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Title	MEMOIRS of the Institute of Scientific and Industrial Research, Osaka University Volume 64
Author(s)	
Citation	MEMOIRS of the Institute of Scientific and Industrial Research, Osaka University. 2007, 64, p. 1-436
Version Type	VoR
URL	https://hdl.handle.net/11094/77444
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The University of Osaka

ISSN 0369-0369

VOLUME 64,2007

MEMOIRS OF THE

Institute of Scientific and Industrial Research

OSAKA UNIVERSITY

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Foreword

For the development of "Honorable Science" and "Advantageous Technology"

Tomoji Kawai
Director, The Institute of Scientific and Industrial Research

The Institute of Scientific and Industrial Research (ISIR), Osaka University was founded in 1939, 68 years ago, with only 3 departments by the financial support from Industries of Kansai area to promote basic science for the development of industry. From then, ISIR has emphasized basic and applied researches to promote the multidisciplinary science for ultimate contribution to the industries in 3 main research areas, i.e., material science, information science, and bio-sciences. At present, we have 7 divisions including 28 departments and 3 research Centers, "Nanoscience and Nanotechnology Center" , "Materials Analysis Center" and "Materials Science & Technology Research Center for Industrial Creation". “Nanoscience and Nanotechnology Center” is focusing the researches on advanced materials and devices, beam-science for nanotechnology which is key technology now and future and then it’s one of the leading research organizations in Japan.

ISIR has also close contact with several faculties of Osaka University such as Faculties of Science, Engineering, Engineering Science, Pharmaceutical Science, Information Science and Technology, Frontier Biosciences, and supervises their graduate students. From 2002 through 2006, the Institute was selected as the 21st Century COE in the fields of new and interdisciplinary area.

This publication "Memoirs of the Institute of Scientific and Industrial Research (ISIR)" is our annual publication summarizing the scientific activities of ISIR. We have particulate plan for the future, and our challenges are never ending. We hope this annual publication will be useful and stimulating for all researchers and young scientists outside as well as inside our Institute.

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

Outline of ISIR

1. Research Activities

1) History and Organization

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

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

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

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

In 2002, Nanoscience and Nanotechnology Center has started with restructuring Research Center for Intermaterials and Radiation Laboratory. The new Center focuses its researches on nanomaterials and devices, beam science for nanotechnology and industrial nanotechnology. In 2006, Materials Science & Technology Research Center for Industrial Creation has started and at present, ISIR has 7 divisions including 28 departments and 3 research Centers, "Nanoscience and Nanotechnology Center" , "Materials Analysis Center" and "Materials Science & Technology Research Center for Industrial Creation". In April 2006, Academia Industry Relation Office (AIR-Office) has been settled in order to strengthen cooperation between the Institute and Industries.

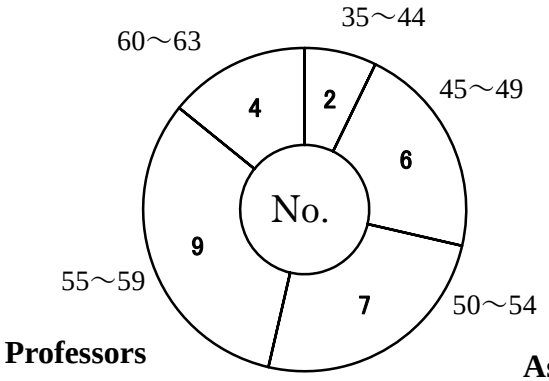
Divisions	Departments
Quantum Engineering	Quantum Molecular Devices Photonic and Electronic Materials Semiconductor Electronics Condensed Matter Physics
Advanced Materials Science & Technology	Structural Characterization and Design Metallic Materials Process Atomic Scale Science Functional Ceramic Materials 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)

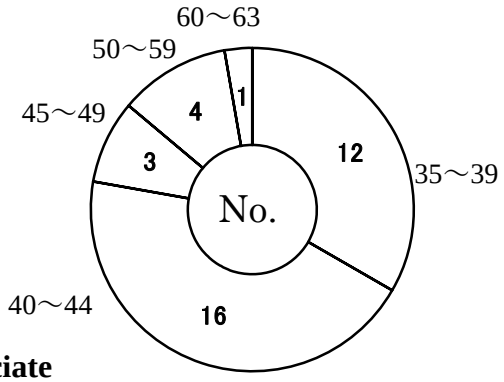
Nanoscience and Nanotechnology Center	**Nanomaterials and Nanodevices** Artificial Nanomaterials for Bio-Information Systems Single-Molecular Integrated Devices Supramolecular Chemistry Nanobiology Nanosystem Design

	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 Research Center for Industrial Creation	**Materials Research Project** 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**

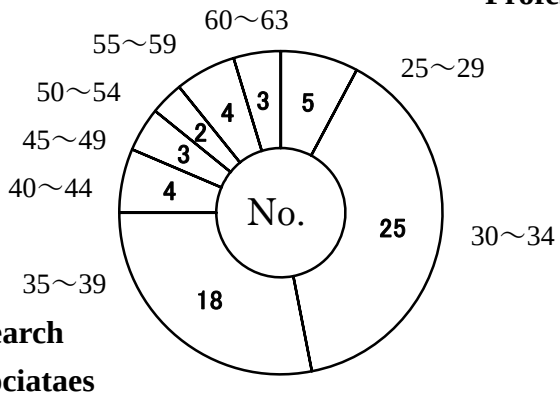
Staffs' Age (years old) –As of 3.31.2007



Professors

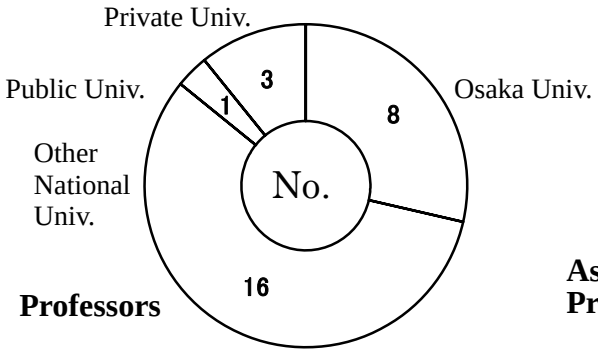


Associate Professors

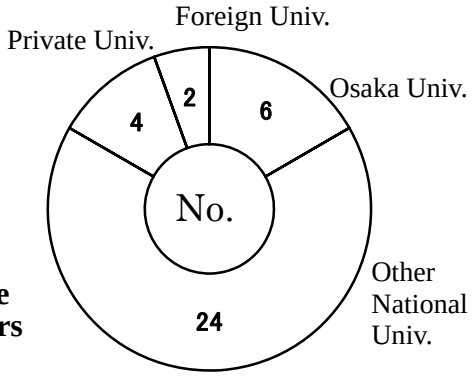


Research Associataes

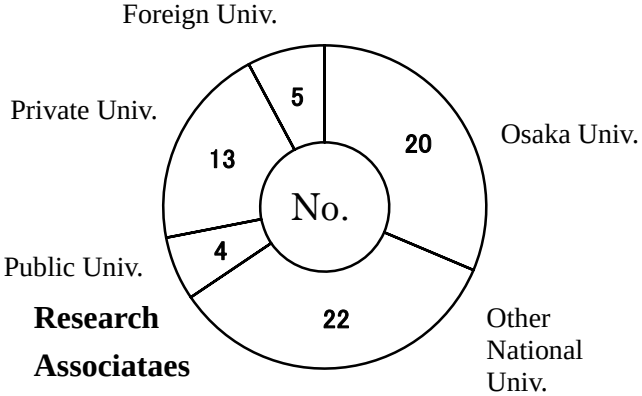
Staffs' Alma Mater –As of 3.30.2007



Professors



Associate Professors



Research Associataes

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, 2007 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 stet 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.

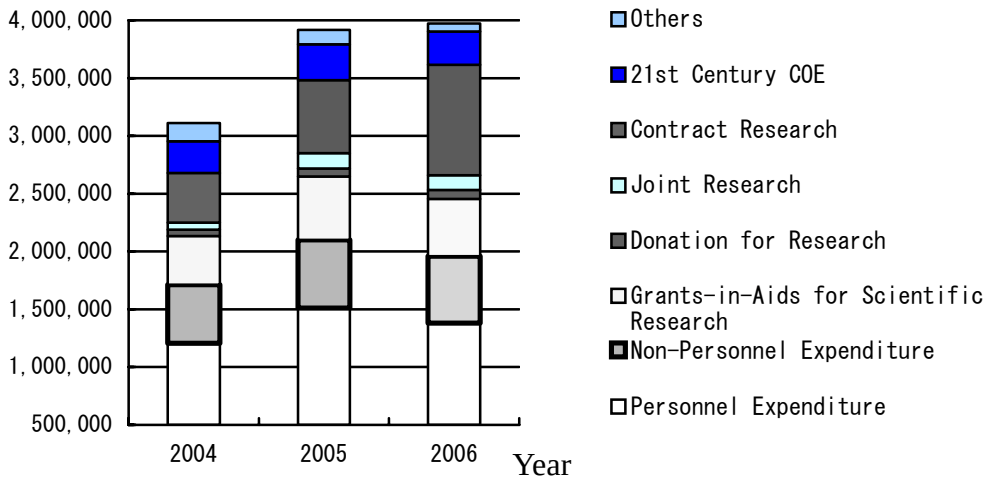
In 2002, the following project has been selected as a 21st Century Center of Excellence (COE) program from the Ministry of Education, Culture, Sports, Science and Technology.

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 2006 is 497,540,000 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
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)
2006	4,500 (3)	13,141 (17)	16,400 (13)	10,100 (8)

Division / Year	Biological Science	Quantum Beam Science and Technology	Nanoscience and Nanotechnology center	Others	Total
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)
2006	9,250 (7)	0 (0)	10,700 (9)	13,300 (5)	77,391 (62)

4) Cooperative Research

Cooperative Researches and Contract Researches in the fiscal year 2006-2007 are as follows: Cooperative Researches are carried out with 57 organizations. The budget for the fiscal year 2006-2007 is 127,556,000 yen. Contract Researches are 63. The budget for the fiscal year 2006-2007 is 957,672,000 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)
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

- The workshop on porous materials (No. 1/'06-'07) (Aug 31, 2006)
- The 14th JSPS-KOSEF Core University Program(CUP) Seminar – New Nanostructured and Nanocomposite Materials with Multiple Functionality (Oct 18-20,2006)
- 16th Microelectronics Symposium (MES2006), Osaka, 2006 (Oct 26-27)
- Joint meeting between ISIR SANKEN, Osaka University and the Forschungszentrum Juelich (Oct 30, 2006)
- 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 2006, the Symposium was held on November 24. The topics were "Advanced Industrial Science and International Relationship".

- Fifth International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” (Dec 8-9,2006)

- The 15th JSPS-KOSEF Core University Program(CUP) Seminar in conjunction with The 8th International Symposium on Eco-Materials Processing and Design(ISEPD2007) (Jan 11-13,2007)

- Second SANKEN-Chungnam National University, Korea(CNU) Joint Symposium on Nanoscience and Nanotechnology (Jan 25-26,2007)

- Seminar on Soft Material Research Group(G2) of Materials Science & Technology Research Center of Industrial Creation(MSTec) (Jan 28,2007)

- Symposium on 2006 Research Progress on Materials Science & Technology Reseach Center for Industrial Creation(MSTec) in SANKEN (Jan 31,2007)

- The workshop on porous materials (No.2/’06-’07) (Feb 8,2007)

- 21st Century COE Korea Workshop (Feb 25,2007, Dongguk University)

- Symposium on 2006 Reseach Progress on Materials Science & Technology Research Center for Industrial Creation(MSTec), Coodinated Reseach Center between SANKEN and Institute of Multidisciplinary Reseach for Advanced Materials, Tohoku University (TAGENKEN) in Gakushi-kaikan (Mar 2,2007)

- The workshop on porous materials (No.3/’06-’07) (Mar 22,2007)

Other Lectures and Seminars

14 Apr 2006	Hermenegildo Garcia (University Politechnica of Valencia,Professor)	Photocatalytic Activity of Structured Mesoporous Ti02 Materials
17 Apr 2006	Heitz D. Roth (Rutger University, Professor)	Generation and Reactions of Organic Radical Cations in Zeolites
15 May 2006	Ayyappanpillai Ajayaghosh (Regional Research Laboratory, Travandrum, India, Professor)	Soft Organic Materilals with Sol-Gel Tunable Optical Properties
17 May 2006	Tarun Kumar Sharma (Raja Ramanna Center for Advanced Technology, India,Scientific Officer)	Physics and Applications of MOVPE grown Nanostructures
31 May 2006	Joji Oshita (Hiroshima University, Professor)	Simple Synthesis of Orfanic Halosilanes and Alkozysianes
2 Jun 2006	Joji Oshita (Hiroshima University, Professor)	Property Control of Oligothiophenes by Silicon Substitution and its Application to EL and FET Materials
12 Jun 2006	Tamas Horvath (University of Bonn and Fraunhofer Institute AIS,Germany, Professor)	Frequent Subfraph Mining in Outerplanar Graphs
19 Jun 2006	Gyorgy Turan (University Illinois at Chicago, USA, Professor)	Nearest neighbor representations for Boolean functions
19 Jun 2006	Yutaka Kano (Osaka University, Professor)	How statisticians think of casual inference
13 Jul 2006	Michael E. Houle (National Institute for Informatics, Tokyo, Visiting Professor)	A Generic Query-Based Model for Scalable Clustering
14 Jul 2006	Dae Won Cho (Chosun University,Korea, Professor)	Intramolecular Exciplex and Intermolcular Excimer Formation of 1,8-Naphthalimide-linker-Phenoth--iazine
18 Jul 2006	Sing Bing Kang (Microsoft Corporation, Senior Researcher)	Animating Chinese Paintings through Stroke-Based Decomposition

17 Aug 2006	Yu Qiang (Yokohama National University, Associate Professor)	Reliability Estimation for Micro Joints in Electronics Devices Using Computer Aided Engineering (CAE)
18 Aug 2006	Hou Xue-Long (Shanghai Institute of Organic Chemistry, Professor)	Towards Control of Selectivities in Asymmetric Catalysis
24 Aug 2006	Fumitoshi Kakiuchi (Keio University, Professor)	A New Stream of Organic Synthesis – Transition Metal-catalyzed Functionalization of C-H Bonds
24 Aug 2006	Hou Xue-Long (Shanghai Institute of Organic Chemistry, Professor)	Transformations of Imines and Aziridines
28 Aug 2006	J. Herfort (Paul-Drude-Institut, Germany, Scientific Researcher)	Epitaxial Heusler alloys on GaAs substrates
28 Aug 2006	Saso Dzeroski (Jozef Stefan Institute, Slovenia, Professor)	Inductive Queries on Global Models
6 Sep 2006	David C.Dunand (Northwestern University, Professor)	Processing and Properties of Advanced Metallic Foams
7 Sep 2006	Tapan Ganguly (Indian Association for the Cultivation of Science, Professor)	Attempts for the productions of longer-lived charge separated species within model donor-acceptor systems. Compounds of Artificial Photosynthesis and Solar Energy Conversion
22 Sep 2006	Fumitoshi Kakiuchi (Keio University, Professor)	A New Method for the Formation of C-C Cond via C-H Bond Cleavage
28 Sep 2006	Lian Gao (Shanghai Institute of Ceramics,Chinese Academy of Science, Shanghai, China, Professor)	Preparation and Properities of Carbon Nanotube Ceramic Composites
17 Oct 2006	Masahiko Yamamoto (Osaka University, Professor)	Magnetic memory, magnetic logic operation and new measurement method for magnetization state of small magnet
25 Oct 2006	Steven Kraines (The University of Tokyo, Associate Professor)	A Web-based platform for scientific knowledge sharing, discovery, and integration

