of Surface Science and Nanotechnology (Advisory Board)

Publications in Domestic Meetings

The Japan Society of Applied Physics	7 papers
Electronic Materials Symposium	1 paper

Sponsorship

Grant-in-Aid for Scientific Research on the Priority Area (A) (2)

Y.K. Zhou	Study on Synthesis of GaN-Based Transparent Ferromagnetic Semiconductors	¥2,700,000
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Nanotechnology Process Foundry

Professor:	Tomoji KAWAI
Visiting Associate Professor:	Masakazu MURASUGI Toshio KAWAHARA
Visiting Research Associates:	Takahiro OHNO Yoshinori MATSUI Kazumasa OKAMOTO
Supporting Staff:	Keiko ENMI

Outlines

Nanotechnology Process Foundry was founded in Nanoscience and Nanotechnology Center on the basis of Nanotechnology Support Project, supported by MEXT, Japan.

The purpose to start up the foundry is to build a platform supporting Nanotechnology R&D totally in Japan, especially for researchers outside Osaka University. It was the 4th year of this project in 2005, and most of our efforts resulted in supporting 33 research themes.

The Nanotechnology Support Project system was organized to realize the requests that researchers in private laboratories and R&D projects needed opportunities to use special facilities and equipments for their Nanotechnology R&D.

Institute of Science and Industrial Research, Osaka University has played an important role in Nanotechnology field by means of providing technology and information. In particular, thin film deposition works covering oxides and organic materials were presented a lot of impressed results. Based on the excellent works, Nanotechnology Process Foundry focuses the following supports.

- (1) Thin film deposition of oxides, organic materials, and high melting point metals.
- (2) Nanofabrication for oxide and organic material devices.
- (3) Characterization of thin films and devices made of oxides and organic materials.

Achievements

The 144 research themes have been supported since the foundry started its support.

Considering they were applied by researchers in companies, universities, and national laboratories, we can see that the foundry activates Nanotechnology field clearly. There were three points on our achievements in the followings:

1. Bring-up Nanotechnology Process Foundry.

The foundry was founded to support Nanotechnology researchers through thin film deposition, nanofabrication, and characterization. These supports are provided in the type of (a) consulting, (b) collaboration, (c) equipment use, and (d) research support.

2. Break-through toward functional Nanotechnology R&D.

The foundry supports advanced Nanotechnology R&D as well as fundamental research. The research on functional integration and system building based on nanomaterial is acceptable in the foundry.

3. Fusion between top-down and bottom-up Nanotechnologies.

Many useful equipments for top-down and bottom-up Nanotechnologies are in operation. The fusion between top-down and bottom-up Nanotechnologies will bring a lot of important progresses on Nanotechnology in the near future.

Publications

Original Papers

Fluoropolymer Outgassing in Focused Ion Beam Micromachining, Y. Matsui, S. Seki and S. Tagawa: J. Photopolym. Sci. Technol., 18 (2005) 501-502.

Nanopatterning of polyfluorene derivative using electron-beam lithography, Y. Doi, A. Saeki, Y. Koizumi, S. Seki, K. Okamoto, T. Kozawa and S. Tagawa: J. Vac. Sci. Technol. B, 23 (2005) 2051-2055.

Tunneling Spectroscopy Analysis of Hexachloro-Fluorescein Phosphoramidite Fluorescent Dye Attached to Deoxyribonucleic Acid, T. Kawahara, T. Takahashi, H. Tanaka and T. Kawai: Jpn. J. Appl. Phys., 44 (2005) 5386-5389.

Resist thickness effect on acid concentration generated in poly(4-hydroxystyrene) film upon exposure to 75 keV electron beam, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto and S. Tagawa: Jpn. J. Appl. Phys., Part 2, 44 (2005) L1298-L1300.

Effects of Dielectric Constant on Acid Generation in Chemically Amplified Resists for Post-Optical Lithography, T. Kozawa, K. Okamoto, A. Saeki and S. Tagawa: Jpn. J. Appl. Phys., 44 (2005) 3908-3912.

Requirements for Laser-Induced Desorption/Ionization on Submicrometer Structures, S. Okuno, R. Arakawa, K. Okamoto, Y. Matsui, S. Seki, T. Kozawa, S. Tagawa and Y. Wada: Anal. Chem., 77 (2005) 5364-5369.

Structural analysis for hydrogenated a-Si films by reverse monte carlo simulation, N. Tabuchi, T. Kawahara, T. Arai, J. Morimoto and H. Matsumura: Jpn. J. Appl. Phys., 44 (2005) 3808-3812.

Reaction Mechanism of Brominated Chemically Amplified Resists, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato and H. Komano: Jpn. J. Appl. Phys., Part 2, 44 (2005) L842-L844.

Study on acid generation from polymer, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato and H. Komano: J. Vac. Sci. Technol. B, 23 (2005) 2728-2732.

Potential Cause of Inhomogeneous Acid Distribution in Chemically Amplified Resists for Post Optical Lithography, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato and H. Komano: Jpn. J. Appl. Phys., Part 1, 44 (2005) 5836-5838.

Synchronization of Femtosecond UV-IR Laser with Electron Beam for Pulse Radiolysis Studies, A. Saeki, T. Kozawa, S. Kashiwagi, K. Okamoto, G. Isoyama, Y. Yoshida and S. Tagawa: Nucl. Instrum. Meth. A, 546 (2005) 627-633.

Dependence of Acid Yield on Acid Generator in Chemically Amplified Resist for Post-Optical Lithography, A. Nakano, K. Okamoto, Y. Yamamoto, T. Kozawa, S. Tagawa, T. Kai and H. Nemoto: Jpn. J. Appl. Phys Part 2, 44 (2005) 5832-5835.

Patents

The Control of Nano-Step Structure on the Sapphire Ware Surface, Y. Matsui, M. Murasugi, S. Seki, S. Tagawa, W. Hara, M. Yoshimoto, A. Takeuchi, N. Aota, H. Koyama, T. Kotaki, K. Sunagawa, Y. Yaguchi, S. Namiki, Tokugan2005-378335

International Conferences

Fluoropolymer Outgassing in Focused Ion Beam Micromachining, *Y. Matsui, S. Seki and S. Tagawa. The 22nd conference of photopolymer science and technology/The International symposium 2005 materials & processes for advanced microlithography and nanotechnology, Chiba, Japan, June. 21-24, 2005

Tunneling Spectra for Single Molecules of HEX-Fluorescent Dye Attached to DNA Adsorbed on Cu(111) Surfaces, *T. Kawahara, T. Takahashi, N. Kubo, H. Tanaka, M. Taniguchi and T. Kawai, 13th International Congress on Thin Films, 8th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures, Stockholm, Sweden, June. 19-23, 2005

Tunneling Spectroscopic Study for the Fluorescein Derivatives Attached to Deoxyribonucleic Acid, *T. Kawahara, Y. Nojima, H. Tanaka and T. Kawai, 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques, Sapporo, Japan, July. 3-8, 2005