31 Oct 2006	Hideki Matsui (Institute for Materials Research, Professor)	Study on Materials for Nuclear Fusion Furnace
11 Nov 2006	Dieter Enders (RWTH Aachen University, Professor)	Biomimetic Asymmetric Organocatalysis
13 Nov 2006	Peter K ündig (University of Geneva, Professor)	Advanced in Transition Metal Lewis Acid-Mediated and – Catalyzed Reactions
13 Nov 2006	Takashi Onoda (Central Research Institute of Electric Power Industry, Tokyo, Senior Researcher)	Foundations and Applications of Support Vector Machines
11 Nov 2006	Matej Vesenjak (University of Maribor)	Computational modeling of cellular structures accounting for fluid fillers
22 Nov 2006	Tsuyoshi Kawagoe (Osaka Kyoiku University,Associate Professor)	Magnetic Imaging of 3d-Transition Metal Thin Film by Spin-Polarized STM/STS
29 Nov 2006	Josef Pola (Institute of Chemical Process Fundamentals(ICPF),Prague)	CW CO_2 laser-induced formation of nano-sized iron particles
7 Dec 2006	Laren Malcolm Tolbert (Georgia Institute of Technology, Professor)	Molecular Lithography
11 Dec 2006	Bo-Young,Hur (Gyeongsang National University,Professor)	Rheolgical characteristics of Molten Metal for Casting Design
25 Dec 2006	Joji Oshita (Hiroshima University, Professor)	Preparation of Silene from Novel Acylpolysilanes
27 Dec 2006	Joji Oshita (Hiroshima University, Professor)	Substituent Effects of Silicone Substituenet on π-Electronic Systems and its Application to Functionallized Materials
5 Jan 2007	Dae Won Cho (Chosun University, Korea, Professor)	Photoinduced Electron Transfer Processes in 1,8-Naphthalimide-linker-Phenothiazine Dyads
22 Jan 2007	Sumio Kozawa (New Energy and Industrial Technology Development Organization)	Materials Technology and Its Application
24 Jan 2007	Koiwa Masahiro (Kyoto University, Professor)	Step in the Progress of Difusion Study
24 Jan 2007	Wayne P. Hess (Pacific Northwest National Laboratory, Associate Director)	Functional Oxide Surfaces: structures and reactivity

13 Feb 2007	Seung Joo LEE (Dongguk University, Korea, Professor)	Diluted Magnetic Semiconductors
13 Feb 2007	Michael E. Houle (National Institute for Information, Tokyo, Visiting Professor)	SASH: Fast Approximate Similarity Search in Extremely High-Dimensional Date Sets
26 Feb 2007	Albert S. C. Chan (The Hong Kong Polytechnic University, Professor)	Catalytic Asymmetric C-C bond Formation
28 Feb 2007	Makoto Snagawa (Teikyo-Heisei University, Professor)	Research on the Drug Development Ⅰ
3 Mar 2007	Zoran Ren (University of Maribor, Professor)	Computational and Experimental Verification of Roadside Safety Barrier in Europe
6 Mar 2007	Yoshiyuki Nakata (Iwaki Meisei University, Professor)	Transmission electron microscopy obserbations of Sb-Te alloys
19 Mar 2007	J.Kumar (Anna University, India, Professor)	Semiconductor Nanostructures
19 Mar 2007	Makoto Snagawa (Teikyo-Heisei University, Professor)	Research on the Drug Development Ⅱ
22 Mar 2007	Kaori Ando (University of the Ryukyus, Professor)	Application of Theoretical Calculation to Organid Synthesis

7) Public Information Activity

Public information activity of ISIR in 2006 is as follows:

- Bulletin of ISIR (2006 (in both Japanese and English)
- Memoirs of the Institute of Scientific and Industrial Research, Osaka University (Vol.62 2006 (in English)
- Annual Report of ISIR (2006 (in Japanese)
- SANKEN News Letters, 28-30(in Japanese)
- Report on SANKEN TECHNO SALON (2006 (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 2006 is 463. The details are described in the part of activity of divisions and facilities.

9) Scientific Awards

Y.K..ZHOU	Best Paper Award （IUMRS-ICA-2006）
Y.HIROTSU	Metallography Award (The Japan Institute of Metals)
M.ISHIMARU	Metallography Award (The Japan Institute of Metals)
M.NAITO	Metallography Award (The Japan Institute of Metals)
M.ISHIMARU	Honda Memorial Young Scientist Award (Honda Memorial Foundation)
A.HIRATA	Best Poster Young Researcher Presentation Award (5th International Conference on Bulk Metallic Grasses)
M.TANE	Young Scientist Award (The Japan Institute of Metals)
Dept. of Frontier Materials Creation	Poster Award, The 2nd Asia-Oceania Ceramic Federation (AOCF) Conference
Dept. of Frontier Materials Creation	Best Presentation Award, The 8th International Symposium on Eco-Materials Processing and Design
Y.HAYASHI	ICCE2006 Best paper award (The 14th International Conference on Computers in Education)
R.MIZOGUCHI	ICCE2006 Best paper award (The 14th International Conference on Computers in Education)
S.ISOTANI	ICCE2006 Best student paper award (The 14th International Conference on Computers in Education)
R.MIZOGUCHI	ICCE2006 Best student paper award (The 14th International Conference on Computers in Education)
S.ISOTANI	Second Place Award of the ACM Student Research Competition at SIGCSE (the Association for Computing Machinery)
Y.YAGI	Distinguished Poster (5th International Conference on Capsule Endoscopy)
Y.YAGI	Finalist for T.J.Tarn Best Paper in Robotics (IEEE International Conference on Robotics and Biomimetics)
S.SEKI	Hitachi-Kasei Award (The Society of Polymer Science, Japan)

S.TUKUDA Poster Award
(Japanese Society of Radiation Chemistry)
H.YAMAMOTO Poster Award
(Microprocess and Nanotechnology Conference 2006)

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, 2007 is as follows.

G.S. / Course	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Course	35	53	14	5	13	8	128
Doctor Course	19	45	8	4	8	0	84
Total	54	98	22	9	21	8	212

Number of students who had obtained Master's or Doctor's Degree in 2007 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 15

organizations.
○Faculty of Natural Science, Otto-von-Gueriche University Magdeburg (Germany)
○College of natural Science,Chungnam National University (Korea)
○Forschungszentrum Jülich GmbH (Germany)
○University of Maryland at COLLEGE PARK (U.S.A.)
○University College London (U.K.)
○College of Natural Sciences, Pusan National University (Korea)
○Research Institue of Industrial Science, Hanyang University (Korea)
○College of Science, National Taiwan University (Taiwan)
○Pacific Northwest National Laboratory (U.S.A.)
○Centre National de la Researche scientifique : CNRS (France)
○Rwth Aachen University (Germany)
○College of Engineering, Gyeongsang National University (Korea)
○College of Natural Science, Chungnam National University (Korea)
○Institute of Romote Sensing and Geographical Information System、Peking University (China)
○College of Science, National Taiwan Normal University (Taiwan)

2) Foreign Researchers and Students

Number of foreign researchers and students staying in ISIR as of March 31, 2007 is 67 in total. Details are: Associate Professors (2), Research Associates (5),Visiting Researchers (1), Part-time Employee (32), Graduate Students (Doctor Course) (19), (Master Course) (8). Their nationalities are : Korea (27), China (17), India (9), Viet Nam (4), U.K. (2), Brasil (2), Bangladesh (1), Taiwan (1), Indonesia (1), Philippines (1), Canada (1), Venezuela (1)
Foreign visitors in 2006 are as follows:
U.S.A. (16), Korea (8),U.K. (3), Italia (2), Germany (2), Austria (2), France(2), Spain (1), China (1), Thailand (1), Netherlands (1), Australia (1), Canada (1), Ukraine (1), Hong Kong (1), Sweden (1), India (1) Total (45).

3) International Conferences and Symposiums

Number of presentations (plenary, invited, oral and poster in various international conferences and symposia) by staff of ISIR is 767 in total.

Number of ISIR staffs who have been working as committee members of

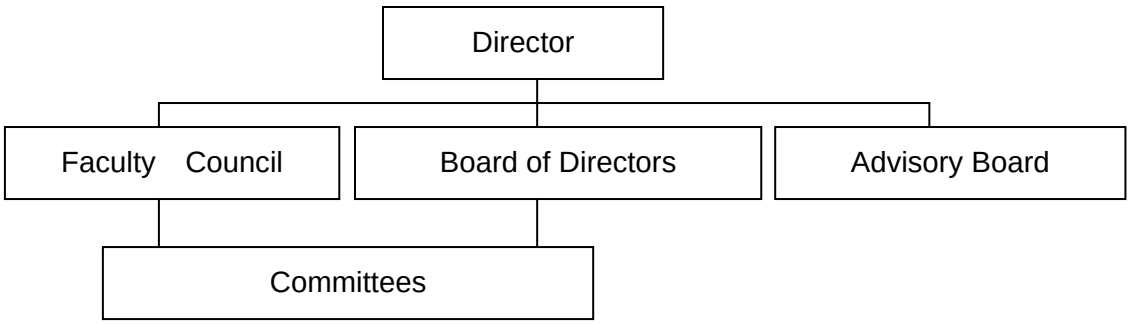
International Conferences or Editorial Board of international academic journals are 190 in total. For more details, see the part of activity of divisions and facilities.

4. Concluding Remarks

(1) Organization and Management System

At present (March.2007), ISIR has 7 divisions including 28 departments and 3 research Centers, "Nanoscience and Nanotechnology Center" , "Materials Analysis Center" and "Materials Science & Technology Research Center for Industrial Creation". In April 2006, Academia Industry Relation Office (AIR-Office) has been settled in order to strengthen cooperation between the Institute and Industries. In the Institute, brilliant staff together from wide-range fields, professors, associate professors and research associates do research and have scientific communication among scientists. All professors are participant in management system, 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.

【Organization of ISIR】



(2) Research Activities

For development of industry, researchers of ISIR are exploiting new and interdisciplinary research through basic science and technology

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.

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.

ISIR's research environment as facilities and equipments has been becoming better. A new building was constructed in 2001 and 2003 to the increased number of scientists and the development of Nanotechnology, respectively and Nanosocience and Nanotechnology Center started in April 2002. In addition, the old first research building will be reconstructed from autumn, 2007.

(3) Education

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

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".

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

(4) Contribution to Societies

As the fast–paced advancement of science and technology and the rapid alteration of social and industrial structures, we must further recognize as the Institute open to society and industry. We consistently strive to deepen our cooperation with society through positively opening of facilities, intellectual properties and achievements to meetings (ex. Sanken Techno Salon) and publications. Through them, we will be able to transfer our industrial seeds for new technology and exchange ideas for new materials. They have been highly evaluated that we have done joint researches with other university/industry.

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

(5) International Exchange

International Exchange is one of indispensable element for our Institute. We are trying to open the door widely to invite more researchers and students from other

countries, and we have 3 kind of International exchange, Academic Exchange, Student Exchange and branches in France and USA. At present (March, 2007), 64 foreign researchers and students join in the Institute. International Conferences sponsored by our Institute have been held twice a year since 1998. It's so important to release our results towards all over the world and have a chance to exchange opinions with foreign scientists.

(6) Future Plan and Prospect

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

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

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

Activities of Divisions

Division of Quantum Engineering

Outline

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

Research areas studied and techniques employed by the Division of Quantum Engineering include atomic and electronic structures of semiconductor surfaces and interfaces, nanofabrication processes using scanning probe microscopy, crystal growth of biomolecules, epitaxial growth of compound semiconductors by molecular beam epitaxy, characterization of structural, electric, optical and magnetic properties of semiconductor materials, formation and characterization of low-dimensional semiconductor quantum structures, fabrication of new semiconductor and quantum structure devices, control of the physical properties of carbon nanotibes 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 Si-, $SrTiO_3$- and protein-crystal surfaces
- Molecular fluorescence of organic films by STM-induced luminescence spectroscopy
- Crystal growth, characterization and device application of new semiconductors including III-nitride-based ferromagnetic semiconductors, Tl-III-V-N, III-nitride nanorod and quantum nanostructures
- Control of the physical properties of carbon nanotibes and the application to Votanometric / Amperometric integrated 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:	Hongwen LIU, Jun NAKAMURA
Post Doctoral Fellows:	Shanmugam KUMARAN, Tiezhu HAN
Graduate Students:	Hitoshi KURIBAYASHI, Noritsune ANAN, Nobuyasu HORI, Mahito YAMAMOT
Under Graduate Students:	Noriyuki NAKAMURA, Hirofumi FUJII, Nobutaka FUKUI
Supporting Staffs:	Yae OKADA, Kiyomi HIRASAWA

Outline

The Department of Quantum Molecular Devices is engaged in study of multi-scale surfaces/interfaces structures and nanoscale properties of materials for development of novel devices that integrate the quantum mechanical features of semiconductors and molecular functions of organic- and bio-molecules. In more concrete terms, we are studying dynamics of 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 Projects

Relaxation Dynamics of Nanoscale Structures on Crystalline Surfaces

Relaxation kinetics of nanoscale structures on $SrTiO_3$(001) surfaces have been studied, using variable temperature scanning tunneling microscopy (STM). Performing real-time observation of thermal relaxation of nanostructures, characteristic features of dynamics of nanoscale structures have been revealed. Shape transformation of microstructures on Si substrates by high temperature annealing has been studied. It has been clarified that step dynamics plays an important role in the shape transformation process.

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, using atomic force microscopy (AFM). The growth mechanism of needle-shaped orthorhombic lysozyme crystals has been studied by AFM. Dependence of interactions between protein molecules on solution conditions has been studied by AFM observation of the molecule arrangement on Thaumatin crystals.

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 show 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. The organic fluorescent materials were supplied by the Aso Lab. for porphyrin molecules, and by Dr. Lifeng Yan for conjugated polymer molecule MEH-PPV respectively.

Patterning of Biomolecules on Si by AFM Anodic Oxidation
Processes for micro-patterning of protein molecules on Si were developed based on the anodic oxidation technique of the Si surface by an AFM probe. The proteins studied are Ferritin and Fibronectin for immobilization of cells.

Publications

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Thermal relaxation of mesoscopic structures, H. Iwasaki, K. Sudoh: Manufacturing and Technology, vol. 58 No.4 (2006) 13-18.

Books
Frontiers of electrodeposition (part), Hiroshi Iwasaki, JYOHO-KIKOU, (2006) 618-628.

Patents
Fabrication of nanostructures, Hiroshi Iwasaki, Li Nan, Japanese patent No. 3888775 registered.
Method and instrument for measurement of semiconductor depletion layer, Hiroshi Iwasaki, Abu Bakar Ismail, Japanese patent No. 3816296 registered.

International Conferences
Cavity Effect on Molecular Fluorescence of a Porphyrin Film Induced by Tunneling Electrons (Oral), *H.W. Liu, Y. Ie, R. Nishitani, T.Z. Han, Y. Aso and H. Iwasaki, International Conference on Nanoscience and Technology, China 2007 (ChinaNANO 2007), Beijing, China, June 4-6, 2007.

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Molecular Fluorescence excited by STM from a PhTPP Film, *H. Liu, Y. Ie, T. Yoshinobu, Y. Aso, K. Sudoh, H. Iwasaki, R. Nishitani, M. Nowicki, 9th Sanken International Symposium 2006 on Advanced Science and Technologh for Materials, Biologh, and Information by Quantum Beams, Feb.8-9, 2006.

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Positive Patterning of Ferritin and Fibronectin Molecules on Silicon, K. Shanmugam, T. Yoshinobu, and *H. Iwasaki, 2006 Scanning Probe Microscopy, Sensors and Nanostructures, Montpellier 3-6 June 2006.

Mechanism and Control Technology of Trench Corner Rounding by Hydrogen Annealingfor Highly Reliable Trench MOSFET, *R. Shimizu, H. Kuribayashi, R. Hiruta, K. Sudoh and H. Iwasaki, 18th International Symposium on Power Semiconductor Devices and ICs, Napoli, Italy, June 6th, 2006.

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Cavity Effect on STM-Induced Light Emission (Oral), *H. Liu, Y. Ie, Y. Aso, H. Iwasaki, R. Nishitani, The 7th International Conference on Nano-Molecular Electronics, Kobe, Japan, Dec. 13-15, 2006.

STM Tip-Enhanced Photoluminescence from Porphyrin Film, *R. Nishitani, H. Liu, H. Iwasaki, The 7th International Conference on Nano-Molecular Electronics, Kobe, Japan, Dec. 13-15, 2006.

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Nano-Patterning and Crystal Growth of Proteins and Fluorescence of Organic Films Studied by Using Scanning Probe Microscopes, K. Sudoh, K. Shanmugam, T. Yoshinobu, H. Liu, Y. Ie, Y. Aso and *H. Iwasaki, 5th 21st COE International Symposium, Awaji, Japan, Dec.8-9, 2006.

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Molecular Fluorescence of Conjugated Polymer on Metal Substrates Induced by STM, *H. Liu, L. Yan, H. Iwasaki, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, Sep. 19-20, 2006.

Bias Dependence of STM-excited Molecular Fluorescence from PhTPP Film on Noble Metal Substrates, *H. Liu, Y. Ie, T. Yoshinobu, Y. Aso, K. Sudoh, H. Iwasaki, R. Nishitani, M. Nowicki, Handai Nanoscience and Nanotechnology International Symposium, Osaka, Japan, Jan. 30 - Feb. 1, 2006.

How Plasmons affect STM-induced luminescence (Oral), *H. Liu, Y. Ie, Y. Aso, H. Iwasaki, R. Nishitani, 21 Century COE Nanobio Group Symposium, Osaka, Japan, Oct.13, 2006.

Time Evolution of Nano-scale Morphology of Silicon Microstructure Surfaces in the Early Phase of Hydrogen Annealing, *R. Hiruta, H. Kuribayashi, R. Shimizu, K. Sudoh and H. Iwasaki, MRS Fall Meeting, Boston, USA, Dec.30, 2006.

Contributions to International Conferences and Journals

H. Iwasaki	Scanning Probe Microscopy, Sensors and Nanostructures June 3-6, 2006, Palais des Congrès, La Grande Motte, France (Committee member)

Publications in Domestic Meetings

The Physical Society of Japan	4 papers
The Japan Society of Applied Physics	2 papers
The Surface Science Society of Japan	1 paper
The Japanese Association for Crystal Growth Cooperation	1 paper

Academic Degrees

Doctor Degree for Engineering

H. Kuribayashi	Control of Silicon Trench Structures by Hydrogen Annealing

Master Degree for Engineering

N. Anan	Study on Growth Mechanism of Lysozyme Needle Crystals

Sponsorships

Grant-in-Aid for Young Scientists (B)

K. Sudoh	Study on Macro-scale Shape Transformation of Three-Dimensional Crystalline Structures via Atomic Step Motion	¥800,000

Entrusted Research

H. Iwasaki	Foundation for Biomedical Research and Innovation	2,3-D Display of Cells and Its Application to Next Generation Analysis System	¥3,850,000

Other Research Fund

H. Iwasaki	Fuji Electric Advanced Technology Co., LTD	¥1,000,000

Department of Photonic and Electronic Materials

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Research Student: Jin-Qiang LIU
Support Staff: Akiko WATANABE

Outline

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

Current Research Projects

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. In 2005, GaCrN/GaN/GaCrN trilayer structure tunnel diodes were fabricated and tunnel magnetoresistance effect was observed at 77 K. Great advances in 2006 are the successful low temperature (300°C) growth of high Gd concentration (12%) GaGdN with improved ferromagnetism and the observation of carrier-induced ferromagnetism in GaGdN/GaN superlattice structures. Successful growth of GaCrN/AlN multiquantum well structures and the observation of increased magnetization as well as PL blue shift

were also realized.

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

In 1995, we proposed new semiconductors TlInGaAs in which the bandgap energy is independent of temperature. We have grown TlInGaAs by MBE and confirmed the small temperature variation of the bandgap energy and refractive index. We also proposed the TlInGaAsN/AlGaAs for both temperature-stable wavelength and threshold current LDs. In 2005, we fabricated the TlInGaAs/TlInP/InP SCH LDs and obtained the small temperature variation of lasing peak wavelength as small as 0.06 nm/K in the relatively wider temperature range. In 2006, to further improve the temperature characteristics we have studied the relationship between growth condition and Tl incorporation and found that the Tl incorporation is much improved by the use of Tl-contained cladding layers and barrier layers and by the co-doping of nitrogen (N) atoms.

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 (FE) characteristics of electrons from GaN/metal samples, which is promising to fabricate the FE electron source devices. We also formed the GaN nano-rod structures on Si substrate and obtained the very small threshold voltage of 1.1 V/μm for the FE. In 2006, to obtain further improved FE characteristics and to develop to high-resolution display devices we have studied the self-formation of GaN nanorods on Si substrate with miron-scale patterns and observed the reduction in FE threshold voltage.

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

The nano-structural and physical properties of short-channel MOSFETs have been studied with scanning tunneling microscopy (STM). In 2005, we have conducted the STM observation on transverse and longitudinal cross-sections of short-channel MOSFETs and have succeeded in the nano-scale characterization of the source/drain structures as well as the fluctuation of the gate along the channel-width direction. In 2006, we have carried out the computer simulation of 3-dimensional potential profiles in short-channel MOSFETs with transverse and tilted cross-sections. The simulation has clarified that the transverse cross-section has almost the same potential profile as that the bulk, while the potential profile on the tilted cross-section differs from that in the bulk. The simulation results are consistent with the STM observation that we have reported previously.

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. The uniformity of δ–doped GaCrN under the adequate growth conditions is confirmed.

Publications

Original Papers

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Electronic Configurations of Ce and Gd in $Ce_xGd_{1-x}N$ Evaluated by XENES and Magnetization Measurements. Hiroaki Nitani, Takashi Nakagawa, T. Onuki,, Y. Suzuki, M. Yamanouchi, Takao A. Yamamoto, and Shuichi Emura, J. Alloys and Compounds 408-412 (2006) 717-720.

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Evaluation of Device Configurations through Cross-Sectional Planes along Gates of 0.1um Metal-Oxide-Semiconductor Field-Effect Transistors by Scanning Tunneling Microscopy/Scanning Tunneling Spectroscopy, S. Hasegawa, W. Doi, A. Yabuuchi and H. Asahi, Jpn. J. Appl. Phys. 45 (3B) (2006) 2033-2036.

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Nature of deep level defects in GaCrN diluted magnetic semiconductor, S. Shanthi, S. Kimura, M.S. Kim, S. Kobayashi, Y.K. Zhou, S. Hasegawa and H. Asahi, Jpn. J. Appl. Phys. 45 (4B) (2006) 3522-3525.
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Yoshinori Arachi, Shuichi Emura, Akira Omura, Masanobu Nunogaki, Takeshi Asai, Shunichi Yamaura, Akihisa Inoue and Yoshiaki Arata. Solid State Ionics 177 (2006) 1861-1864.

MBE growth of TlInGaAs/TlInP/InP SCH LDs and their laser operation, A. Fujiwara, T. Matsumoto, D. Krishnamurthy, S. Hasegawa and H. Asahi, Proc. 18th Int. Conf. on InP and Related Materials (Princeton, USA, 2006) pp.426-428.

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Books

Process Technology in III-V Compound Semiconductors, H. Asahi: in *Electronic Materials*, Ed. by T. Kimura *et al.* (Asakura, 2006) 183-186 (in Japanese).

Patents

Ferromagnetic Materials: Y.K. Zhou and H. Asahi, JP2006-294577.

Magnetism Control Method: S. Emura, H. Asahi and Y.K. Zhou, JP2006-319153.

International Conferences

Growth and fabrication of spintronics/quantum materials and devices by atomic and molecular beams (Invited), H. Asahi, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

ECR-MBE Growth of Pentanary TlGaInNAs-based DQW Structures and Fabrication of LEDs, D. Krishnamurthy, T. Matsumoto, A. Fujiwara, S. Hasegawa and H. Asahi, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

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Formation process of sharp tip-like structures on GaN nanorods during RF-MBE and their field emission characteristics, M. Terayama, K. Uchida, S. Hasegawa, M. Ishimaru, Y. Hirotsu, and H. Asahi, Sanken International Symposium 2006 on Advanced Science and Technology for Materials, Biology, and Information by Quantum Beams, Osaka, Japan, February 8-9, 2006.

Growth of GaCrN/AlGaN/GaCrN Trilayer Structures and Observation of Tunnel Magneto-Resistance Effect (Invited), H. Asahi, M.S. Kim, S. Matsuno, Y.K. Zhou, S. Emura and S. Hasegawa, International Symposium on Hybrid Nano Materials Toward Future Industries, Nagaoka, Japan, February 3-5, 2006.

Optical properties of TlInGaAs/TlInP/InP, A. Fujiwara, T. Matsumoto, S. Hasegawa, H. Asahi, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006.

Ferromagnetism in short-period GaGdN/GaN superlattices grown by RF-MBE, Y.K. Zhou, S.W. Choi, M. S. Kim, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006.

MBE growth of TlInGaAs/TlInP/InP SCH LDs and their laser operation, A. Fujiwara, T. Matsumoto, D. Krishnamurthy, S. Hasegawa and H. Asahi, 18th International Conference on Indium Phosphide and Related Materials, Princeton, USA, May 7-11, 2006.

Crystal and Electronic Structures of the $LiNi1_{1/2}Mn1_{1/2}O_2$ Related Materials, H. Kobayashi, Y. Arachi, Shuichi Emura, K. Itoh, K. Handa, A. Okamoto, M. Shikano, and K.Tatsumi, ILMB2006 Biarritz, France, June 18 – 23, 2006.

Cr atom alignment in Cr-delta-doped GaN, S. Kimura, S. Emura, H. Ofuchi, Y. Nakata,

Y.K. Zhou, C.W. Choi, Y. Yamauchi, S. Hasegawa and H. Asahi, The XIII International Conference on XAFS, Stanford, USA, July 9-15, 2006.

Observation of Valence State Change in Layered $Li_{1-y}Ni_{1/3}Mn_{1/3}Co_{1/3}O_2$. H. Kobayashi, Y. Arachi, S. Emura, K. Handa, K. Tatsumi, The XIII International Conference of XAFS, Stanford, USA, July 9-15, 2006.

Alternation of the Pd Lattice in Nano-Sized-Pd/ZrO_2 Composite during Hydrogen Absorption. Y. Arachi, S. Emura, A. Omura, M. Nunogaki, T. Asai, S. Yamaura, A. Inoue, Y. Arata, The XIII International Conference of XAFS, Stanford, USA, July 9-15, 2006.

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Magnetic properties of GaGdN/GaN superlattices grown by RF-MBE, S. W. Choi, Y. K. Zhou, S. Kimura, S. Emura, S. Hasegawa, and H. Asahi, International Conference on Physics and Applications of Spin Related Phenomena in Semiconductors, Sendai, Japan, August 15-18, 2006.

Electronic State and Local Structure Analysis of GaGdN by HX-PES and XAFS, S. Emura, S.W. Choi, J.J. Kim, S. Kimura, S. Kobayashi, Y.K. Zhou, K. Kobayashi, H. Asahi, N. Teraguchi and A. Suzuki, International Conference on Physics and Applications of Spin Related Phenomena in Semiconductors, Sendai, Japan, August 15-18, 2006.

MBE growth of TlInGaAs/TlInP/InP SCH LD structures and their laser operation with low temperature variation of lasing wavelength, A. Fujiwara, D. Krishnamurthy, T. Matsumoto, S. Hasegawa and H. Asahi, 14th International Conference on Molecular Beam Epitaxy, Tokyo, Japan, September 3-8, 2006.

Growth and Characterization of Ferromagnetic Cubic GaCrN, S. Kimura, S. Kabayashi, Y. Zhou, S. Choi, S. Subashcandran, H. Ofuchi, M. Ishimaru, Y. Hirotsu, S. Emura, S. Hasegawa and H. Asahi, 14th International Conference on Molecular Beam Epitaxy, Tokyo, Japan, September 3-8, 2006.

TlGaInNAs/GaAs Double Quantum Well Structures: Effect of Barrier Layers and Substrate Orientation, D. Krishnamurthy, T. Matsumoto, A. Fujiwara, S. Hasegawa and H. Asahi, 14th International Conference on Molecular Beam Epitaxy, Tokyo, Japan, September 3-8, 2006.

Evolution of Cr-doped and Gd-doped GaN layers grown at low temperatures (Best Paper Awards), Y.K. Zhou, S.W. Choi, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, IUMRS International Conference in Asia 2006, Jeju, Korea, September 10-14, 2006.

Magnetic properties of Gd-doped GaN single layer and GaGdN short period superlattices grown by RF-MBE, S.W. Choi, Y.K. Zhou, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, IUMRS International Conference in Asia 2006, Jeju, Korea, September 10-14, 2006.

Electronic structure of ferromagnetic element Cr in DMS GaCrN observed in X-ray absorption spectra, S. Emura, S. Kimura, M. Hashimoto, S. Kobayashi, S.W. Choi, M.S. Kim, Y.K. Zhou and H. Asahi, IUMRS International Conference in Asia 2006, Jeju, Korea, September 10-14, 2006.

Unique Lattice Alignment around Cr Atoms Doped in GaN under Some Growth Condition, S. Emura, S. Kobayashi, S. Kimura, Y. Yamauchi, S.W. Choi, Y.K. Zhou, H. Ofuchi, S. Hasegawa, H. Asahi, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, September 19-20, 2006.

Growth and characterization of ferromagnetic cubic GaCrN, S. Kimura, S. Emura, H. Ofuchi, S. Shanthi, M. Ishimaru, Y. Hirotsu, Y. K. Zhou, S. Hasegawa and H. Asahi, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, September 19-20, 2006.

Growth of flat AlN layer for GaCrN/AlN/GaCrN trilayer structure, Y. Yamauchi, S. Matsuno, M. Funakoshi, M.S. Kim, S. Hasegawa, and H. Asahi, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, September 19-20, 2006.

Surface Modification of a Metal into a Thick Ceramic Layer and a Model for Analyzing the Increased Hardness. Shuichi Emura, Masanobu Nunogaki and Yoshiyuki Nakata, The Second Asia-Oceania Ceramic Federation [AOCF] Conference, Daegu South Korea, Oct. 18 – 20, 2006.

Design of a New Type of Plasma Processing Device Installed with Sputtering Ion Source. Masanobu Nunogaki, Satoshi Sugimoto and Shuichi Emura, Asia-Oceania Ceramic Federation [AOCF] Conference, Daegu South Korea, Oct. 18 – 20, 2006.

Formation process of sharp-pointed structures on GaN nanorods during RF-MBE growth and their field emission characteristics, M. Terayama, S. Hasegawa, K. Uchida, M. Ishimaru, Y. Hirotsu and H. Asahi, International Workshop on Nitride Semiconductors 2006, Kyoto, Japan, October 22-27, 2006.

Growth and characterization of GaN-based diluted magnetic semiconductors for semiconductor spintronics (Invited), S. Hasegawa, M. Funakoshi, Y. Yamauchi, Y.K. Zhou, S. Emura and H. Asahi, Handai Nanoscience and Nanotechnology International Symposium 2006, Osaka, November 20-22, 2006.

GaN-based diluted magnetic semiconductors for nano-spintronics, H. Asahi, S. Hasegawa, S. Emura and Y.K. Zhou, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo,

December 8-9, 2006.
Growth and characterization of cubic GaCrN, S. Kimura, S. Emura, Y.K. Zhou, S. Shanthi, Y. Yamauchi, Y. Hiromura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Defect analysis on MBE grown ferromagnetic GaCrN epitaxial layers, S. Shanthi, S. Kimura, Y.K. Zhou, S. Emura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Epitaxial growth and magnetic properties of GaGdN/GaN superlattice structures, S.W. Choi, Y.K. Zhou, S. Kimura, M. Funakoshi, S. Emura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Low temperature growth of GaCrN and GaGdN layers and their properties, Y.K. Zhou, S.W. Choi, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Contributions to International Conferences and Journals

H. Asahi	14th International Conference on Molecular Beam Epitaxy (Organizing Committee Vice-Chair, Program Committee Chair)
H. Asahi	15th International Conference on Ternary and Multinary Compounds (Program Committee member)
H. Asahi	The Third International School and Conference on Spintronics and Quantum Information Technology (Spintech III) (Organizing Committee member)
H. Asahi	2006 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	14th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (Publication Committee member)
H. Asahi	18th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	2007 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	19th International Conference on Indium Phosphide and Related Materials (Organizing Committee member, International Steering Committee member)
H. Asahi	International Symposium on Compound Semiconductors 2007 (Organizing Committee member, Program Committee member)
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)
S. Hasegawa 19th International Conference on Indium Phosphide and Related Materials (Local Arrangements Committee member)
S. Hasegawa 9th International Conference on Polycrystalline Semiconductors (Advisory Committee member)

Publications in Domestic Meetings

The Japan Society of Applied Physics	15 papers
The Surface Science Society of Japan	2 papers
Electronic Materials Symposium	2 papers
The Institute of Electronics, Information and Communication Engineers	1 paper

Academic Degrees

Master Degree of Engineering

M. Terayama Study on Formation of GaN Nano-Rod Emitters on Si Substrate and Electric Field Emission Characteristics
M. Funakoshi Study on Crystal Growth of CaCrN and Their Device Application

Master Degree of Science

Y. Yamauchi Study on Fabrication of GaCrN/AlN Multiquantum Well Structures and their Characterization

Doctor Degree of Engineering

A. Fujiwara Study on Growth of Tl-containing III-V Semiconductors and Temperature Stable Lasing Wavelength Semiconductor Laser Diodes
S.W. Choi Study on Properties of Rare-Earth Doped III-Nitride Magnetic Semiconductors

Sponsorships

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

H. Asahi	Study on Room Temperature Ferromagnetic Nitride Semiconductor Nanostructures and Application to Nanospintronics Devices	¥7,500,000

Entrusted Research

S. Hasegawa	Iketani Science and Technology Promotion Foundation	Basic Study on Formation of Surface-Emission-Type Electron Field Emission Electron Source by Use of Nitride Semiconductors	¥1,500,000
S.W. Choi	Marubun Research Promotion Foundation	Study on Fabrication of Rare-Earth Doped Diluted Magnetic Semiconductors and Their Physical Properties	¥1,500,000

Department of Semiconductor Electronics

Professor:	Kazuhiko MATSUMOTO
Associate Professor:	Koichi INOUE
Research Associates:	Kenzo MAEHASHI, Yasuhide OHNO
Post Doctoral Fellows:	Takashi IKUNO, Takafumi KAMIMURA
Graduate Students:	Jun OKUNO, Yoshihiro ASAI, Taiji KATSURA, Kohei NISHIGUCHI
Under Graduate Students:	Yuichi TSUJITA, Satoshi NAGASO
Supporting Staff:	Saori KONO

Outline

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

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

Current Research Programs

Resonant Raman Scattering Spectra of Oxygen Ion-Implanted SWNT s

It is known that semiconducting SWNTs show usually p-type character in the atmosphere. In order to obtain n-type SWNTs, oxygen ions have been implanted into SWNTs at 25 eV which is near to the exchange energy of C atoms in the graphene. By the implantation to the carbon-nanotube field-effect-transistors (CNT-FETs), we have obtained n-type characteristics in source-drain current (I_{DS}) - gate voltage (Vg) curves. In resonant Raman scattering spectra of the implanted samples, the characteristic shift of the resonance energies has been observed. To understand the observed results, the band structures and optical transition energies of SWNTs 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 SWNTs.