Tunneling Spectroscopic Study for the Single Molecule of the Fluorescein Derivatives Attached Deoxyribonucleic Acid, *T. Kawahara, H. Tanaka and T. Kawai, International Workshop on "The Nanoelectronics and Dynamics of DNA", Hawaii, USA, August 28 - September 2, 2005

Fluoropolymer Outgassing in Micro-and Nano-Fabrication(Poster), *Y. Matsui, S. Seki and S. Tagawa, S. Tsuji and T. Itani, PCIFICHEM2005, Hawaii, USA, December 15-20, 2005

Reactivity of Model Compounds of ArF Immersion, ArF, and KrF Resists with Diphenylsulfinyl Radical Cation, a Cage-Escape Product of Photochemistry of Triphenylsulfonium Salts, *Y. Matsui, H. Sugawara, S. Tsuji, T. Itani, S. Seki, T. Kozawa and S. Tagawa, San Jose, USA, February 19-24, 2006

Publications in Domestic Meetings

Journal of the Ceramic Society of Japan

1 paper

Sponsorship

Entrusted Research

T. Kawai	MEXT (RR2002)	Nanotechnology Support Project	¥97,000,000
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Open Laboratory

Professors:	Yoichi YOSHIDA (Chair) Kazuhiko MATSUMOTO Hikaru KOBAYASHI Hiroaki SASAI
Technical Staffs:	Akira YOSHIDA, Kimihiro NORIZAWA
Supporting Staff:	Kayoko OHASHI

Outlines

Open Laboratory supports the comprehensive research for creative and advanced academic study on materials and devices, which should become the foundation of scientific and technological development on nanotechnology. This Open Laboratory is shared by the researchers engaged in nanotechnology in Osaka University.

Achievements

In 2005, the following 28 researchers used Open Laboratory:

Prof. Tomoyuki KAKESHITA	Graduate School of Engineering
Prof. Masahiko YAMAMOTO	Graduate School of Engineering
Prof. Takatomo SASAKI	Graduate School of Engineering
Associate Prof. Yusuke MORI	Graduate School of Engineering
Prof. Masanori OZAKI	Graduate School of Engineering
Prof. Yasufumi FUJIWARA	Graduate School of Engineering
Prof. Katsuaki SUGANUMA	Institute of Scientific and Industrial Research
Prof. Tomoji KAWAI	Institute of Scientific and Industrial Research
Specially Appointed Associate Prof. Isamu Oh	Graduate School of Engineering
Prof. Hitoshi TABATA	Institute of Scientific and Industrial Research
Prof. Hideo NAKAJIMA	Institute of Scientific and Industrial Research
Prof. Yoichi YOSHIDA	Institute of Scientific and Industrial Research
Associate Prof. Seiichi MURASUGI	Institute of Scientific and Industrial Research
Prof. Hiroshi MASUHARA	Graduate School of Engineering
Associate Prof. Tsuyoshi ASAH	Graduate School of Engineering
Prof. Tetsurou MAJIMA	Institute of Scientific and Industrial Research
Prof. Seiichi TAGAWA	Institute of Scientific and Industrial Research
Prof. Satoshi KAWATA	Graduate School of Engineering
Associate Prof. Yoshimitu YAMASAKI	Graduate School of Medicine

Prof. Shun-ichi FUKUZUMI	Graduate School of Engineering
Prof. Yukichi UMAKOSHI	Nanoscience and Nanotechnology Research Center
Associate Prof. Takehiko WADA	Graduate School of Engineering
Prof. Susumu KUWABATA	Graduate School of Engineering
Prof. Mitsuru AKASHI	Graduate School of Engineering
Associate Prof. Yasushi INOUE	Graduate School of Frontier Biosciences
Prof. Hiroshi YOSHIDA	Institute of Scientific and Industrial Research
Prof. Hikaru KOBAYASHI	Institute of Scientific and Industrial Research
Prof. Kiichi FUKUI	Graduate School of Engineering

Radiation Laboratory

Professor, Director:	Goro ISOYAMA
Professors	Seiichi TAGAWA, Tetsuro MAJIMA, Yoichi YOSHIDA
Associate Professors:	Ryuko KATO, Yoshihide HONDA, Shu SEKI, Mamoru FUJITSUKA, Takahiro KOZAWA
Research Associates:	Toshiji IKEDA, Norio KIMURA, Kazuo KOBAYASHI, Sachiko TOJO, Kiyohiko KAWAI, Masayuki ENDO, Shigeru KASHIWAGI, Jinfeng YANG, Akinori SAEKI
Technical Staff:	Tamotsu YAMAMOTO, Kumiko BABA
Support Staff:	Naoko KAWAGUCHI

Outlines

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 two technicians 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.

Achievements

1. 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 2005 is as follows; 118 days including 18 days for maintenance are allocated in the first term and 118 days including 16 days for maintenance in the latter term. The operation days in the year are 205 days in total and the operation time is 2,300 hours. The L-band linac has the highest rate of operation among the three linacs and hence it went wrong frequently, but most of the troubles were properly dealt with or repaired on the same day due to efforts and quick response of persons involved. The most serious troubles occurring this year were leakage of a coolant gas of the cooling water system, and unstable operation and a short

lifetime of a thyatron of the modulator power supply for the klystron. As for the cooling water system, a flow-control valve was replaced with a valve empirically showing high reliability. In the latter case, the thyatron was replaced with one that can stand a higher average current to be operated stably for a longer time.

2. 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. It was operated for 123 hours in this fiscal year. We had many troubles such as output faults of high voltage DC power sources used in klystron modulators, frequent burnouts of fuses used in the DC power sources, leakage of an insulation gas at brazing parts of waveguides, discharges in the waveguides, so that we could not run the linac stably and it took time to fix these problems.

3. RF-gun linac

The formal name of the RF-gun linac is the laser-photocathode S-band RF electron linac. It can accelerate a pico-second electron pulse beam to 40 MeV at maximum and can produce a short-pulse electron beam down to the femto-second region by means of the magnetic pulse compression method. These femto-second or pico-second pulse electron beams are mainly used for studies to investigate reactions induced by quantum beams. In this fiscal year, we designed and fabricated an RF switch for the waveguide system and tested its operation for two months, and then operated the linac for 407 hours in five months. The operation of the linac was satisfactory for the most part.

4. ^{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, and the Faculty of Medicine. The number of research subjects increased compared with that in last year and the facility was extensively used over the university. The total utilization time is 1710 hours, which is shorter than a value in last year, but it is because short-time irradiation experiments increased and the number of days in operation actually increased.

Concerning operation and maintenance, we made inspections and repairs of manipulators and the operation and control system of the irradiation facility also this fiscal year. Movement and conditions of the operation and control system was comparatively good. We changed motors and wiring of the periscope because they were damaged due to an elapse of years and exposure to strong γ -rays for a long time. We plan to maintain area monitors by the end of this year. In these few years, we found malfunctions of area monitors for higher radiation rates and measures are under review.