Formation of CNT-FETs with Si_3N_4 Passivation Films

CNT-FETs have been fabricated with Si_3N_4 passivation films formed on CNT channels by catalytic chemical vapor deposition (Cat-CVD). The characteristics of

CNT-FETs can also be controlled by the selection of a substrate temperature during Si_3N_4 passivation processes. Because the CNT-FETs have been completely protected by the Si_3N_4 passivation films from further effects of ambient gases, we have obtained successfully air-stable both p- and n-type CNT-FETs. By the measurement of I_{DS} - Vg characteristics, it has been concluded that the hysterisis in I_{DS} - Vg curves has been much reduced by the careful cleaning and passivation of the CNT channel.

Formation of Aptamer-Based Biosensors using CNT-FET

To fabricate high-sensitive protein sensors, we have developed aptamer-modified CNT-FETs for sensing Immunoglobulin E (IgE) as a target material. Aptamers are artificial oligonucleotides that have the ability to recognize specific ligands by forming binding pockets. In the experiments, definite changes of I_{DS} have been observed by the introduction of IgE into phosphate buffer solutions (PBS) in which the aptamer-modified CNT channels are immersed. It has been possible to detect the presence of IgE effectively by this FET with IgE concentration as low as 0.25 nM solution.

Publications

Original Papers

Electrical transport characteristic of carbon nanotube after mass-separated ultra-low-energy oxygen ion beams irradiation, Kazuhiro Yamamoto, Takafumi Kamimura, and Kazuhiko Matsumoto, Appl. Surf. Sci. 252 (2006) 5579-5582.

Large magnetoresistance in single-walled carbon nanotubes contacted different ferromagnetic metal electrodes, Yasuhide Ohno, Kazuki Narumi, Kenzo Maehashi, Koichi Inoue and Kazuhiko Matsumoto, J. Physics: Conf. Series 38 (2006) 57?60.

Coherent Transport of Hole and Coulomb Blockade Phenomenon in Long p-Type Semiconductor Carbon Nanotube, Takafumi Kamimura and Kazuhiko Matsumoto, Jpn. J. Appl. Phys. 45 (2006) 338-340.

High-Sensitive Label-Free Biosensors Based on Single-Walled Carbon Nanotubes, Kenzo Maehashi, and Kazuhiko Matsumoto, Proc. SPIE 6127 (2006) 612715/1-4.

Patents

Sensors Based on Carbon Nanotube Electrodes,
K.Matsumoto, K.Maehashi, J.Okuno, E.Tamiya, Y.Takamura: PCT/JP2006/246073

International Conferences

Label-free protein biosensor based on aptamer-modified carbon nanotube field-effect

transistors. *K. Maehashi, T. Katsura, K. Matsumoto, K. Kerman, Y. Takamura and E. Tamiya, The 9th World Congress on Biosensors, Toronto, Canada, May 10 - 12, 2006

High-sensitive label-free amperometric protein biosensors based on single-walled carbon nanotubes array modified microelectrodes. *J. Okuno, K. Maehashi, K. Matsumoto, K. Kerman, Y. Takamura and E. Tamiya The 9th World Congress on Biosensors, Toronto, Canada, May 10 - 12, 2006.

Label-Free Amperometric Biosensors Based on Single-Walled Carbon Nanotube Modified Microelectrodes. *Kenzo Maehaashi, Jun Okuno, Kazuhiko Matsumoto, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya, 64th Device Research Conference Pennsylvania State University, USA, June 26-28, 2006.

Carbon Nanotube Single-Electron Transistors Fabricated with Focused-Ion-Beam Technique. *Kenzo Maehashi, Hirokazu Ozaki, Yasuhide Ohno, Koichi Inoue, Kazuhiko Matsumoto, Shu Seki, Seiichi Tagawa, TMS 2006 Electronic Materials Conference, Pennsylvania State University, USA June 28-30, 2006.

Precise Control of Number of Carbon Nanotube Growth by Digital Growth Process. *Masatoshi Maeda, Takafumi Kamimura and Kazuhiko Matsumoto, TMS 2006 Electronic Materials Conference, Pennsylvania State University, USA June 28-30, 2006.

High-Sensitive Detection of Immunoglobulin E Using Atamer-Modified Carbon Nanotube Field-Effect Transistor. *Taiji Katsura, Kenzo Maehashi, Kazuhiko Matsumoto, Kagan Kerman, Yuzuru Takamura and Eiichi Tamiya, TMS 2006 Electronic Materials Conference, Pennsylvania State University, USA June 28-30, 2006.

Real-Time Sensing of Proteins by Using a Top-Gate CNT-FET Biosensor. *Masuhiro Abe, Katsuyuki Murata, Atsuhiko Kojima, Yasuo Ifuku, Mitsuaki Shimizu, Tatsuaki Ataka and Kazuhiko Matsumoto, TMS 2006 Electronic Materials Conference, Pennsylvania State University, USA June 28-30, 2006.

Electronic states of Single-walled carbon nanotubes with substitutional impurities. *Koichi Inoue, Yasuhide Ohno, Kenzo Maehashi and Kazuhiko Matsumoto, 28th International Conference on the Physics of Semiconductors, Vienna, Austria, July 24 - 28, 2006.

Spin injection to single-walled carbon nanotubes through thin tunnel barriers. *Yasuhide Ohno, Kazuki Narumi, Kenzo Maehashi, Koichi Inoue and Kazuhiko Matsumoto, 28th International Conference on the Physics of Semiconductors, Vienna, Austria, July 24 - 28, 2006.

Edge-Contact Carbon Nanotube Field-Effect Transistors with No Hysteresis Characteristics. *Kohei Nishiguchi, Yasuhide Ohno, Kenzo Maehashi, Koichi Inoue and Kazuhiko Matsumoto, 28th International Conference on the Physics of

Semiconductors, Vienna, Austria, July 24 - 28, 2006.

High-Sensitive Protein Biosensors Using Single-Walled Carbon Nanotubes. *K. Maehashi, J. Okuno, T. Katsura, K. Matsumoto, K. Kerman, Y. Takamura and E. Tamiya, International Conference on Nanoscience and Technology, NANO9 meets STM'06, Basel, Switzerland, July 30 - August 4, 2006.

Selective Detection of Proteins by Using Top-Gate Carbon Nanotube Field Effect Transistor. *M. Abe, K. Murata, A. Kojima, Y. Ifuku, M. Shimizu, T. Ataka and K. Matsumoto, International Conference on Nanoscience and Technology, NANO9 meets STM'06, Basel, Switzerland, July 30 - August 4, 2006.

Growth of Suspended Single-Walled Carbon Nanotubes by Laser-Irradiated Chemical Vapor Deposition. *Y. Asai, Y. Fujiwara, K. Maehashi, Y. Ohno, K. Inoue, K. Matsumoto, International Conference on Nanoscience and Technology, NANO9 meets STM'06, Basel, Switzerland, July 30 - August 4, 2006.

Ideal Control of Carbon Nanotube Field Effect Transistor Characteristics. K. Matsumoto, International Conference on Nanoscience and Technology, NANO9 meets STM'06, Basel, Switzerland, July 30 - August 4, 2006.

High-Sensitive and Label-Free Detection of Biomolecules Using Single-Walled Carbon Nanotube Modified Microelectrodes. *J. Okuno, K. Maehashi, K. Matsumoto, K. Kerman, Y. Takamura and E. Tamiya, 2006 International Conference on Solid State Device and Materials, Kanagawa, Japan, September 13 - 15, 2006.

DNA Aptamer-Based Biosensing of Immunoglobulin E Using Carbon Nanotube Field-Effect Transistors. *T. Katsura, K. Maehashi, K. Matsumoto, K. Kerman, Y. Takamura and E. Tamiya, 2006 International Conference on Solid State Device and Materials, Kanagawa, Japan, September 13 - 15, 2006.

First Selective Detection of Proteins Using Top-Gate Carbon Nanotube Field Effect Transistor. *M. Abe, K. Murata, A. Kojima, Y. Ifuku, M. Shimizu, T. Ataka and K. Matsumoto, 2006 International Conference on Solid State Device and Materials, Kanagawa, Japan, September 13 - 15, 2006.

Formation of Carbon Nanotube Field-Effect Transistors with Low Hysteresis Characteristics. *K. Nishiguchi, Y. Ohno, K. Maehashi, K. Inoue and K. Matsumoto, Sanken International Symposium on Nanoscience and Nanotechnology 2006 -Perspective on Interdisciplinary Nanobiology and Industrial Nanotechnology- Osaka, Japan, September 19 - 20, 2006.

Growth of Single-Walled Carbon Nanotubes by Laser-Irradiated Chemical Vapor Deposition. *Y. Asai, Y. Fujiwara, K. Maehashi, Y. Ohno, K. Inoue and K. Matsumoto, Sanken International Symposium on Nanoscience and Nanotechnology 2006 -Perspective on Interdisciplinary Nanobiology and Industrial Nanotechnology- Osaka, Japan, September 19 - 20, 2006.

Label-Free Protein Biosensors Using DNA-Aptamer-Modified Carbon Nanotube Field-Effect Transistors. *T. Katsura, K. Maehashi, K. Matsumoto, K. Kerman, Y. Takamura and E. Tamiya, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium Awaji, Japan, December 8 - 9, 2006.

Fabrication of Label-Free High-Sensitive Biosensors Using Direct-Grown Carbon Nanotube Arrayed Electrode. *J. Okuno, K. Maehashi, K. Matsumoto, K. Kerman, Y. Takamura and E.Tamiya
5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, December 8 - 9, 2006.

Single-Walled Carbon Nanotube Field-Effect Transistors with Oxidized Metal Insulator, *Y. Ohno, Y. Asai, K. Maehashi, K. Inoue and K. Matsumoto, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium Awaji, Japan, December 8 - 9, 2006.

Carbon Nanotubes Grown by Thermal CVD Method and their Applications to Some Devices, *K. Inoue, K. Maehashi, Y. Ohno and K. Matsumoto, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium Awaji, Japan, December 8 - 9, 2006.

Publications in Domestic Meetings

The Japan Society of Applied Physics	14 papers
The physical Society of Japan	1 paper

Academic Degrees

Master Degree of Engineering

J. Okuno	Carbon Nanotube Amperometric Biosensors

Sponsorships

Grant-in -Aid for Basic Research (C)

K.Inoue	Study on the Carbon Nanotubes by Double-Excitation Method	¥2100,000

Other Research Fund

K.Matsumoto	Japan Science and Technology Agency	Carbon nanotube single electron electron single spin measurement systems	¥129,000,000

K.Matsumoto	New Energy & Industrial Technology Development Organization	Development of CNT High Sensitive Biosensor for Personal QOL System	¥19,550,000

Department of Condensed Matter Physics

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Outline

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 Projects

Ab intio 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, laser excitation and electron beam excitation. We have simulated the enhancement of the atomic diffusion of boron (B), hydrogen (H), and oxygen (O) in silicon under the electronic excitation in order to fabricated the future nano-electronics materials.

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 $CuAlO_2$.

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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-Tc Nano-superstucture 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-T_C phase.

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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 Bi_2Te_3 compounds. We obtained good agreement between the calculation and experiment. We have design high-efficient thermoelectric power for p-type $CuAlO_2$.

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.

Atomic Geometries and Electronic Properties of Metal/Organic Interfaces.

We have studied the atomic geometries and electronic properties of the tris-(8-hydroxyquinoline) aluminum (Alq_3)/Al interface using density functional calculations. The calculated interface dipoles agree reasonably well with the experiments and the origin of the interface dipole formation mainly comes from the alignment of the permanent dipoles of Alq_3 molecules. The HOMO levels of the Alq_3 molecules significantly depend on the orientation of the molecular permanent dipoles and the interfacial gap state observed by experiments is ascribed to the co-existence of the two orientations of the molecular dipoles.

N dissolution in Ga_xNa_{1-x} liquid alloys.

The origin of the drastic enhancement of the N solubility in Na-rich Ga_xNa_{1-x} liquid alloys compared to pure Ga and Ga-rich alloys is clarified using density functional theory. Liquid simulations show that Ga atoms tend to aggregate in Ga-rich alloys,

while Ga atoms are isolated or form small clusters in Na-rich alloys. The calculated N solubility for model crystals shows good agreement with the experimental results. In Ga-rich alloys, the interaction between Ga and N is weak because Ga interacts strongly with surrounding Ga atoms. In Na-rich alloys, Ga–N bond becomes strong because Ga is chemically active, leading to the enhancement of the N solubility.

Theoretical Study of H Adsorption and Desorption on TiO_2(110) surfaces.

Metal oxides are used for catalysis or its support materials. It is important to reveal elementary processes of chemical reactions on metal oxide surfaces and identify the most important factor determining the reactivity of surfaces. Rutile TiO_2(110) is a stable and atomically well characterized surface and many experimental and theoretical studies have concentrated on this surface. However, experimental results of hydrogen desorption from the TiO_2(110) surface are controversial [1-4]. In this study, we intend to clarify the desorption processes of hydrogen from the TiO_2(110) surface by using first-principles theoretical calculations. We investigated 1) the adsorption energies of H_2O and H_2 on TiO_2(110), 2) potential energy surfaces of H on TiO_2(110). All calculations were carried out using a program package STATE (Simulation Tool for Atom TEchnology).

First-principles Molecular Dynamics Simulations of Chemical Reactions at Water/Metal Interfaces.

Current-voltage analysis of electrochemical reactions has a very long history to understand overall reaction mechanisms. Recent development of the experimental techniques makes it possible to study on the reaction mechanism in the microscopic level. However, a consensus has not been reached yet on the reaction mechanism even for the simplest electrochemical process, i.e. the hydrogen evolution reaction (HER), $2H^+ + 2e^- \rightarrow H_2$, on the Pt electrode. In this study, we have carried out first-principles molecular dynamics (FPMD) simulations of chemical reactions at water/Pt(111) interface to elucidate the microscopic mechanism of the HER on the Pt(111) electrode, reaction intermediates, and reaction pathways. We have succeeded in simulating the Volmer process by the FPMD under the applied bias for the first time. The hydrogen atom adsorbs to the atop site, which is considered to be an active site. Upon adsorption the charge transfer takes place from the Pt electrode to the lowest unoccupied orbital (LUMO) of the hydronium ion.

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First-Principles Study of Alq_3/Al Interfaces: Origin of the Interfacial Dipole (Oral), *S. Yanagisawa and Y. Morikawa, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

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First-Principles Theoretical Study of Thiols adsorbed on Au(111), *A. Nagoya, I.

Hamada, Y. Morikawa, International Symposium on Theories of Organic/Metal Interfaces 2007 (ISTOMI'07), Osaka Univ., Osaka, Japan, Jan.15-17, 2007.

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Application of van der Waals Density Functional to the Physisorption of n-butane on Cu(111) and Au(111), *K. Lee and Y. Morikawa, International Symposium on Theories of Organic/Metal Interfaces 2007 (ISTOMI 2007), Icho-Kaikan, Osaka University, Suita, (Osaka), Jan. 15-17, 2007.

First-Principles Theoretical Study of Adsorption of Hydrogen on TiO_2(110), *M. Hiramatsu and
Y. Morikawa, International Symposium on Theories of Organic/Metal Interfaces 2007 (ISTOMI'07), Osaka Univ., Osaka, Japan, Jan.15-17, 2007.

Single-Molecular Spectroscopy of Purine Base Molecule using STM/STS, *N. Kubo, A. Nagoya,
Y. Morikawa, H. Tanaka and T. Kawai, International Symposium on Theories of Organic/Metal Interfaces 2007 (ISTOMI'07), Osaka Univ., Osaka, Japan, Jan.15-17, 2007.

First-Principles Theoretical Simulations for Surfaces and Interfaces (Invited), *Y. Morikawa, I. Hamada, S. Yanagisawa, K. Lee, M. Hiramatsu, A. Nagoya, T. Takeuchi, M. Otani, O. Sugino, Y. Okamoto and T. Ikeshoji, JSPS-DST Asia Academic Seminar on Molecular and Supramolecular Materials with Designed Functions, Feb. 23-28, 2007, Pune, India

First-Principles Study of Al/Alq_3 and Al/LiF/Alq_3 Interfaces (Oral), *S. Yanagisawa, K. Takeuchi and Y. Morikawa, Fourth International Conference on Molecular Electronics and Bioelectronics (M&BE4), Takeda Hall, Hongo Campus, The University of Tokyo, Tokyo, Japan, Mar. 14-16, 2007.

Contributions to International Conferences and Journals

H. Katayama-Yoshida	24rd International Conference on Defects in Semiconductors : ICDS24 (Advisory committee members)
H. Katayama-Yoshida	The First international conference on Quantum Design and simulation (Organizing Committee)
H. Katayama-Yoshida	4th 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)

Y. Morikawa	CREST Workshop on Physics of Single Molecules: Transport properties of single molecules, atomic wires and DNA (Organizing Committee)
Y. Morikawa	International Symposium on Theories of Organic/Metal Interfaces 2007 (ISTOMI07) (Organizing Committee Chair)

Publications in Domestic Meetings

The Physical Society of Japan	19 papers
The Japan Society of Applied Physics	7 papers
The Electrochemical Society of Japan	1 papers

Academic Degrees

Doctor Degree for Engineering

K. Matsukawa	Materials design for the gettering of diffusive 3d transition elements in silicon

Doctor Degree for Science

N. Mitsuda	First principles study on the bonding states and diffusion of CN molecule in crystalline silicon

Master Degree for Engineering

K. Takeuchi	First-principles Molecular Dynamics Simulations of Al/Alq_3 Interfaces: Atomic Geometries and Electronic Properties.
A. Nagoya	First-principles Simulation of Self-Assembled Monolayers on Au.
M. Hiramatsu	First-Principle Theoretical Study of Adsorption of Hydrogen on the Rutile TiO_2(110) surface

Master Degree for Science

H. Dekura	Metalization of solid boron by impurity doping and its electronic structure
H. Minai	Ab initio study on the ferromagnetism and magnetic excitations in dilute magnetic semiconductors

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas

Y. Morikawa	Development and releasing of quantum simulator for submicron scale systems	¥2,300,000
Y. Morikawa	Development of efficient parallel quantum dynamics simulator	¥14,500,000
Y. Morikawa	Theory of nano-scale linked molecules	¥2,900,000

Grant-in-Aid for Creative Scientific Research (K. Seki)

Y. Morikawa	Elucidation and Control of Interfaces Related to Organic Electronic Devices		

Entrusted Research

H. Katayama-Yoshida	JSPS Core-to-Core Program –Integrated Action Initiative-	Computational Nano-Materials Design	¥16,000,000
Y. Morikawa	Japan Science and Technology Corporation Core Research for Evolutional Science and Technology	Contact effects and transport properties of single molecules	¥11,500,000
Y. Morikawa	Japan Science and Technology Corporation Core Research for Evolutional Science and Technology	Electrode Chemistry at Interfaces Between Two Phases	¥10,300,000

Other Research Fund

H. Katayama-Yoshida	Japan Science and Technology Corporation	Case study on advanced measurements and analysis	¥1,960,000
H. Katayama-Yoshida	Japan Atomic Energy Agency	Analysis and Materials design simulation in Grid computing	
H. Katayama-Yoshida	Institute for Materials Research, Tohoku Univ.	Materials design, fabrication and device application for transparent high-T_C ferromagnetic semiconductors spintronics	
Y. Morikawa	Nihon Insulators, LTD.	First-principles Simulations for GaN Crystal Growth by the Na-flux Method	¥1,000,000
Y. Morikawa	Toyota Central R&D Labs., INC.	First-principles Theoretical Study on Emission Control Catalysts	¥1,800,000

Division of Advanced Materials Science and Technology

Outline

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

Achievements

- Phase stabilization mechanisms of Fe- and Pd-based metallic glasses
- Low temperature fabrication and characterization of $L1_0$-type hard magnetic nanoparticles
- Ion beam synthesis of new functional 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 SiO_2/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 low-dimensional nano-structural control and their application
- Multi-functionalization of oxide nanotubes and their application for energy/environmental systems
- 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 Associate:	Kazuhisa SATO, Akihiko HIRATA
Post Doctoral Fellows:	Andras KOVACS
Graduate Students:	Jong Han WON, Han Wool RYU, Satoru KUBOYA Hayato HASUI, Naoto KAWAHARA, Yousuke KIMURA
Supporting Staff:	Shigeko TOMII

Outline

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 Projects

Local atomic structure and crystallization process in bulk metallic glasses

We have investigated medium-range-order structures in glass states and crystallization processes induced by annealing for Pd- and Zr-based bulk metallic glasses by means of transmission electron microscopy. The obtained results are as follows: (1) We have found a complex local structural change where an fcc-type medium-range-order structure transforms into a compound-like one in the pre-crystallization stage of the $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass. This complex change is considered to contribute to the high glass stability, because it is hard to observe such change in the low-stable glasses. (2) A new crystalline phase with a large monoclinic unit cell has been found to appear without a large compositional fluctuation in the primary crystallization stage of the $Zr_{55}Cu_{30}Al_{10}Ni_5$ bulk metallic glass. The monoclinic structure can explain almost all peaks in the corresponding X-ray diffraction profile which has been interpreted as the multiple phases in some previous studies.

Fabrication and Characterization of $L1_0$-type Hard Magnetic Nanoparticles

We have been developing a new fabrication method of thin films with oriented $L1_0$ hard magnetic nanoparticles. The following results were obtained in this year: (1) Atomic ordering process of 10-nm-sized FePt and FePtCu nanoparticles has been studied by *in-situ* selected area electron diffraction and nanobeam electron diffraction. Ordering initiates at temperatures higher than 723K for FePt nanoparticles. Nanobeam electron diffraction revealed the particle size dependence of atomic order in FePtCu

nanoparticles. (2) Perpendicular magnetic anisotropy as well as enhancement of saturation magnetization have been achieved by small amount of Co addition into FePd nanoparticles. These properties are sensitive to the Co concentration. (3) 10-nm-sized $L1_0$-FePtCu nanoparticles with orientation and high-density dispersion were fabricated by rf-magnetron sputtering under the lower substrate temperatures between 563 and 673K. The substrate temperature dependence of structure and morphology of the FePtCu nanoparticles has been studied by high-resolution TEM and nanobeam electron diffraction.

Ion Beam Synthesis of New Functional Materials

We have performed high-dose iron (Fe) ion implantation into a single crystalline silicon (Si) substrate in order to synthesize a beta-$FeSi_2$/Si heterostructure. Si(001) substrates were implanted with 120 keV Fe ions at 623 K to a fluence of $4x10^{17}$ /cm^2, followed by thermal annealing at temperatures ranging from 773 K to 1073 K. Implantation-induced microstructures as well as annealing-induced ones were examined by means of x-ray diffraction (XRD) and transmission electron microscopy (TEM) in combination with energy-dispersive x-ray spectroscopy. Grazing-incidence XRD and cross-sectional TEM observations indicated that a continuous iron silicide layer consisting of epsilon-FeSi and beta-$FeSi_2$ is formed in as-implanted samples. With increasing annealing temperature the epsilon-FeSi phase transformed into the beta-$FeSi_2$ one, and finally a continuous beta-$FeSi_2$ polycrystalline layer was formed on the topmost layer of the Si substrate. Pole figure XRD measurements revealed that the beta-$FeSi_2$ crystallites are not randomly oriented but possess a preferred orientation. We discussed structural evolution upon thermal annealing as well as the damage recovery processes in high-dose Fe ion implanted Si.

Publications

Original Papers

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Local Atomic Structure of Pd-Ni-P Bulk Metallic Glass Examined by High-Resolution Electron Microscopy and Electron Diffraction, A. Hirata, Y. Hirotsu, T. Ohkubo, T. G. Nieh and N. Tanaka, Intermetallics 14 (2006) 903-907.

Voronoi Analysis of the Structure of Cu-Zr and Ni-Zr Metallic Glasses, T. Fukunaga, K. Itoh, T. Otomo, K. Mori, M. Sugiyama, H. Kato, M. Hasegawa, A. Hirata, Y. Hirotsu and A.C. Hannon, Intermetallics 14 (2006) 893-897.

Mechanism of Nanocrystalline Microstructure Formation in Amorphous Fe-Nb-B Alloys, A. Hirata, Y. Hirotsu, E. Matsubara, T. Ohkubo and K. Hono, Phys. Rev. B 74 (2006) 184204(1)-184204(6).

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Characteristic Features of the Fe_7Mo_6-Type Structure in a Transition-Metal Alloy Examined using Transmission Electron Microscopy, A. Hirata, A. Iwai and Y. Koyama, Phys. Rev. B 74 (2006) 054204(1)-054204(4).

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Application of Energy Filtering TEM to Nanocrystallization Process in Amorphous $Fe_{84}Nb_7B_9$ alloy, A. Hirata and Y. Hirotsu, J. Mater. Sci. (2006) 2597-2600.

Compositional Dependence of Local Atomic Structures in Amorphous $Fe_{100-x}B_x$ (x=14,17,20) Alloys Studied by Electron Diffraction and High-Resolution Electron Microscopy, A. Hirata, Y. Hirotsu, T. Ohkubo, T. Hanada and V. Bengus, Phys. Rev. B 74 (2006) 214206(1)- 214206(9).

Structural Characterization of Iron Silicides Nanoparticles Grown on Si Substrate: Annealing Rate Dependence, J. H. Won, K. Sato, M. Ishimaru and Y. Hirotsu, J. Mater. Sci. 41 (2006) 2611-2614.

Structural Investigation of Ge-Sb-Sn Thin Film using Transmission Electron Microscopy, M. Naito, M. Ishimaru, Y. Hirotsu, M. Takashima and H. Matsumoto, J. Mater. Sci. 41 (2006) 2615-2616.

Order-Disorder Transformation in $L1_0$-FePd Nanoparticles Studied by Electron Diffraction, K. Sato and Y. Hirotsu, Mater. Trans. 47 (2006) 59-62.

Fabrication of Oriented $L1_0$-FeCuPd and Composite bcc-Fe/$L1_0$-FeCuPd Nanoparticles: Alloy Composition Dependence of Magnetic Properties, H. Naganuma, K. Sato and Y. Hirotsu, J. Appl. Phys. 99 (2006) 08N706(1)-08N706(3).

Direct Synthesis of Oriented High-Density Islands of $L1_0$-FePtCu Alloy at 613K, W. H. Ryu, H. Naganuma, K. Sato and Y. Hirotsu, Jpn. J. Appl. Phys. 45 (2006) L608-L610.

Perpendicular Magnetic Anisotropy of Epitaxially Grown $L1_0$-FePdCu Nanoparticles with Preferential c-Axis Orientation, H. Naganuma, K. Sato and Y. Hirotsu, J. Appl. Phys. 100 (2006) 074914(1)-074914(7).

Transmission Electron Microscopy Study on $FeSi_2$ Nanoparticles Synthesized by Electron-Beam Evaporation, J. H. Won, K. Sato, M. Ishimaru, and Y. Hirotsu, J. Appl. Phys. 100 (2006) 014307(1)-014307(6).

Chemical Short-Range Order in Ion-Beam-Induced Amorphous SiC: Irradiation

Temperature Dependence, M. Ishimaru, I.-T. Bae, A. Hirata, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, Nucl. Instrum. Meth. B 242 (2006) 473-475.

Epitaxial Growth of Ferromagnetic Cubic GaCrN on MgO Substrate, S. Kimura, S. Subashchandran, Y. K. Zhou, M. S. Kim, S. Kobayashi, S. Emura, M. Ishimaru, Y. Hirotsu, S. Hasegawa and H. Asahi, Jpn. J. Appl. Phys. 45 (2006) 76-78.

Formation Process of beta-$FeSi_2$/Si Heterostructure in High-Dose Fe Ion Implanted Si, M. Ishimaru, K. Omae, I.-T. Bae, M. Naito, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, J. Appl. Phys. 99 (2006) 113527(1)-113527(7).

Solid Phase Crystallization of Amorphous Fe-Si Layer Synthesized by Ion Implantation, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, Appl. Phys. Lett. 88 (2006) 251904(1)-251904(3).

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, Nucl. Instrum. Meth. B 250 (2006) 283-286.

Structural Evolution in Fe Ion Implanted Si upon Thermal Annealing, K. Omae, I.-T. Bae, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, Nucl. Instrum. Meth. B 250 (2006) 300-302.

Electron-Beam Radial Distribution Analysis of Ion-Beam-Induced Amorphous SiC (invited), M. Ishimaru, Nucl. Instrum. Meth. B 250 (2006) 309-314.

Structural Changes of SiC under Electron-Beam Irradiation: Temperature Dependence, I.-T. Bae, M. Ishimaru and Y. Hirotsu, Nucl. Instrum. Meth. B 250 (2006) 315-319.

Annealing Effect on Structural Defects in Low-Dose Separation-by-Implanted-Oxygen Wafers, M. Tamura, M. Ishimaru, K. Hinode, K. Tokiguchi, H. Seki and H. Mori, Jpn. J. Appl. Phys. 45, 7592-7599 (2006).

Low-Temperature Crystallization Caused by Ultrasound in $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ and $Pd_{40}Ni_{40}P_{20}$ Bulk Metallic Glasses, T. Ichitsubo, E. Matsubara, K. Anazawa, N. Nishiyama, M. Naito and Y. Hirotsu, Mater. Sci. Eng. A 442 (2006) 273-277.

HRTEM analysis of anti-phase boundary formation in $L1_0$-FePd phase, A. Kovacs, K. Sato and Y. Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1520.

Characterization of 2D-dispersed FeCuPd Alloy Nanoparticles, H. Naganuma, K. Sato and Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1545.

Low Temperature Synthesis of High-Density FePtCu Nanoparticles Fabricated by Rf-magnetron Sputtering, H. W. Ryu, H. Naganuma, K. Sato and Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1548.

Nanobeam Electron Diffraction Analysis of Medium Range Order Structures in Zr-Based Metallic Glasses, A. Hirata, T. Morino and Y. Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1606.

Amorphous Structure of Ion-Beam-Synthesized Fe-Si Thin Layer, M. Naito, M. Ishimaru and Y. Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1771.

High-Dose Fe Ion Implanted Si: Ion-Beam-Induced and Annealing-Induced Microstructures, M. Ishimaru, K. Omae, I.-T. Bae, M. Naito and Y. Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1856.

Review Papers

Chemical Short-Range Order in Ion-Beam-Induced Amorphous SiC, M. Ishimaru and Y. Hirotsu, Microscopy 41 (2006) 156-159 (in Japanese).

Observation of Local Atomic Structure in Pd-Ni-P Bulk Metallic Glass using Cs-corrected TEM, A. Hirata, Y. Hirotsu, T. Ohkubo, N. Tanaka and T. G. Nieh, Materia Japan 45 (2006) 848 (in Japanese).