5. Join-use

The number of joint-uses this fiscal year is 24 subjects from our institute, 15 subjects from other departments in the university, and 4 subjects from groups including members outside the university, and these are adding up to 43 subjects in total. Among them, the

total number of subjects is 23 for the L-band linac, 21 for ^{60}Co γ -ray irradiation facility, and 7 for facilities other than the aforesaid. We held two workshops; “Nanoscience by means of Chemical Applications of Quantum Beams” held on November 14, 2005, and “Generation of Highly Brilliant and Stable, and Extremely Short Quantum Beams and Related Basic Technologies” held on January 16, 2006. In addition, we held the annual meeting for presenting results obtained in the fiscal year 2005 on March 13, 2006 at the auditorium of the institute. We received more than 260 visitors to the Radiation Laboratory.

6. Radiation safety management

The number of radiation users related to the Radiation Laboratory is 43 persons in the fiscal year 2005 and 7 persons among them are newly certificated users. An education and training course for new users was held on May 16, 2005 at the seminar room in the Radiation Laboratory.

Electron Microscope Laboratory

Professor, Director: Yoshihiko HIROTSU

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 2005, the 300kV TEM served as an important equipment for the nano-structure characterization researches of 9 laboratories in ISIR with operation times as many as 448.

Electronic Processing Laboratory

Professor: Hajime ASAH
Associate Professor: Shigehiko HASEGAWA
Associate Professor: Takuya MATSUMOTO
Associate Professor: Koichi SUDOH
Research Associate: Yi-Kai ZHOU
Research Associate: Kenzo MAEHASHI

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.

Nanofabrication Shop

Director: Katsuaki SUGANUMA
Technical Staffs: Kimiaki TANIHATA, Takeshi ISIBASHI
Specially Appointed Researcher:
Shouichi SAKAKIHARA

Outlines

Nanofabrication Shop was established in 2005 in order to promote researches by use of equipments and technologies for nano-fabrication belonging to ISIR. Besides this shop fabricates nano-devices for the ISIR researchers and develops devices for researchers who want to apply nano-devices for their nanotech experiments.

Achievements

This workshop has offered one hundred samples to one laboratory in the year 2005. In addition, we held a practice seminar which formed a part of COE project.

Materials Analysis Center

Professor Director: Hiroaki SASAI
Associate Professor: Takeyuki SUZUKI
Support Staff: 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 oxidative dimerization and Tishchenko reaction**

For the synthesis of dimeric esters, oxidative dimerization of primary alcohols is an important method as well as the Tishchenko reaction of aldehydes. Recently we have developed an Ir aminoalkoxide complex, which catalyzes the oxidative lactonization of diols and Oppenauer oxidation of primary alcohols. This time we found the Ir complex-catalyzed oxidative dimerization of various primary alcohols at room temperature. This reaction is also the first example of the use of ketone as a cooxidant. The reaction proceeds with 1–2 mol % of the catalyst and 0.3 mol equiv of K_2CO_3 in 2-butanone at room temperature to give the corresponding dimeric esters in 30–93% yield. Tishchenko reaction of the corresponding aldehydes were developed using the same catalyst. The reaction proceeds with 1 mol % of the catalyst and 20–30 mol % of K_2CO_3 in acetonitrile at room temperature to give the corresponding dimeric esters in good yield. Furthermore, we have developed two intramolecular cyclization of ketoaldehydes. The intramolecular Tishchenko reaction of ketoaldehyde proceeds with 5 mol % of Ir catalyst under reflux in *t*-BuOH, leading to the formation of 3,4-dihydroisocoumarin in 70% yield. Changing the reaction condition afforded the first oxidative lactonization of ketoaldehyde for the synthesis of isocoumarin in excellent yield.

Publications

Original Papers

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Catalytic Enantioselective Michael Reaction of 1,3-Dicarbonyl Compounds via Formation of Chiral Palladium Enolate, Y. Hamashima, D. Hotta, N. Umebayashi, Y. Tsuchiya, T. Suzuki, M. Sodeoka, Adv. Synth. Catal. 347 (2005) 1576–1586.

Publications in Domestic Meetings

The Chemical Society of Japan	1 paper
The Pharmaceutical Society of Japan	3 papers

Sponsorship

Grant-in-Aid for Young Scientist (B)

T. Suzuki	Development of Novel Catalytic Asymmetric Reaction Using Group 9 Transition Metal Complexes for the Synthesis of Biologically Active Substances	¥1,500,000
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Entrusted Research

T. Suzuki	KRI	Research of Materials Analysis	¥300,000
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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. A. Yamaguchi

G4 Human Interface Research Group: Group leader: Prof. H. Tabata

Achievements

Development of mass production method of lotus-type porous metals

Functionalization of lotus-type porous materials

Development of fabrication technique of lotus-type porous ceramics

Low temperature technique for environmentally conscious Pb-free electronics packaging

Development of wiring technique for nanopaste and ondemand

Functional nano-scale wires using biomolecular building blocks

Development of Multifunctional Asymmetric Catalysts

Multifunctional Asymmetric Organocatalysts

Studies on Excited radicals for Nanomaterial preparation

DNA Beam Chemistry

Identification of the exporters that mediates secretion of lipophilic signal transducing molecules.

Investigation of the expression regulation of multidrug exporters by indole as an intracellular signal transduction molecule.

Control of the shape and the intensity of the electron beam for the Intensity modulated radiation therapy by using the laser photo cathode RF gun.

Generation of the intensity-modulated electron pulse beam with high spatial resolution for medical treatment.

Development of novel single-molecule experimental system for rotary motor proteins driven by membrane potential

Nano structured biosensor chip

Knowledge sharing technology for manufacturing support

Strategic new industry prediction accompanying change of industrial structure

Adaptive interface by the sensor network and machine learning

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.

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

- Fabrication and property elucidation of lotus-type porous metals
- Functionalization of lotus-type porous ceramic
- Development of on-demand printing circuit technology with nanopaste
- Development of low temperature interconnection technology
- 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

Hard Materials Research Group

Professor: Hideo NAKAJIMA, Katsuaki SUGANUMA
Designated Associate Professor: Soong-Keun HYUN
Designated Research Associate: Keun-Soo KIM, Shunkichi UENO

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 developed by this department are unique materials which exhibit extraordinary superior mechanical strength. The materials are fabricated by unidirectional solidification of the melts under pressurized gases. Main issues are to investigate properties of lotus-type porous metals and to develop the engineering applications. In this year, we have established the fabrication method for porous metals using continuous casting technique, fabricated porous ceramic.

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 low temperature interconnection technology.

Current Research Programs

1. Fabrication and Property Elucidation of Lotus-type Porous Metals

We developed a new “Lotus continuous casting (LCC) technique”, by which long lotus-type porous plate or rod can be fabricated. From this technique, we successfully fabricated the lotus copper, which the pore size can be controlled by the solidification velocity. This is a promising technique for low cost and mass-production to commercial application of the lotus metals and provides various products for applications.