Books

Nanostructure Analysis of Metallic Materials (in Japanese), K. Hono and Y. Hirotsu, AGNE Gijutsu Center (2006)

Practical Electron Microscopy and Its Application to Materials (Edited by Iron and Steel Institute of Japan & The Japan Institute of Metals) (in Japanese), K. Sato, H. W. Ryu, Y. Hirotsu (2006) 233

Practical Electron Microscopy and Its Application to Materials (Edited by Iron and Steel Institute of Japan & The Japan Institute of Metals) (in Japanese), A. Makino, T. Bitoh, Y. Hirotsu, K. Sato (2006) 234

Practical Electron Microscopy and Its Application to Materials (Edited by Iron and Steel Institute of Japan & The Japan Institute of Metals) (in Japanese), A. Hirata and Y. Koyama (2006) 247

Patents

Ferromagnetic Particles and Their Production Methods, Y. Hirotsu, A. Kovács and K. Sato: Tokugan 2006-220037.

International Conferences

Direct Synthesis of Isolated $L1_0$-FePtCu Nanoparticles by RF-Magnetron Sputtering (Oral), *H. W. Ryu, K. Sato and Y. Hirotsu, International Workshop on Designing of Interfacial Structures in Advanced Materials and Their Joints, Osaka (May18-20, 2006).

Exchange interactions in hydrogen-induced amorphous YFe_2 (Invited), *K. Suzuki, K.

Ishikawa, K. Aoki, J. M. Cadogan, M. Ishimaru and Y. Hirotsu, 8th International Workshop on Non-Crystalline Solids, Gijón, Spain (June 20-23, 2006).

Change of Nanostructure in $(Fe_{0.5}Co_{0.5})_{72}B_{20}Si_4Nb_4$ Metallic Glass on Annealing (Invited), *Y. Hirotsu, A. Hirata, K. Amiya, N. Nishiyama and A. Inoue, International Conference on Processing & Manufacturing of Advanced Materials (THERMEC' 2006), Vancouver, Canada (July 4-8, 2006).

Formation process of beta-$FeSi_2$/Si heterostructure in high-dose Fe ion implanted Si (Invited), *M. Ishimaru, 19th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas, USA (August 20-25, 2006)

Magnetic Properties and Microstructure of FePt-M-B (M=Zr, Nb, La) Films, *H. Okumura, S. Nishinakagawa, T. Bitoh, A. Makino, K. Sato and Y. Hirotsu, The 17th International Conference on Magnetism, Kyoto (August 20-25, 2006).

Particle Size Dependence of Atomic Ordering and Magnetic Properties of $L1_0$-FePd Nanoparticles, *H. Naganuma, K. Sato and Y. Hirotsu, The 17th International Conference on Magnetism, Kyoto (August 20-25, 2006).

Effects of Additive Elements on Atomic Ordering and Hard Magnetic Properties of $L1_0$-Type FePt and FePd Alloy Nanoparticles (Invited), *Y. Hirotsu, K. Sato, H. W. Ryu and A. Kovács, 48th IUVSTA Workshop, Innovatial Training Course on “Influence of Trace Elements on the Nucleation and Growth of Thin Films”, Budapest, Hungary (August 26-31, 2006).

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Amorphization of SiC under radiation environments (Plenary), *M. Ishimaru, Satellite Conference on Materials Behaviour: Far From Equilibrium, Mumbai, India (December 15-16, 2006).

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Contributions to International Conferences and Journals

Y. Hirotsu	5th International Bulk Metallic Galsses Conference (Co-Chair)
Y. Hirotsu	16th International Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	The IUMRS International Conference in Asia 2006 (Session Organizer)
Y. Hirotsu	International Conference on Magnetism 2006 (Organizing Committee)
Y. Hirotsu	6th Japan-Polish Joint Seminar on Materials Analysis (Organizing Committee)
M. Ishimaru	Japanese Journal of Applied Physics (Associate Editor)
M. Ishimaru	16th International Conference on Electron Microscopy (Session Organizer)

Publications in Domestic Meetings

The Japan Institute of Metals	6 papers
The Japan Society of Applied Physics	1 paper
Others	3 papers

Academic Degrees

Doctor Degree for Engineering

J. H. Won	Fabrication and Structural Analysis of Environmental-Friendly Semiconducting beta-$FeSi_2$

Master Degree for Engineering

S. Kuboya	Local Structural Change and Crystallization Process of Pd-Ni-P Bulk Metallic Glasses
H. Hasui	Formation of Metastable Phase during the Crystallization in Zr-Cu-Al-Ni Bulk Metallic Glasses

Sponsorships

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

Y. Hirotsu	In situ observation of atomistic structures in metallic liquid and metallic glass	¥8,400,000

Grant-in-Aid for Scientific Research (S)

Y. Hirotsu	Fabrication and characterization of hard magnetic alloy nanoparticles produced by vapor quenching	¥11,100,000

Grant-in-Aid for Encouragement of Young Scientists (B)

K. Sato	Quantitative Analyses of Nanostructure and	¥700,000

	Magnetic Properties of $L1_0$-FePt and FePd Nanoparticles by Transmission Electron Microscopy		

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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Outline

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 in pressurized gases. The main issues are to investigate properties of lotus-type porous metals and to develop the engineering applications. In this year, we have fabricated lotus metals and alloys using continuous casting technique and porous aluminum using moisture, and have investigated the fatigue behavior of lotus copper and Equal-Channel Angular Extrusion (ECAE) of lotus-type porous copper. Furthermore, we have investigated the formation of hollow oxide nanoparticles through oxidation of metal nanoparticles.

Current Research Projects

Fabrication of Lotus-type Porous Metals and Alloys by Continuous Casting Technique

We developed a continuous casting technique in a high-pressure gas chamber which enables to fabricate long lotus-type porous plates or rods. Using this technique, we successfully fabricated the lotus copper, aluminum, magnesium, and carbon steel. The pore size and the porosity can be controlled by the solidification rate and the gas pressure. 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, biomaterials, and machine tools, etc.

Equal-Channel Angular Extrusion (ECAE) of Lotus-type Porous Copper
Lotus-type porous copper rods were extruded through an ECAE–die to improve the mechanical properties, and the deformation behavior was investigated. As a result, we can control the morphologies of the pores by varying the process parameters such as the channel angle of the die, the pass number of the extrusion, and the pass route. The conditions where the Vickers hardness of the lotus-type porous copper increased without changing the pore morphologies were found out.

Fabrication of Lotus-type Porous Aluminum by Using Hydrogen Decomposed from Moisture
Lotus-type porous aluminum was fabricated by using hydrogen decomposed from moisture. In a vacuum, pure aluminum was melted and cast into a mold containing a small amount of moisture, which results in formation of unidirectional pores in aluminum ingots. Pores formed in the ingots depend on the melting temperature. By decreasing the melting temperature, we successfully fabricated lotus aluminum with homogeneous pore structure.

Fatigue Behavior of Lotus-type Porous Copper
Fatigue strength of lotus-type porous copper was investigated via constant stress fatigue tests. The fatigue strength shows anisotropy originating from anisotropic pore morphology. The fatigue strength in the direction parallel to the longitudinal axis of pores is higher than that in the perpendicular direction. The fatigue strength is closely related to the ultimate tensile strength; the fatigue strength is proportional to the ultimate tensile strength regardless the loading direction.

Formation of hollow oxide nanoparticles through oxidation of metal nanoparticles
The formation mechanism of hollow oxides through oxidation of several metallic nanoparticles such as Cu, Al, Zn and Ni was studied by TEM. A nano-pore inside the oxide particles is considered as a vacancy cluster which is formed as a result of mass transport during metal oxidation reaction. Hollow oxide nanoparticles can be obtained under the condition that outward diffusion of metal ions is considerably faster than inward diffusion of oxygen ions.

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Fabrication of Porous Materials with Micro and Nano Pores (Invited), *H. Nakajima, The 8th International Symposium on Eco-materials Processing and Design (ISEPD2007), Kitakyusyu International Conference Center, Kitakyushu, Japan, Jan. 11-13, 2007.

Hollow Amorphous Formation via Oxidation of Al Nanoparticles at Low Temperatures (Oral), *R. Nakamura, J.-G. Lee, D. Tokozakura, H. Mori, and H. Nakajima, The 8th International Symposium on Eco-materials Processing and Design (ISEPD2007), Kitakyusyu International Conference Center, Kitakyushu, Japan, Jan. 11-13, 2007.

Fabrication of Lotus-type Porous Nickel Using Moisture Reaction between Casting Mould and Metal (Oral), *H. Onishi, Y. Suematsu, S.K. Hyun, and H. Nakajima, The 8th International Symposium on Eco-materials Processing and Design (ISEPD2007), Kitakyusyu International Conference Center, Kitakyushu, Japan, Jan. 11-13, 2007.

Fabrication of Lotus-type Porous Ni-(15, 28 and 31) at.% Al Alloys by Unidirectional Solidification in Hydrogen Atmosphere, *S.K. Hyun, T. Ikeda, and H. Nakajima, The 8th International Symposium on Eco-materials Processing and Design (ISEPD2007), Kitakyusyu International Conference Center, Kitakyushu, Japan, Jan. 11-13, 2007.

Formation of Nano-scaled Hollow Oxide Particles Using Oxidation Reaction (Oral), *R. Nakamura, D. Tokozakura, J.-G. Lee, H. Mori, and H. Nakajima, 136th TMS Annual Meeting, Walt Disney Swan and Dolphin Hotel, Orland, FA, USA, Feb.25-Mar.1, 2

Contributions to International Conferences and Journals

H. Nakajima	Materials Letters (Principal Editor)
H. Nakajima	Scripta Materialia (Guest Editor)
H. Nakajima	Fifth International Conference on Porous Metals and Metal Foaming Technology (MetFoam2007) (International advisory Board member)
H. Nakajima	High Temperature Materials and Process (Editorial Board)
H. Nakajima	High Temperature Materials and Processes (Guest Editor)
H. Nakajima	Advanced Engineering Materials (Guest Editor)
H. Nakajima	Materials Transactions (Guest Editor)
H. Nakajima	Diffusion and Defect Data (Editorial board member)
H. Nakajima	Materials Science Foundations (Editorial board member)
H. Nakajima	Fifth Pacific Rim International Conference on Materials (PRICM-5) (Organizing Committee Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	International Conference on Processing & Manufacturing of Advanced Materials (THERMEC’2006) (Organizing committee member)
H. Nakajima	International Conference on Diffusion in Materials (International advisory Board member)
H. Nakajima	2nd International Conference on Diffusion in Solids and Liquids (International advisory Board member)
H. Nakajima	International Conference on Eco-Materials Processing and

	Design VIII (International advisory Board member)
H. Nakajima	International Symposium on Synergistic Effects of Materials and Processing (ISSEMP2006) (International advisory Board member)

Publications in Domestic Meetings

The Japan Institute of Metals	29 papers
The Japan Copper and Copper Alloys Research Association	2 papers
The Japan Institute of Light Metals	1 paper
High Temperature Society of Japan	1 paper

Academic Degrees

Master Degree for Engineering

D. Tokozakura	Hollow Oxide Formation via Oxidation of Cu Nanoparticles
L.M. Lin	Study on a Lotus-type Porous Alumina and Its Mechanical Properties

Sponsorships

Grant-in-Aid for Scientific Research

H. Nakajima	Fabrication of Novel Nano-hollow Sphere Metals and Metallic Nano-tube and Elucidation of Physical Propertie	¥32,110,000
R. Nakamura	Fabrication of Hollow Metallic Nanoparticles and Elucidation of their Formation Mechanism	¥2,500,000

Entrusted Research

H. Nakajima	Development of High Performance Machinery Processing System	¥4,685,100

Other Research Fund

H. Nakajima	The Iron and Steel Institute of Japan	Database of porous metals	¥490,655
H. Nakajima	The Japan Institute of Light Metals	Grant-in-Aid from The Japan Institute of Light Metals	¥250,000
H. Nakajima	Japan Science and Technology Agency	Development Project for Seeds Innovation Development of Porous Silicon Heat Sink	¥3,107,000

H. Nakajima	Murayama Co.,LTD.	Development of Hydrostatic Bearing	¥1,000,000
R. Nakamura	Iketani Science and Technology Foundation	Elucidation of Formation Mechanism of Nano-hole in WMetallic Nanoparticles	¥1,500,000

Department of Atomic Scale Science

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Outlines

This research group studies both nano-science and nanobio-technology in its activity, directs toward innovation of "excellent functional material, device systems". Design and synthesis of atomically controlled materials via a "Laser Molecular Beam Epitaxy (LMBE) technique enable us to fabricate novel materials with elegant structures and functions, which were not achieved by previous methods, with intention being to develop "Super Five Senses Sensor" and "Brain-Like Memory". Use of "Scanning probe microscopy (SPM)" allows observation, manipulation and spectroscopy of atoms and molecules including DNA. The knowledge obtained from such microscopic study would be extended to developments of bio-devices and biochips. Computational simulation studies are also employed to predict the phase transition and the electric states of condensed materials. Main subjects are (1) Fabrication of Function Harmonized Artificial Lattices and nanostructures, via LMBE process, (2) SPM observation and manipulation of biomolecules such as DNA (3) Development of Bio-tip, and (4) Development of bio-molecular device constructed from DNA.

Current Research Projects

Fabrication of harmonized functional artificial lattice and oxide nanostructures by laser process

We fabricated oxide spin devices (ferromagnetic FETs and diodes) using novel strongly correlated ferromagnetic oxides $(Fe,M)_3O_4$ (M=Zn, Mn). In addition, we developed novel techniques to fabricate metal oxide nanostructures, such as Mo nano-mask AFM lithography and Nano-imprinting. These techniques allow us to fabricate ultra high resolution patterns (30-100nm) and large area pattern formations. Furthermore, we have fabricated oxide nanowires (less than 10nm) using self-assembling technique.

Development of NanoBiosensor

We confirmed the addressable localization of biological molecules utilizing the self-assembly process for enhancing the signal accuracy, where a miniaturization of analytical biochips can accommodate millions of assays in developing new drugs. We also succeeded in creating a master mold by using Nano-imprint lithography to etch a nanopattern in hydrogel film. We will demonstrate that a specific modified surface for selective binding, for instance, polyethylene glycolpolymer, was enough to prevent non-specific adsorption of biomolecules. Then we will develop a technology, which we termed hybrid assembly that attaches and patterns biocompatible copolymer in nano scale on various materials,
i.e., gold, silicon, glass, polyimide and ceramic.

Nano-science by using of Scanning Probe Microscopes.

Scanning tunneling microscopy (STM) data revealed the unique electronic feature of guanine that enables the assignment of guanine out of the rests, and on the distinctive imaging of cytosine and thymine base molecules by the shape that enables the differentiation between the pyrimidine base molecules. Although the detail of its origin is not yet clear, among the four base molecules, only guanine of DNA/PNA adsorbed on Cu(111) produces sharp peak in tunneling characteristics dI/dV at a negative sample bias in the range between -1.6 to -1.9 V. High resolution STM images enable us to differentiate the sugar phosphate chain and nucleobase, resulting in discrimination of cytosine and thymine which are thought to be difficult to discriminate by shape due to their small size.

Publications

Original Papers

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Soft lithographic patterning of supported lipid bilayers onto a surface and insideb microfluidic channels, P.N.Kim, S.E.Lee, H.S.Jung, H.Y.Lee, T.Kawai, and K.Y. Suh: Lab on a chip, 6 (2006) 54-59.

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Atomic Force Microscopy Observation of Highly Arrayed Phospholipid Bilayer Vesicle on a Gold Surface, H.S.Jung, J.M.Kim, J.W.Park, S.E.Lee, H.Y.Lee, R.Kuboi, and T.Kawai: J.Biosci.Bioeng., 102 (2006) 28-33. (Fig.2; A Cover of JBB vol.102, No.1)

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Thickness Dependence of Structure and Magnetization of $BiFeO_3$ Films on $(LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$ (001) Substrate, Rana, D.S., K.Takahashi, K.R.Mavani, I.Kawayama, H.Murakami, M.Tonouchi, T.Yanagida, H.Tanaka and T.Kawai, Phys. Rev. B, 75 (2007) 060405

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Time-Resolved Electrical Conductance Spectroscopy of Chemical Reactions on Nano-Space,K. Yokota, M. Taniguchi, T. Kawai,Chem. Phys., 330, (2006), 184-189.

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Self-Organized Interconnect Method for Molecular Devices, M. Taniguchi, Y. Nojima, K. Yokota, J. Terao, K. Sato, N. Kambe, T. Kawai, J. Am. Chem. Soc. ,128 , (2006) , 15062-15063 (Commun).

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Electronic states of the DNA polynucleotides poly(dG)poly(dC) in the presence of

iodine, M. Furukawa, H. S. Kato, M. Taniguchi, K. Kawai, T. Hatsui, N. Kosugi, T. Yoshida, M. Aida, M. Kawai, Phys. Rev. B 75 (2007) 045119-0451267.