2. Functionalization of Lotus-type Porous Ceramic

For the increasing use of the Lotus-type porous ceramic, the fabrication of porous ceramics by unidirectional solidification were conducted using optical floating zone furnace. Porous alumina and mullite were successfully prepared by the solidification. The porosity and pore diameter can be controlled by the viscosity of the melt and other experimental conditions such as environmental gas, solidification rate, etc.

3. Development of on-demand printing circuit technology with nanopaste

Wring 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. For nanopaste interconnection, the sintering process of Ag nanopaste was proposed. Interface nano structures were identified by HREM and the precise interface formation mechanism was proposed.

4. Development of low temperature interconnection technology

Sn-Zn low temperature solder can be degraded by oxidation in high humidity condition. We proposed Sn-Zn-X solder instead of conventional Sn-Zn and Sn-Zn-Bi solders. The new Sn-Zn-X solder can withstand the high humidity condition.

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Contributions to International Conferences and Journals

H. Nakajima	Materials Letters (Principal Editor)
H. Nakajima	Fourth International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005) (Organizing Committee Chairman)
H. Nakajima	High Temperature Materials and Process (Editorial Board)
H. Nakajima	Diffusion and Defect Data (Editorial Advisory Board)
H. Nakajima	Materials Science Foundations (Editorial Advisory Board)
H. Nakajima	Pacific Rim International Conference on Materials (Organizing Committee Member)
H. Nakajima	International Symposium on Structural and Functional Materials Design (Organizing Committee Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	THEMEC'2006 Symposium on Metallic Foams (Organizing Committee Member)
H. Nakajima	International Conference on Diffusion in Materials (Organizing Committee Member)
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
K. Suganuma	High Density Packaging and Components Failure Analysis (HDP'05), International Advisory Board

Publications in Domestic Meetings

The Japan Institute of Metals

15 Papers

The Iron and Steel Institute of Japan	3 Papers
High Temperature Society of Japan	2 Papers
Japan Institute of Electronics Packaging	7 Papers
Others	3 Papers

Sponsorship

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	¥20,400,000
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Grant-in-Aid for Encouragement of Young Scientists

S.K. Hyun	Fabrication and mechanical properties of Lotus-type porous intermetallics	¥800,000
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Grant-in-Aid for Inter-university Cooperative Research Program of the Institute for Materials Research

S.K. Hyun	Research on electrical and magnetic properties of Lotus-type porous intermetallics	¥300,000
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Soft Materials Research Group

Professors

Tetsuro MAJIMA (group leader),
Hiroaki SASAI

Specially Appointed Associate Professor:

Masayuki ENDO (2005.6.16-)

Specially Appointed Research Associates:
(2005.8.1-)

Katsuya MATSUI, Masanori SAKAMOTO

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 Programs

Functional nano-scale wires using biomolecular building blocks

Programmable arrangement of the biomolecular building blocks through self-assembly is one of the most fascinating features for the supramolecular chemistry and nanotechnology. To construct the nano-scale structures and integration of functionalities, we created the DNA and protein supramolecular and nanostructures by designing the building blocks. First, we designed and characterized DNA tube structures by using the DNA tile system and four-way branched DNA-porphyrin connector. By self-assembling the DNA tiles and DNA-porphyrin connector, we successfully obtained the DNA fiber structures (20 μm), and the detailed analysis by AFM indicates the well-defined tube formation. Using this system, we developed the construction of the DNA nanotubes, and this strategy can be applicable for design and construction of functionalized nano-materials. Second, we investigated the effect of the aromatic molecules on the formation and stability of the tobacco mosaic virus (TMV) structures. Pyrene was used as a chromophore and introduced to the four specific amino acids in the pore of the TMV rod-structure. We examined the rod-structure formation by AFM, and the two pyrene-modified mutants into about 2 μm length of the rod-structures, which is 6-8 times longer than the native TMV rod. The interaction of the pyrene moieties in the TMV pore were investigated by detecting the characteristic fluorescence of pyrene excimer. By the analysis of the spectroscopic data, the pyrene moieties effectively stabilizes the rod-structures by π -stacking interaction, and the one pyrene moiety introduced into the monomer can affect the overall formation of TMV rod-structure. The TMV supramolecular system described in this report allows the integration of aromatic molecules into the cavity of the TMV scaffold and serves for creating well-ordered self-assembled molecular wires for the creation of the π -stacked supramolecular nano-scale materials.

Development of Multifunctional Asymmetric Catalysts and Multifunctional Asymmetric Organocatalysts

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. The aza-MBH reaction is a C-C bond-forming reaction of activated alkenes with imines catalyzed by Lewis bases, such as amines or phosphines, to give highly functionalized allylic amines. Two types of chiral bifunctional organocatalysts for enantioselective aza-MBH reaction of α,β -unsaturated carbonyl compounds with *N*-tosylimines, which possess Brønsted acid unit and Lewis base unit, have also been developed. The enantioselective reactions promoted by the chiral organocatalysts proved to be deeply influenced by the position of the Lewis base unit on the BINOL skeleton. Especially, in the (S)-3-(*N*-isopropyl-*N*-3-pyridinylaminomethyl)BINOL catalyzed aza-MBH reaction, the acid-base functionalities are required for not only the activation of the substrate but fixing the conformation of the organocatalyst.

Excited Radicals for Preparation of Nanomaterials

Radicals were one of the most important intermediates in the photochemistry and closely related with our familiar phenomena. The high reactivity of radicals was applied to the many industrial techniques. When radicals in the ground state are excited with photo irradiation within the lifetimes, those in the excited state are generated. Radicals in the excited state show specific emissions depending on the structure and the reactivity was different from those in the ground states. Therefore, studies on the radicals in the excited state were expected to give a new kind of photochemical reactions. In this year, we investigated the properties and reactivity of several short-lived radicals in the excited state using the nanosecond-picosecond two-color two-laser flash photolysis. The emissions from xanthone and azaxanthone ketyl radicals in the excited state were investigated. The anomalous emitting property of azaxanthone ketyl radical in the excited state was found for the first time. The investigation of reactivity benzophenone derivatives ketyl radicals in the excited state revealed that the excited ketyl radicals have high reducing power. The unique intermolecular electron transfer from benzophenone derivatives ketyl radicals in the excited state to the parent molecules was found for the first time.

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New Concepts for Immobilization of Asymmetric Catalysts (Invited), *H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

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Development of Effective Enzyme Mimics Utilizing Dendrimers (Poster), *D. Jayaprakash, R. N. Nadaf, H. Sasai, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30-Feb. 1, 2006.