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Review Papers

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Books

Thin film formation (Chapter 4), Hidekazu Tanaka, et al., ”thin film formation technique”（2006）42-51

Patents

DIRECT IMMOBILIZATION METHOD OF CARBOHYDRATES ON SURFACE OF SOLID SUBSTRATE, H.J.Choa, J.H.Seo B.K.Lee, K.Adachi, H.Y. Lee, T.Kawai, Korean Institute Number: 2006-0105908

Development of direct immobilization of polysaccharides on surface for various application of carbohydrate, B.K.Lee, K.Adachi, H.Y. Lee, T.Kawai, S.Matsuura, H.J.Choa, J.H.Seo, Japanese Institute Number: 2006-288952.

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International Conferences

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DNA Nanowires; Molecular Imaging, Transport Properties and Device Applicaion, T.Kawai（Plenary talk）: The Seventh International Symposium on Functional π -Electron Systems, Osaka, Japan, May 15-20, 2006.

DNA Based Nano-bioelectronics, T.Kawai: Winnipeg Symposium on Charge Migration in DNA, Winnipeg, Manitoba, Canada, June 6-9, 2006

Programmed Self-organization for Creation of Bio-inspired Nano-Devices, T.Kawai:, Nagoya, Aichi, June 13, 2006.

Advanded Bio Devices, T.Kawai: Workshop on Nanoscience and Nanotechnology between Sanken and CNRS Towards Creating New Industrius Based on Inter-Nanoscience, Orsay, France, July 17, 2006.

High Resolution STM Imaging of DNA and Related Bio-molecules; Recent Developments, T.Kawai: International Coference on Nanoscience and Technology, Basel, Switzerland, July 30 - August 4, 2006.

DNA Nanotechnology in Kawai Laboratory, T.Kawai: Nanoelectronics and dynamics of DNA, Hawaii, U.S.A., August 20-22, 2006.

Phase Transition Control in Strained Vanadium Dioxides Thin Films, T.Kawai: XIII International Workshop on Oxide Electronics, Ischia, Italy, October 8-11, 2006.

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DNA Nanowires; Molecular Imaging, Transport Properties and Device Application, T.Kawai（Plenary talk）: 2006 Joint International Meeting, ECS 210th Meeting, Cancun, Mexico, October 29 － November 3, 2006.

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DNA NANOTECHNOLOGY: Molecular Imaging, Self-Organization and NanoBioDevices, T.Kawai: PNU Symposium on Material Chemistry 2006, Busan, Korea, November 17-18, 2006.

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High resolution imaging, manipulation and device formation using DNA and protein molecules on surfaces, T.Kawai: Gordon Research Conference, Ventura, CA, U.S.A., February 11-16, 2007.

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Well-Oriented NanoWell Array Metrics for Integrtaed Digital Nanobiosensore (Invited), *H.Y.Lee and T. Kawai:Center of Scientific Orsay, Paris University, Paris, France, June 26, 2006.

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Interaction of Pore Forming Protein Streptolysin O (SLO) with Supported Lipid Bilayers : Nanoscale pore formation and Enhanced electric signal, Kota Sreenivasa Rao, Bong-Kuk Lee, Hea-Yeon Lee, Tomoji Kawai The 3rd International Workshop on Biochips and Environmental Monitoring, Osaka, Japan, August 17, 2006

Self-Organized Nanopatterning of Poly-Vinyl Alcohol Hydrogel using Capillary Lithography, Bong-Kuk Lee, Hea-Yeon Lee, Tomoji Kawai: Sanken International Symposium 2006, Osaka, Japan, September19, 2006.

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Investigation on Ferromagnetism of (La,Ce)MnO_3 Thin Films, Yanagida, T., H.Tanaka and T.Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2006, Osaka, Japan, February 8-9 (2006)

Influence of Ambient Atmosphere on Transport Properties and Phase Transition of Strained Vanadium Dioxides Ultra Thin Films, Nagashima, K., T.Yanagida, H.Tanaka and T.Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2006, Osaka, Japan, February 8-9 (2006)

Functional Nano Oxides, Yanagida, T., H.Tanaka and T.Kawai, Workshop on Nanoscience and Nanotechnology between Sanken and CNRS, Paris, France, July 21 (2006) (Invited Talk)

Synthesis of Ultra Small MgO Nanowires, Yanagida, T., K.Nagashima, H.Tanaka and T.Kawai, 13th International Workshop on Oxide Electronics, Ischia, Italy, October 8-11 (2006)

Can Ce-doped Manganites be Electron-doped Ferromagnet?, Yanagida, T., H.Tanaka, T.Kawai, Y.Saitoh, Y.Takeda and A.Fujimori, 13th International Workshop on Oxide Electronics, Ischia, Italy, October 8-11 (2006)

Phase Transition Control in Strained Vanadium Dioxides Thin Films, Kawai, T., K.Nagashima, T.Yanagida and H.Tanaka, 13th International Workshop on Oxide Electronics, Ischia, Italy (Invited Talk), October 8-11(2006)

Fabrication of Small MgO Nanowires by Pulsed Laser Deposition, Yanagida, T., K.Nagashima, H.Tanaka and T.Kawai, Material Research Society Fall Meeting, Boston, USA, November 27-December 1 (2006)

Origin of Ferromagnetism in Ce-doped Manganites, Yanagida, T., H.Tanaka, T.Kawai, Y.Saitoh, Y.Takeda and A.Fujimori, Material Research Society Fall Meeting, Boston, USA, November 27-December 1 (2006)

Modulation of Metal-Insulator Transition in Strained Vanadium Dioxides Thin Films, Yanagida, T., K.Nagashima, H.Tanaka and T.Kawai, Material Research Society Fall Meeting, Boston, USA, November 27-December 1 (2006)

Room Temperature Control of Phase Transition in Strained Vanadium Dioxide Thin Films, Nagashima, K., T.Yanagida, H.Tanaka and T.Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2006, Osaka, Japan, September 19-20 (2006)

Thickness Dependence of Stress Relaxation Effect on Transport Properties of Strained Vanadium Dioxide Epitaxial Thin Films, Nagashima, K., T.Yanagida, H.Tanaka and T.Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2006, Osaka, Japan, September 19-20 (2006)

Synthesis of Ultra Small MgO Nanowires by Laser MBE, Nagashima, K., T.Yanagida, H.Tanaka and T.Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2006, Osaka, Japan, September 19-20 (2006)

Strain Effects on Metal-Insulator Transition of VO_2 Thin Films, Yanagida, T., K.Nagashima, H.Tanaka and T.Kawai, Kyoto Conference on Solid State Chemistry -Transition Metal Oxides: Past, Present and Future-, Kyoto, Japan, November 14-18 (2006)

MgO Nanowires by Pulsed Laser Deposition, Yanagida, T., K.Nagashima, H.Tanaka and T.Kawai, Kyoto Conference on Solid State Chemistry -Transition Metal Oxides: Past, Present and Future-, Kyoto, Japan, November 14-18 (2006)

Precise Modulation of Metal-Insulator Transition of Strained VO_2 Thin Films, Nagashima, K., T.Yanagida, H.Tanaka and T.Kawai, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9 (2006)

Magnesium Oxide Nanowire Growth by Pulsed Laser Deposition, Yanagida, T., K.Nagashima, H.Tanaka and T.Kawai, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9 (2006)

Transport Properties of $ZnFe_2O_{4-d}$, Marcu, A., T.Yanagida, K.Nagashima, H.Tanaka and T.Kawai, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9 (2006)

Arbitrary Control of Magnesium Oxide Nanowire Growth and the Underlying Mechanism, Nagashima, K., T.Yanagida, H.Tanaka and T.Kawai, Second SANKEN-CNU Joint Symposium on Nanoscience and Nanotechnology, Osaka, Japan, January 25-26 (2007)

Functional Nano Oxides, Yanagida, T., H.Tanaka and T.Kawai, Workshop on Nanoscience and Nanotechnology between Sanken and CNRS, Paris, France, February 19 (2007) (Invited Talk)

Highly Conductive $(Fe,Mn)_3O_4$ Thin Films with Spin Polarization at Room Temperature and Their Application to Nano Spintronic Devices by AFM Lithography(Invited), *Hide. Tanaka, T. Kawai, 2006 MRS (Materials Research Society) Spring Meeting, San Francisco, USA, April 17-22, 2006

Oxide Nano-Spintronics (Invited), *Hide. Tanaka, T. Kawai, Commemorative Workshop of Opening SANKEN USA Branch in San Francisco, San Francisco, USA, December 15-16, 2006

Electronic structures of electron doped ferromagnetic oxides, -Perovskite manganite and spinel ferrite-(Invited), *Hide. Tanaka, T. Kawai, The 2nd Indo-Japan Seminar “Novel Magnetic Materials and their Electronic Structures”, Tokyo, Japan, February 27-March 1, 2007

Room-Temperature Spin-Polarized $(Fe,Mn)_3O_4$ Thin Films Grown on $Nb:SrTiO_3$ Substrates by Pulsed-Laser Deposition Method, I. Satoh, Hide. Tanaka, and T. Kawai, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006

Electrical and magnetic properties of $(La,Pr,Ca)MnO_3$ manganite nano-channel fabricated by AFM lithography technique, Y. Yanagisawa, L. Pellegrino, Hide. Tanaka, M. Hirooka, T. Kawai, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006

Electronic Structure of Ferromagnetic Perovskite Manganite Thin Films Investigated by Hard X-ray Photoemission Spectroscopy, Hide. Tanaka, T. Yanagida, M. Ohnishi, T. Kawai, Y. Takata, K. Horiba, M. Taguchi, S. Shin, D. Miwa, K. Tamasaku, Y. Nishino, T. Ishikawa, E. Ikenaga, M. Kobata, J-J. Kim, S. Ueda, M. Awaji, A. Takeuchi, K. Kobayashi, The 2nd International Workshop on Hard X-ray Photoelectron Spectroscopy, Hyogo, Japan, September 19- 20, 2006

Electronic Structure of $Fe_{3-x}MxO_4$ (M=Zn, Mn) Spinel Oxide thin films as Tunable Ferromagnetic Semiconductor Investigated by Hard X-ray Photoemission Spectroscopy, J. Takaobushi, M. Ishikawa, I. Satoh, T. Yanagida, Hide. Tanaka, T. Kawai, S. Ueda, J-J. Kim, M. Kobata, E. Ikenaga, K. kobayashi, Y. Takeda, Y. Saitoh, The 2nd International Workshop on Hard X-ray Photoelectron Spectroscopy, Hyogo, Japan, September 19-20, 2006

Heterostructured Oxide Spin Devices using Tuneable Ferromagnetic Semiconductor of High TC Spinel $Fe_{3-x}Mn_xO_4$ Films, Hide. Tanaka, I. Satoh, M. Ishikawa, Y. Yanagisawa, L. Pellegrino, and T. Kawai, XIII International Workshop on Oxide Electronics, Ischia, Italy, October 8-11, 2006

Room-Temperature Spin-Polarized (Fe,Mn)3O4 Thin Films and Their Spin Polarization Properties Studied by $(Fe,Mn)_3O_4/Nb:SrTiO_3$ Schottky Contacts, I. Satoh, Hide. Tanaka,

and T. Kawai, XIII International Workshop on Oxide Electronics, Ischia, Italy, October 8-11, 2006

Electrical and magnetic properties of perovskite manganite nano-channel fabricated by AFM lithography technique, Y. Yanagisawa, L. Pellegrino, M. Hirooka, Hide. Tanaka, and T. Kawai, XIII International Workshop on Oxide Electronics, Ischia, Italy, October 8-11, 2006

Preparation of Transition Metal Oxides Nano-Array by Imprint Technique using MgO Nano-Mask, Hide. Tanaka, N. Suzuki, Y. Yanagisawa, S.Yamanaka, K. Ojima, B.K. Lee, J.H. Seo, H.Y. Lee , M. Kanai, T. Kawai, 2006 MRS (Materials Research Society) Fall Meeting, Boston, USA, November 27 - December 1, 2006

Heterostructured Oxide Spin Devices using Tunable Ferromagnetic Semiconductor of High TC Spinel $Fe_{3-x}Mn_xO_4$ Films, T. Kawai, Hide. Tanaka, I. Satoh, M. Ishikawa, Y. Yanagisawa, L. Pellegrino, 2006 MRS (Materials Research Society) Fall Meeting, Boston, USA, November 27 - December 1, 2006

Nano-patterning of epitaxial oxide films by molybdenum lift-off, N. Suzuki, Hide. Tanaka, S. Yamanaka, B. K. Lee, H. Y. Lee and T. Kawai, 5th 21st COE International symposium, Awaji, Japan, December 8-9, 2006

Tunable Current-Voltage Characteristics of $(Fe,Mn)_3O_4/Nb:SrTiO_3$ Schottky Barrier Diode, I. Satoh, J. Takaobushi, Hide. Tanaka, and T. Kawai, 5th 21st COE International symposium, Awaji, Japan, December 8-9, 2006

Hard X-ray Photoelectron Spectroscopy of Heterojunction Interface Based on Halfmetal Oxide、I. Satoh, M. Ohnishi, Hide. Tanaka, and T. Kawai, 5th 21st COE International symposium, Awaji, Japan, December 8-9, 2006

Design of Ferromagnetic Oxide Field Effect Transistor, J. Takaobushi, Hide. Tanaka, and T. Kawai, 5th 21st COE International symposium, Awaji, Japan, December 8-9, 2006

Electronic Structure of $Fe_{3-x}MxO_4$ (M=Zn, Mn) Spinel Oxide thin films as Tunable Ferromagnetic Semiconductor Investigated by Hard X-ray Photoemission Spectroscopy, J. Takaobushi, M. Ishikawa, I. Satoh, T. Yanagida, H. Tanaka, T. Kawai, S. Ueda, J.-J. Kim, M. Kobata, E. Ikenaga, K. Kobayashi, Y. Takeda, Y. Saitoh, 5th 21st COE International symposium, Awaji, Japan, December 8-9, 2006

Functional Oxides in Nano-scale, Hide. Tanaka, and T. Kawai, 5th 21st COE International symposium, Awaji, Japan, December 8-9, 2006

Nano-patterning of epitaxial oxide films by molybdenum lift-off, N. Suzuki, Hide. Tanaka, S. Yamanaka, B. K. Lee, H. Y. Lee and T. Kawai, nano tech 2007 ,Tokyo, Japan,

February 21-23, 2007

$Fe_{3-x}MxO_4$ (M=Zn, Mn) Spinel Oxide Thin Films as Ferromagnetic Semiconductor with Strongly Correlated Electron System, J. Takaobushi, M. Ishikawa, I. Satoh, Hide. Tanaka, T. Kawai, S. Ueda, K. Kobayashi, J.-J. Kim, M. Kobata, E. Ikenaga, Y. Nishino, D. Miwa, K. Tamasaku, M. Yabashi, T. Ishikawa, The 2nd Indo-Japan Seminar, "Novel Magnetic Materials and their Electronic Structures", Tokyo, Japan, February 27-March 1, 2007

Influence of Sequences and Salts on Electrical Conductivity, M. Taniguchi, T. Kawai, CREST workshop on Physics of single molecules; Transport properties of single molecules, atomic wires and DNA,May 16-18, (2006), Shonan, Japan

Influence of Sequences and Salts on Electrical Conductivity, M. Taniguchi, T. Kawai, 2006 Osaka Univ./LANL International Workshop on “The Nanoelectronics and Dynamics of DNA”, August 21-22, (2006), Hawaii, U.S.A.