Contribution to International Conferences

T. Majima, International Symposium on "Chemistry, Biological Chemistry, and Material Science towards Creating New Science and Industry based on Inter-Nanoscience" 2005 (CBMS2005) (Chairperson)

T. Majima, 2004 Korea-Japan Symposium on Frontier Photoscience “Photochemistry and Nanotechnology” (Chairperson)
 T. Majima, PACIFICHEM 2005 (Session organizer)

Publications in Domestic Meetings

Photochemistry Meeting	7 papers
Radiation Chemistry Meeting	11 papers
Advanced Radiation Chemistry Meeting	3 paper
Japan Photomedical Science and Photobiology	1 paper
85th Japan Chemical Society Meeting	26 papers
Surface Photochemistry Meeting	18 papers
4th Symposium on Reaction Control of Dynamic Complexes	1 paper
1st Symposium on Ionic Liquid	1 paper
Symposium on Organometallic Chemistry	2 papers
Symposium on Combinational Chemistry	1 paper
Congress of Heterocyclic Chemistry	2 papers
Symposium on Progress in Organic Reactions and Syntheses	1 paper
Symposium on Organic Synthesis	1 paper
The 1st Symposium on Creation of Biologically Functional Molecules	1 paper

Sponsorship

Grand-in-Aid for Scientific Research (S)

T. Majima Nanoscience of Photofunctionalized DNA
 ¥46,400,000

Grand-in-Aid for Scientific Research in Special Area (2)

T. Majima Fundamental Science and Technology of
 ¥10,600,000

	Photofunctional Interfaces	
H. Sasai	Development of Enantioselective Cascade Reaction	¥2,900,000
H. Sasai	Development of Artificial Enzyme with Synergistic Multicooperation in Active Sites	¥2,000,000
M. Endo	Fundamental Science and Technology of	
¥2,600,000	Photofunctional Interfaces	

Grand-in-Aid for Basic Scientific Research

T. Majima Formation of Carbon Nanotubes Arrays based on
 ¥2,400,000
 DNA Self-assembly

Grand-in-Aid for Encouragement of Young Scientists (B)

M. Endo Apoptosis and its Application to Cancer Therapy
 ¥800,000

Based on Photofunctional Biomolecules

Grant-in-Aid for JSPS Fellows

T. Majima	High Efficient Formation of Long-lifetime Charge Separated State in DNA and its Application to DNA Molecular Devices	¥900,000
T. Majima	Mechanism of Charge Separation and DNA Damage of TiO ₂ -DNA Nanoconjugates	¥1,100,000
T. Majima	Hydration of DNA Structure Studied by Dynamic Stokes Shift	¥1,100,000
H. Sasai	Development and Application of Novel Asymmetric Spiro Catalysts	¥1,500,000
H. Sasai	Polymer-Supported Artificial Enzyme with Dendritic Systems	¥800,000

Other Research Fund

H. Sasai	Yamada Science Foundation	Development of Enzyme-like Asymmetric Bifunctional Organocatalyst	¥2,000,000
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Human Interface Research for Safety and Security Project

Outlines

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, novel biosensors and software systems. In addition, we also investigate a new industrial prediction.

Achievements

- Identification of the exporters that mediates secretion of lipophilic signal transducing molecules.
- Generation of the gradation electron beam for the Intensity modulated radiation therapy.
- Virulence and drug resistance roles of xenobiotic transporters of *Salmonella enterica* serovar *Typhimurium*.
- Development of novel single-molecule measurement systems.
- Research of a nano structured biosensor chip.
- Research on the knowledge sharing technology for manufacturing support.
- Research on the strategic new industry prediction accompanying change of industrial structure.
- The adaptive interface by the sensor network and machine learning.

Medical Sciences Research Group

Professor: Akihito YAMAGUCHI, Yoichi YOSHIDA
Specially Appointed-
Research Associate: Tsuyoshi NISHI, Takafumi KONDOH, Ryouta IINO,
Kunihiko NISHINO
Specially Appointed-
Researcher: Shouichi SAKAKIHARA

Outlines

The main research objective of our group is understand 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.

We are also developing the new single molecular measurement system to analyze the cells and enzyme function and the electron beam control technology to realize the next generation intensity modulated radiation therapy for cancer therapy with a laser photo cathode RF gun LINAC.

Current Research Programs

Identification of the exporters that mediates secretion of lipophilic signal transducing molecules.

We develop a monoclonal antibody that recognized the ABCA5 proteins and found that ABCA5 is localized in vesicle like organelle localized near the apical membrane of the thyroid cells. This localization is similar to that of thyroglobulin that is essential for thyroid hormone biosynthesis. This result suggested the possible contribution of ABCA5 protein in thyroid hormone synthesis.

We are also trying to identify a sphingosine-1-phosphate exporter(s) from platelet. We success to show that sphingosine-1-phosphate is exported with specific transporter(s), is not mediated by exocytosis, from the platelet. Using the semi-intact platelet cells and specific inhibitors for known transporters, we proposed that ABC A-type transporters may participate the export of sphingosine-1-phosphate.

Generation of the gradation electron beam for the Intensity modulated radiation therapy

The Intensity modulated radiation therapy reduces dose to the scarfskin and the normal tissue, and that is remarkable as the effective therapy of cancer. In this research, the generation technology of the intensity modulated electron beam (gradation beam) was developed by the laser photo cathode RF gun LINAC at ISIR. The gradation beam was generated by processing of incident laser light to the photocathode. The gradation electron beam has the high spatial resolution for the medical application.

Virulence and drug resistance roles of xenobiotic transporters of *Salmonella enterica* serovar Typhimurium.

Xenobiotic transporters play a major role in resistance to a wide range of noxious compounds in several Gram-negative species. We investigated the drug resistance and

virulence phenotypes of *Salmonella* mutants defective in xenobiotic transport systems. We determined that nine potential xenobiotic transporters contribute to drug resistance of *Salmonella* and found that the *Salmonella*-specific MdsABC system conferred resistance to a variety of toxic compounds. The RND-type MdsAB system could function with either MdsC, which is encoded in the same operon, or TolC as the outer membrane component. Although the *Salmonella* EmrAB, MdfA, and MdtK are 90% identical in their amino acid sequences to their *Escherichia coli* homologues, the drug specificity of *Salmonella* transporters was different from that reported for equivalent *E. coli* transporters. Deletion of the *macAB* genes attenuated *Salmonella* virulence and a strain lacking all drug efflux systems was avirulent when mice were inoculated by the oral route. The promoter region of the *macAB* drug efflux system genes harbors a binding site for the response regulator PhoP, which functions to regulate *macAB* transcription. The PhoP/PhoQ two-component system is a major regulator of *Salmonella* virulence, which underscores the connection between drug efflux systems and virulence.

Development of Novel Single-Molecule Measurement Systems

Direct observation of rotation of F-type ATP synthase: To investigate the rotation mechanism of F-type ATP synthase driven by proton motive force, we have developed novel experimental system combining planar membrane method and single-molecule optical microscopy. At present, ATP-driven rotation of F-type ATP synthase reconstituted in planar membrane have been observed.

Single-Molecule observation by use of micro-heater: We have fabricated the micro-heater which can locally heat the sample plane of microscope and applied it to single-molecule observations. In the year 2005, heat-activation of F₁-ATPase and denature of single DNA molecule were directly observed under the microscope.

Publications

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Genome-Wide Analyses of *Escherichia coli* Gene Expression Responsive to the BaeSR Two-Component Regulatory System, K. Nishino, T. Honda and A. Yamaguchi: *J. Bacteriol.*, 187 (2005) 1763-1772.

Indole Induces The Expression Of Multidrug Exporter Genes in *Escherichia coli*, H. Hirakawa, Y. Inazumi, T. Masaki, T. Hirata and A. Yamaguchi: *Mol. Microbiol.*, 55 (2005) 1113-1126.

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Chemomechanical Coupling in Single-Molecule F-Type ATP Synthase, R. Iino, Y. Rondelez, M. Yoshida, and H. Noji : J. Bioeng. Biomem. 37, (2005) 451-453.

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Regulation of Xenobiotic Exporter Gene Expression and Multidrug Resistance in *Escherichia coli* (Poster), *H. Hirakawa, A. Kobayashi, T. Hirata and A. Yamaguchi, 4th 21st Century COE program "Towards Creating New Industries Based on Inter-Nanoscience" International symposium, Toba, Mie, Japan, November 18, 2005.

Regulation of Xenobiotic Exporter Gene Expressions by Environmental Response systems in *Escherichia coli* (Poster), H. Hirakawa, A. Kobayashi, T. Kodama, T. Hirata and *A. Yamaguchi, Gordon Research Conference on Multi-Drug Efflux Systems, Magdalen college, Oxford, UK, Augst 28 - September 2, 2005.

Bacterial Xenobiotic Exporter World: From Molecular Structure to Physiological Implications (Invited), *A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Identification of the Residues Involved in Substrate Recognition in RND-Type Multidrug Efflux Transporter (Poster), *N. Kobayashi, N. Tamura, S. Murakami and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

Molecular Design of the Super Carbenicillin Resistance AcrB (Poster), *A. Iwata, N. Kobayashi, N. Tamura, Y. Ohkawa, F. Ishibashi, S. Murakami and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

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Fur (Ferric Uptake Regulator) Controls the Expression of AcrD and MdtABC, Multidrug Efflux Transporters in *Escherichia coli* (Poster), *T. Masaki, H. Hirakawa, T. Hirata and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, August 8-10, 2005.

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2005.

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Characterization of ABCA5 Protein with Its Specific Monoclonal Antibody and Knockout Mice (Poster), *M. Ohigashi, C. Takenaka, T. Nishi and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji, Aug. 9, 2005

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Localization of Novel RND-Type Proteins in Culture Cells and Mice Tissues (Poster), *S. Hashimoto, Y. Kubo, T. Nishi, T. Hirata and A. Yamaguchi, International Symposium on Biological Membrane Transport 2005, Awaji, Aug. 9, 2005

Analysis of the Mechanism of Proton Translocation through the Integral Vo Domain of the Vacuolar (H⁺)-ATPases (Poster), S. Kawasaki-Nishi, *T. Nishi and A. Yamaguchi, 4th 21st Century COE “Towards Creating New Industrial Based on Inter-Nanoscience” International Symposium, Toba Hotel international, Mie, Japan, Nov. 18, 2005

Development of Femtosecond and Atto-Second Pulse Radiolysis by Using Laser Photocathode RF Gun S-Band Electron Linac (Poster), *Y. Yoshida, J. Yang, and T. Kondo, The 2005 Particle Accelerator Conference, Knoxville, Tennessee, USA, May 16-20, 2005

An Advantage of the Equivalent Velocity Spectroscopy for Femto Second Pulse Radiolysis (Poster), *T. Kondoh, J. Yang, T. Kozawa, S. Tagawa, H. Tomosada, and Y. Yoshida, The 2005 Particle Accelerator Conference, Knoxville, Tennessee, USA, May 16-20, 2005

Generation of a Gradation Electron Beam Pulse by a Photo Cathode RF Gun LINAC for Single Shot Pulse Radiolysis Measurement (Poster), *T. Kondoh, J. Yang, K. Kan, Y. Kuroda, S. Takemoto, A. Asano, A. Yoshida, T. Yamamoto, T. Kozawa, Y. Yoshida, and S. Tagawa, 4th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Toba, Mie, Japan, November 18-19, 2005

Femto-Second Bunch Length Measurement Using Spectral Broadening of Undulator Radiation (Poster), *T. Kondoh, J. Yang, A. Yoshida, Y. Yoshida and a. Ogata, 4th 21st

Century COE “Towards Creating New Industries Based on Inter-Nanoscience”
International Symposium, Toba, Mie, Japan, November 18-19, 2005

Femtosecond Pulse Radiolysis Study on Primary Process of Radiation Chemistry of Polymer(Oral), *Y. Yoshida, J. Yang, T. Kondoh, A. Yoshida, T. Kozawa, and S. Tagawa, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005

Selective Polymerization of 5,7-Dodecadiyne-1,12-Diol Bis[Phenylcarbamate](TCDU) Crystals and Concentration of the B-Phase Chain in TCDU-1 Crystals Using the Electron Beam Excitation (Poster), *T. Kondoh, C. Itoh, J. Yang, Y. Yoshida, and K. Tanimura, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 15-20, 2005

Generation of 98-FemtoSecond Single Electron Bunch in Photocathode Linear Accelerator (Oral), *Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006

Generation of a Gradation Electron Beam Pulse Toward the Intensity Modified Radiation Therapy (IMRT) (Poster), *T. Kondoh, J. Yang, A. Yoshida, T. Yamamoto, Y. Yoshida and S. Tagawa, SANKEN International Symposium 2006 (SIS-2006) on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006

Chemo-Mechanical Coupling in F-Type ATP Synthase (Invited). *R. Iino. FASEB summer research conferences. Transport ATPases: Genomics, Mechanisms, and Relevance to Diseases. Saxtons River, Vermont, USA. July 16-21, 2005.

Imaging of Heat Denature of Single DNA Molecules in Femtoliter Chambers on a Micro Heating Device: Toward a Single-Molecule Detection of PCR (Poster), *K. Ishizuka, H. Arata, S. Sakakihara, C. Bergaud, K. V. Tabata, Y. Rondelez, S. Takeuchi, H. Fujita, H. Noji, μ TAS 2005, Boston, USA, Oct. 9-13, 2005.

Avoidance of Fe(III) Toxicity Mediated by the PmrA/B Two-Component Regulatory System in *Salmonella enterica* (Poster), *K. Nishino and E. A. Groisman, American Society for Microbiology 105th General Meeting, Atlanta, GA, USA., Jun. 5-9, 2005.

Modification of the Cell Membrane and Avoidance of Metal Toxicity (Invited), K. Nishino, Washington University School of Medicine, Molecular Microbiology & Microbial Pathogenesis Program 2005 at Rend Lake Conference Center, Whittington, IL, USA., Oct. 1, 2005.

How Bacteria Resist Killing by Fe(III) and Al(III) (Invited). K. Nishino, The 8th Japan-Korea International Symposium on Microbiology, Kanazawa, Japan, Mar. 29.

Contributions to International Conferences and Journals

A. Yamaguchi International Symposium on Biological Membrane Transport 2005
(Area Editor)

Publications in Domestic Meetings

The Japanese Biochemical Society:	10 papers
The Molecular Biology Society of Japan:	6 papers
Symposium of Biomembrane-Drug Interaction	3 papers
Biophysical Society of Japan	5 papers
The Institute of Electrical Engineers of Japan	1 paper
Japanese Society for Bacteriology	4 papers
The Pharmaceutical Society of Japan	4 papers
Japan Society for Bioscience, Biotechnology, and Agrochemistry	1 paper
The 8 th Japan-Korea International Symposium on Microbiology	1 paper
21st Century COE nano-baio group symposium	5 papers
31 th Japanese Bioenergetics Group	4 papers
Sakigake Live 2004	1 paper
2 nd 21st Century research conference on <i>Escherichia coli</i>	1 paper
Atomic Energy Society of Japan:	4 papers
Japanese Society of Radiation Chemistry:	7 papers
Particle Accelerator Society of Japan:	3 papers
RF gun meeting:	2 papers
Symposium on Advanced Radiation Chemistry:	1 paper

Sponsorship

Grant-in-Aid for Scientific Research on Priority Area (B)

A. Yamaguchi Studies on the Nano-structure and Transport Mechanism of Antiport-type Efflux Transporter for Organic Compounds. ¥28,500,000

Grant-in-Aid for Scientific Research (S)

A. Yamaguchi Post-genome Analysis of Bacterial Xenobiotic Exporter and Studies on the Novel Resistance Mechanism. ¥15,200,000

Grant-in-Aid for Scientific Research (A)

Y. Yoshida Basic Research on Subfemtosecond and Attosecond Pulse Radiolysis ¥5,900,000

Entrusted Research

A. Yamaguchi	Japan Science and Technology Corporation. (CREST)	Investigation of the Structure and Function for Xenobiotics Transporters and Clarification of Multidrug Resistance Mechanism	¥10,400,000
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T. Nishi	Japan Science and Technology Corporation. (PRESTO)	Analysis of Cellular Networks Organized with the Tissue Specific Isoforms	¥650,000
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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	The University of Tokyo	Development of the high brightness and high-speed response metal oxide electron beam monitor.	
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.	

Other Research Fund

A. Yamaguchi	Japan Science and Technology Corporation. (CREST)	Investigation of the Structure and Function for Xenobiotics Transporters and Clarification of Multidrug Resistance Mechanism	¥38,416,000
T. Nishi	Japan Science and Technology Corporation. (PRESTO)	Analysis of Cellular Networks Organized with the Tissue Specific Isoforms	¥6,350,000

Human Interface Research for Safety and Security Project

Human Interface Research Group

Professor: Hitoshi TABATA, Masayuki NUMAO, Hiroshi YOSHIDA,
Riichiro MIZOGUCHI

Specially Appointment Staff

Professor: Sunao TAKAFUJI

Associate Professor: Takashi Kei SAITO

Research Associate: Makoto NAKAZAWA, Yasushi MAKIHARA,
Ken-ichi FUKUI, Munetoshi SEKI

Outlines

Materials Science & Technology Research Center for Industrial Creation, MSTeC is the newly established cooperative organization with ISIR and the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University from 2005. Our research interests are building novel biosensors and software systems, which enable analyzing genotype, phenotype, and social information. Furthermore, we also perform econometrical researches on a new industrial prediction and strategically intellectual property accompanying from the information about industrial structure transitions. We will integrate those research efforts to establish a human-oriented future type an interface network system as novel human interfaces.

Current Research Programs

Research of a nano structured biosensor chip (Tabata, Saito, Seki)

1) As a prototype of the large-scale integrated cell fusion device by nano self-organization material, we prepared the substrate of zinc oxide nano rods which modified with the photosensitizer and successfully performed large scale cell-membrane penetration to neural cell line PC12 colonies.

2) We acquired an external fund (the local new consortium, Ministry of Economy, Trade and Industry) with CLUSTER TECHNOLOGY CO., LTD., based on the collaborative efforts.

3) A practical robot as a substantial human interface, which can perform test and demonstration of our research efforts was developed. We demonstrated by International Robot Exhibition etc., and are performing some joint development with a company and local government.

Research on the knowledge sharing technology for manufacturing support (Mizoguchi, Takafuji)

1) The prototype software of the representation tool of knowledge which united the xfy technology of JUSTSYSTEMS Corp. (next generation core technology of XML) and ontology engineering was established. The software was also incorporated the newest result of the ontology engineering

2) In order to support an engineer's representation of the knowledge, the framework software for building a functional concept efficiently using natural-language-processing

technology was established.

Research on the strategic new industry prediction accompanying change of industrial structure (Yoshida, Nakazawa)

1) We focused the relationship of a gross assets and the growth rate of a company as an index of industrial analysis and found that a growth rate did not depend on the gross assets of a degree in the previous year. The effort shows the start of novel quantitative analysis of Japanese economy.

2) A model of two dimensional classification tools for the technology analysis from the keywords which appeared in patents and papers, with multidimensional scaling method etc was developed. It enables prediction of new industry generating fields as a synchronized position of industrial needs and seeds.

The adaptive interface by the sensor network and machine learning (Numao, Fukui, Makihara)

1) Based on the mobile object information acquired from fixed Web cameras in rooms, the algorithm which extracts automatically main courses and points in a life space was proposed, and the validity was checked.

2) In the infrared sensor network, sensor contiguity relations were automatically gained using the relation before and after sensor ignition, and the validity to the person pursuit under two or more person activity was verified.

3) Although the personal authentication technology using individual gait was mostly restricted in the observation direction of the side, we extended the direction conversion model, and succeeded in attestation by the walk of various directions.

Publications

Original Papers

High-temperature Cluster Glass State and Photomagnetism in Zn- and Ti-substituted NiFe_2O_4 Films, M. Seki, A.K.M. Akther Hossain, T. Kawai and H. Tabata : J. Appl. Phys., 97 (2005) 083541(6pages)

Photocontrol of Magnetization in Al-substituted Fe_3O_4 Thin Films, M. Seki, Akther A.K.M. Hossain, H. Tabata, T. Kawai : Solid State Commun., 133 (2005) 791-796.

Visualizing Dynamics of Hot Topics Using Sequence-Based Self-Organizing Maps, K. Fukui, K. Saito, M. Kimura, M. Numao, Lecture Notes in Artificial Intelligence, 3684 (2005) 745-751.

Predicting High-level Student Responses Using Conceptual Clustering, R. Legaspi, R.Sison, K. Fukui, M. Numao, Frontiers in Artificial Intelligence and Applications, 133, IOS Press, (2005) 761-764.

International Conferences

High Temperature Photoinduced Magnetization in Spinel and Garnet Ferrite Thin Films,
*M. Seki, K. Tsuruta, T. Kawai, and H. Tabata, The 8th International Symposium on
Sputtering & Plasma Processes (ISSP 2005), Kanazawa, Japan, Jun. 8-10, 2005

Photocontrol of Cluster-glass States in Spinel and Garnet Ferrite Thin Films (Poster),
*M. Seki, K. Tsuruta, H. Tabata, T. Kawai, The 12th International Workshop on Oxide
Electronics(WOE12), Chatham, USA, Oct. 2-5, 2005

Photo-control of Magnetization at Room Temperature in Spinel Ferrite Thin Films, *M.
Seki, K. Tsuruta, and H. Tabata, International Symposium on Hybrid Nano Material
Toward Future Industries (HNM 2006), Nagaoka, Japan, Feb. 3-5, 2006
Semantic Document Processing with xfy Technology, S. Takafuji, Workshop on the
Semantic Computing Initiative(SeC2005), WWW2005, Chiba, Japan. May 10-14, 2005.

Functional metadata schema for engineering knowledge management, S. Takafuji,
Workshop notes of Activities on Semantic Web Technologies in Japan (WS11),
WWW2005, Chiba, Japan. May 10-14, 2005.

Matching Gait Image Sequences in the Frequency Domain for Tracking People at a
Distance R. Sagawa, Y. Makiyama, T. Echigo, Y. Yagi, In Proc. 7th Asian Conf. on
Computer Vision, 2, 141-150, Hyderabad, India, Jan. 13-16, 2006.

Agent-Based Human-Environment Interaction Framework for Ubiquitous Environment,
S. Kurihara, S. Aoyagi, T. Takada, T. Hirotsu, T. Sugawara, M. Numao, Proceedings of
2nd International Workshop on Networked Sensing Systems (INSS2005), San Diego,
California, USA, Jun. 27-28, 2005.

A Cluster-based Predictive Modeling to Improve Pedagogic Reasoning, R. Legaspi, R.
Sison, K. Fukui, M. Numao, Proc. IADIS International Conference on Cognition and
Exploratory Learning in Digital Age, Porto, Portugal. Dec. 14-16, 2005.

Publications in Domestic Meetings

Information Processing Society of Japan	1 paper
Special Interest Group of Intelligence and Complex Systems	2 papers
The Japan Society of Applied Physics	2 papers
The Physical Society of Japan	1 paper
The Society of Materials Science, Japan	1 paper

Other Research Fund

T. K. Saito	Toyama Prefectural government, Japan	Snowplow Robot (collaborative project)	¥2,000,000
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Activities of Facilities

Workshop

Director Professor: Tetsuro MAJIMA

Technical Staff

Machine Shop: Michiaki KAKUICHI, Masayoshi OHNISHI

Glassworks: Hiroaki MATSUKAWA, Noriyuki OGAWA

Outlines

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, 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.

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, and held a practice course of carved seals. The 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 and held a practice course using an additional budget allowed for the Workshop.

We renewed a cutting machine of the Machine Shop and a drying machine of the Glassworks on the budget of the Work Shop in the fiscal year 2005. We also equipped the Machine Shop with peripheral devices and tools for the machining center for precise machining.

The Glassworks receives staff members of universities in the Kansai area for

technical training in glass work and in 2005 it received a person from Kobe University and coached him for handing skills and technique down to the next generation.

1. Number of jobs

Machine Shop: 148 jobs (150 jobs in the previous year).

Glassworks: 216 jobs (155 jobs).

2. Number of users in the open shop

Machine Shop: 50 users (60 users in the previous year).

Glassworks: 50 users (50 users).

3. Number of visitors during Icho-Sai

Machine Shop: 40 persons (35 persons in the practice course).

Glassworks: 70 persons (70 persons).

4. Number of persons being trained

Machine Shop: 5 persons.

Glassworks: 7 persons for 17 subjects, including 17 subjects out of the institute.

Office of Information Network

Professor: Akihito YAMAGUCHI

Outlines

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: Katsuyuki TANIZAWA

Outlines

This laboratory is specially designed for biochemical and molecular biological experiments using radioactive compounds labeled with ^3H , ^{14}C , ^{32}P , ^{35}S . The main equipments are liquid scintillation counters and an image scanner. This laboratory is essential for the research in the field of biochemistry, molecular biology, and cell biology. Contributions of the facilities to each project 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: Yoshio ASO
Staff: Taiko FURUTA

Outlines

The ISIR Library houses only 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 and magazines, 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 April 1, 2006)

	Number of books	Journals	Newspapers
Japanese	12,498	293 titles	4 titles
Foreign	44,521	974 titles	1 title

Academia Industry Relations Office

Professor: Mototaka SENDA
Professor: Hirokazu SHIMIZU

Outlines

The Academia Industry Relations Office (AIR Office) was opened on October 1, 2005 at the Institute of Scientific and Industrial Relations (ISIR), Osaka University. AIR Office is part of ISIR and its role is to coordinate research activities of the institute via a multi-directional networking procedure. This important mission of the Japanese University to our society is clearly stated in the policy of 2nd and 3rd period Science and Technology Roadmap by the Science and Education Administration of the Japanese Government. A goal of AIR Office is to build up a seamless relationship between academia and industry. 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 complimentary 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.

[http:// www.sanken.osaka-u.ac.jp/labs/air/](http://www.sanken.osaka-u.ac.jp/labs/air/)

Lecture Series

Promotion to communicate with a foreign culture on Science and Technology

Three speakers were invited from Silicon Valley, California, consisting Dr. Patricia Malin (Founder & CEO, Cellstat, Inc.), Dr. Benjamin Borson (Patent Lawyer, LLP) and Dr. Nobi Kambe (Founder & CTO, NanoGram, Inc.). Dr. Malin lectured about US venture business to global biotechnology industry from her experience of her own entity, CellStat, Inc. Dr. Borson from Flisler & Meyer LLP lectured about intellectual property and law compliance in the USA by the scope of academia and industry research. Dr. Kambe stated current nanotechnology venture business in Silicon Valley from his own business (NanoGram, Inc.) experience.

Public Relations Office

Professor, Director: Tetsuro Majima

Administrative Associate: 1 officer

Outlines

Public Relations Office works for the following matters at ISIR. We provide the right information of our Research Institute for the public effectively.

- (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 page 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: Hitoshi YAMADA

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 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.

Publications in Domestic Meetings

The 53rd Annual Conference on Mass Spectrometry, Saitama, Japan, 2005	1paper
Symposium on Technology and Engineering in Instruments and Analysis Technique, Iwate, Japan, 2005	1paper
Japanese Society of Radiation Safety Management	1paper