Contributions to International Conferences and Journals

Tomoji Kawai	Nanotech (Chairman)
Tomoji Kawai	Surface Science (Editorial Board)
Tomoji Kawai	The 2006 Asian Conference on Nanoscience and Nanotechnology
Tomoji Kawai	9th International Conference on Atomically Controlled Surfaces, (Organizing Committee)
Tomoji Kawai	Interfaces and Nanostructures (ACSIN9) (Organizing Committee)
Tomoji Kawai	International Advisory Board of NANOTEC
Hidekazu Tanaka	The Japan Society of Applied Physics, magnetic materials and devices, program coordinator.
Hidekazu Tanaka	The Japan Society of Applied Physics, spin electronics and nano magnetics, program coordinator.
Hiroyuki Tanaka	The 2nd Nanoelectronics and Dynamics of DNA, Maui, Hawaii, August 20-22, 2006. Organizing member

Publications in Domestic Meetings

The Physical Society of Japan	25 paper
The Japan Society of Applied Physics	2 papers
The Chemical Society of Japan	1 paper
Others	7 papers

Academic Degrees

Doctor Degree for Science

Y. Yanagisawa	Fabrication of transition metal oxide nano-structure using AFM lithography and its electrical property	

Master Degree for Science

K. Yokota	Studies on electronic physical properties for single molecular electronics	

Master Degree for Engineering Science

N. Kubo	Single-molecular spectroscopy of Guanine molecule using STM/STS	

Sponsorship

21st Century Center of Excellence

T. Kawai	Toward Creating New Industries Based on Inter-Nanoscience	¥255,000,000

Grant-in-Aid for Scientific Research (A)

T. Kawai	Studies on fabrication and properties of DNA nanostructure.	¥15,600,000

Grant-in-Aid for Scientific Research (B)

Hidekazu Tanaka	Creation of room temperature spintronics devices by oxide nanostructures with strongly correlated electron system	¥4,000,000

Grant-in-Aid for Scientific Research on Priority Areas

Hidekazu Tanaka	Construction of opt-magnetic nano materials by Programmable DNA self-organization	¥7,700,000

Grant-in-Aid for Scientific Research on Exploratory Research

Hidekazu Tanaka	Development of 3 dimensional epitaxy technique by nano-particle via solution	¥2,200,000

Grant-in-Aid for Young Research (B)

T.Yanagida	Fabrication of well-defined transition metal oxide nanowires and their physical properties	¥2,100,000

Fund for JSPS Research fellowships for Young Scientist

Marcu Aurelian	Investigation on oxide film growth by pulsed	¥1,200,000

	laser deposition and the applications to functional materials		
M. Tsutsui	Investigation of single molecule photo-switching characteristics using mechanically controllable break junction technique		¥1,200,000
I. Satoh	Creation of room temperature spintronics devices by oxide nanostructures with strongly correlated electron system		¥1,100,000
M. Ohnishi	Construction of ferromagnetic Field Effect Transistor working at Room Temperature by strongly correlated oxides		¥900,000 (Refunded)
F. Yamada	Development of nano-magnetic particles array formation using programmed self assemble phenomena for an exploration of new magnetic properties		¥900,000

Entrusted Research

T. Kawai	NEDO:Development of Bio-diagnostic tool utilized development project	TORAY: Development of high sensitive gene multi-type detection biochip system which load the pre-treatment equipment	¥9,545,000 (Direct)

Other Research Fund

Hidekazu Tanaka	Kato science foundation	Preparation of ferromagnetic oxide semiconductor using Spinel Ferrite toward magnetic memory operated by electric field	¥2,000,000
Hidekazu Tanaka	Japan Science and Technology Agency, Research for Promoting Technological Seeds	Search for new strongly correlated ferromagnetic oxide and their a application for magnetic memory operated by electric field	¥2,000,000
T. Yanagida	2006-Leader-ship Funds, Researches	Fabrication system for functional low-dimensional nanostructures	¥1,500,000
T. Yanagida	Young Research Funds (A) by 21 century COE,	Fabrication of nanoporous array materials and their mechanical and transport properties	¥2,000,000

Department of Functional Ceramic Materials

Professor:	Hikaru KOBAYASHI
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Research Associates:	Kohji NOBUGAI, Taketoshi MATSUMOTO
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Graduate Students:	Yukio ISHIKAWA, Sung-Soon IM, Muhammad MADANI, Hiroaki NARITA, Kentaro IMAMURA, Masahide URAGOU, Takeru SHISHIDO
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Support Staff:	Chika KUROSAKI, Reiko NOZAKURA

Outline

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

Current Research Projects

Low Temperature Fabrication of Thick SiO_2/Si Structure by Use of Chemical Method and its Application to Thin Film Transistors (TFT)

TFT is fabricated by the deposition of SiO_2 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. SiO_2 layers formed by deposition methods possess poor characteristics, and moreover, it is impossible to form SiO_2 layers with uniform thickness on rough polycrystalline Si surfaces. Consequently, the formation of thick SiO_2 layers of ~50 nm thickness is required to achieve sufficiently low leakage current densities. Moreover, the interfacial characteristics of deposited SiO_2 layers are poor, resulting in a decrease in the mobility. Due to the large SiO_2 thickness, the electricity consumption for the TFT operation increases.

We have developed a low temperature formation method of thick SiO_2 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 SiO_2 layers with thickness more than 20 nm at ~120 °C. The SiO_2 layers formed by the first immersion possess nano-size pores, and nitric acid is decomposed at the nano-size pores during the second

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

We have produced an apparatus for nitric acid oxidation of poly-Si deposited on glass substrates with 30×42 cm^2 in size for TFT, and SiO_2 thin layers were formed on poly-Si surfaces with the apparatus. The thickness of the thin layers was 12.5±0.5 nm, and the dispersion was as small as ±0.7%. X-ray photoelectron spectroscopy (XPS) measurements showed the thin SiO_2 layers with high quality were produced. The azeotropic nitric acid oxidation method is also applied to improve characteristics of SiO_2 layers produced by the CVD method on the glass substrates of the same size. TFTs were produced successfully using the nitric acid oxidation method. Oxidation by nitric acid vapor was used to form SiO_2 layers at low temperature. SiO_2 layers grow to a thickness of more than 4 nm by oxidation with nitric acid vapor at 400°C, while conventional oxidation methods with such as dry and wet oxygen at 400°C increased the thickness of SiO_2 layers only to 2.5 nm. As for exploration of insulators which possess lower density leakage current than those of SiO_2, SiON and HfO_2 on Si layers have been investigated. SiON layers with high relative dielectric constant are produced by electrochemical oxidation in HCN aqueous solutions at room temperature, while they are generally formed by chemical reaction around 1000°C. HfO_2 layers produced on Si surfaces usually show a high interface state density due to the formation of Hf-Si bonds leading to a high density current leakage, but SiN layers between HfO_2 and SiO_2 are found to suppress these phenomena.

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/cm^2 order. Due to the great cleaning ability of the solution, the semiconductor cleaning can be performed at room temperature (cf. conventional cleaning solutions: 50~80 °C), and moreover, the cleaning solutions even with concentration as low as 0.02 % possess sufficiently high cleaning ability. Furthermore, defect states such as Si dangling bonds are passivated by the cleaning solutions, leading to improvements of characteristics of semiconductor devices such as LSI, TFT, and solar cells.

We have proved that the developed semiconductor cleaning solutions can remove

various kinds of metal contaminants such as Cu, Ni, Fe, Co, Mn, Zn, Ca, and Na from SiO_2 and Si surfaces. The mechanism of the Cu removal has been clarified. Measurement of interface states by XPS and solar cells treated with defect passivation etch-less cleaning solutions clearly showed the effect of defect passivation. We have also improved the semiconductor cleaning and defect passivation apparatus to apply to 30×42 cm^2 glass substrates for TFT.

Publications

Original Papers

Mechanism of Ni removal from Si materials using hydrogen cyanide aqueous solutions, Y.-L. Liu, M. Takahashi, H. Kobayashi, J. Electrochem. Soc. 154[1] (2006) H16-H19.

Low temperature formation of SiO_2/Si structure by nitric acid vapor, K. Imamura, O. Maida, K. Hattori, M. Takahashi and H. Kobayashi, J. Appl. Phys. 100 (2006) 114910−1-114910−4.

Interface states for HfO_2/Si structure observed by XPS measurements under bias, O. Maida, K. Fukayama, M. Takahashi, H. Kobayashi, Y.-B. Kim, H.-C. Kim and D.-K. Choi, Appl. Phys. Lett. 89[18] (2006) 122112−1-122112−3.

Room temperature formation of silicon oxynitride/silicon structure by use of electrochemical method, S.-S. Im, M. Takahashi and H. Kobayashi, J. Appl. Phys. 100 (2006) 044101−1-044101−5.

Formation of 10~30 nm SiO_2/Si structure with a uniform thickness at ~120 °C by nitric acid oxidation method, Asuha, S.-S. Im, M. Tanaka, S. Imai, M. Takahashi, H. Kobayashi, Surf. Sci. 600 (2006) 2523-2527.

Mechanism of copper removal from SiO_2 surfaces by hydrogen cyanide aqueous solutions, N. Fujiwara, Y.-L. Liu, M. Takahashi and H. Kobayashi, J. Electrochem. Soc. 153 [5] (2006) G394-G398.

Reaction of cyanide ions with copper on Si surfaces and its use for Si cleaning, Y.-L. Liu, N. Fujiwara, H. Iwasa, M. Takahashi, S. Imai and H. Kobayashi, Surf. Sci. 600 (2006) 1165-1169.

Nitric acid oxidation of Si method for the formation of high quality Si/SiO_2 structure at ~120 °C, H. Kobayashi, Asuha, S.-S. Im, S. Imai and M. Takahashi, Algerian J. Adv. Mater. 3 (2006) 104-108.

Si Cleaning Method Having Defect Passivation Effect by Use of HCN Aqueous Solutions, M. Takahashi, Y.-L. Liu, H. Narita and H. Kobayashi, Algerian J. Adv. Mater. 3 (2006) 131-134.

Methods of observation and elimination of semiconductor defect states, H. Kobayashi,

Y.-L. Liu, A. Asano, Y. Yamashita, J. Iváncho and M. Takahashi, Solar Energy 80 (2006) 645-652.

A method of observation of low density interface states by means of X-ray photoelectron spectroscopy under bias and passivation by cyanide ions, H. Kobayashi, T. Sakurai, Y. Yamashita, T. Kubota, O. Maida and M. Takahashi, Appl. Surf. Sci. 252 (2006) 7700-7712.

Passivation of Si and a-Si:H surfaces by thin oxide and oxy-nitride layers, E. Pinčík, H. Kobayashi, J. Rusnák, M. Takahashi, R. Brunner, M. Jergel, A. Morales-Acevedo, L. Ortega and J. Kákoš, Appl. Surf. Sci. 252 (2006) 7713-7721.

On a presence of Si_mH_n clusters in a-Si:H/c-Si structures, M. Kopani, E. Pinčík, H. Kobayashi, M. Takahashi, N. Fujiwara, R. Brunner, M. Jergel and L. Ortega, Appl. Surf. Sci. 252 (2006) 7722-7725.

Formation of atomically smooth SiO_2/SiC interfaces at ~120 °C by use of nitric acid oxidation method, S. Imai, M. Fujimoto, Asuha, M. Takahashi, and H. Kobayashi, Surf. Sci. 600 (2006) 547-550.

Silicon cleaning and defect passivation effects of hydrogen cyanide aqueous solutions, M. Takahashi, Y.-L. Liu, N. Fujiwara, H. Iwasa, and H. Kobayashi, Solid State Commun. 137 (2006) 263-267.

Patents

Methods and apparatuses of formation of insulating films, production of semiconductor apparatuses, semiconductor apparatuses and, treatment methods of SiC surfaces, H. Kobayashi, Tokugan 2006-218012.

Photosemiconductor apparatuses and production method of the apparatuses, H. Kobayashi, Y. Shimizu, Tokugan 2006-239646.

Method of formation of oxide films, semiconductor apparatuses with the oxide films, production method of semiconductor apparatuses, H. Kobayashi, PCT/JP2006/314232.

International Conferences

New defect passivation method for solar cells, H. Kobayashi, The 8th International Symposium on Eco-Materials Processing and Design, Kitakushu, Japan, Jan. 11-14, 2007.

Si defect passivation and cleaning method by use of new chemistry (Invited), M. Takahashi, International Congress on Materials Science and Engineering 2006 (CISGM4), Algeria, May. 2-4, 2006.

Two-step nitric acid oxidation of Si and SiC (NAOS) method for the formation of SiO_2/Si and SiO_2/SiC structures at 120 ºC (Invited), H. Kobayashi, 5th International

Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

Semiconductor surface cleaning and passivation by the chemical treatment in solutions of hydrogen cyanide (Invited), *M. Takahashi, 5th International Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

Improvement of Si solar cell characteristics by new defect passivation method, H. Kobayashi, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Low temperature fabrication of 3C-SiC/SiO_2 MOS structures by nitric acid oxidation, *M. Takahashi, S.-S. Im, Asuha, H. Kobayashi, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Improved Cleaning Method of SiC Using HCN Aqueous Solutions and 100 % H_2 Treatment, *M. Madani, Y.-L. Liu, S.-S. Im, M. Takahashi, H. Kobayashi, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Low Temperature Oxidation of 4H-SiC by Use of Nitric Acid Oxidation Method, *Y. Ishikawa, Asuha, S. Imai*, M. Takahashi, H. Kobayashi, 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Contributions to International Journals

H. Kobayashi	Applied Surface Science (Editor)

Publications in Domestic Meetings

The Physical Society of Japan	2 papers
The Japan Society of Applied Physics	6 papers
Surface Electronics Society / Seminar on spectroscopic investigation for adsorbed molecules	1 paper
The Japan Vacuum Society	1 paper
Japan Society of Powder and Powder Metallurgy	1 paper
The Surface Science Society of Japan	1 paper
IMAGINE seminar	1 paper
Kansai Semiconductor Analysis Technology Society	1 paper

Academic Degrees

Doctor Degree of Science

S.-S. Im — Low Temperature Formation of Insulating Layers for Si and SiC-based Metal-Insulator-Semiconductor Structure

Master Degree of Science

H. Narita — Adsorption of Cu and removal of Cu particles with HCN solution on Si surfaces

Sponsorships

Entrusted Research

H. Kobayashi	Japan Science and Technology Organization	Development of semiconductor cleaning solutions with defect passivation effect	¥38,480,000
H. Kobayashi	Japan Science and Technology Organization	Low temperature formation of TFT gate oxide layers and lower power consumption by the nitric acid oxidation method	¥74,100,000
M. Takahashi	Japan Science and Technology Corporation	Suppression of Charge Carrier Recombination in Polycrystalline Si by Cyanide Treatment	¥1,170,000

Department of Frontier Materials Creation

Associate Professor:	Tohru SEKINO
Research Associate:	Takafumi KUSUNOSE
Post Doctoral Fellows:	Seung-Ho KIM
Graduate Students:	Myoung-Jae CHO, Youn-Gyu HAN, Hideki HASHIMOTO, Sook-Young MOON, Shinya ITANO, Nobuaki SAKAYANAGI, Asuka HAYASHI, Takako SHIMIZU, Xingping YE
Research Student:	Dong-Jin PARK (2006.10.1-2007.3.31)
Under Graduate Students:	Hayato HIJIKATA
Supporting Staff:	Rie SUEHIRO

Outline

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 structures 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 metalic and organic materials. Thus the target of these researches is to develop a new class of hyper-functionalized materials, which ranges ceramic, metal and organic materials.

Current Research Projects

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 a 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 temperatures. Developments of new ceramic nanocomposites possessing superplasticity, machinability are also achieved by synthesizing nanostructured and nanocomposite powders, and/or by using conventional sintering methods, 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 nanotubes such as carbon nanotubes. These 3D networks were used for the conductive pathway of electric current that realized conductive structural ceramics. Various compounds were formed as the grain-boundaries of AlN, ZrO_2 and so son, 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 nad excellent electrical properties such as electro-discharge machining capability like metals, that would open a 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 Al_2O_3/W,Mo,Ni,Cu,Co,Fe, ZrO_2/Ni,Mo, MgO/Fe,Co,Ni, and also for ceramic/intermetallic compound such as ZrO_2/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 s metal substrate and performances have been investigated. In addition, novel low-temperature processing and oxide/monoxide nanocomposite have been developed to realize s 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 a small amount of ceramic or metallic nanoparticles into $BaTiO_3$, ZnO, c-ZrO_2 can significantly improve their mechanical strength, hardness and toughness which are very important to realize high reliable electric devices operating in severe environmental conditions. 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 the resultant enhancement of thermoelectric performance at high temperatures has bee 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 temperatures 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 quiet 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 have succeeded to synthesize Titania (TiO_2) 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 an open-end structure. This new-type of material has attracted much attention because of its low-dimensional nanotube structure of oxide semiconductor and the resultant high surface area, and we have clarified it has excellent photocatalytic properties and high capability as the electrode of solar cell and ion battery. Also, various cations have been successfully doped into the nanotubes, and the electrical conductivity was increased with incorporation of a 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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Books

Patents

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Aluminum Nitride/ Boron Nitride Nanocomposite Powder and Their Fabrication Methods, T. Kusunose, T. Sekino, N. Sakayanagi, S. Kikutani, M. Azuma, JP2006-170508.

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International Conferences

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Thermal properties and Microstructure of Zirconia/Monazite-type $LaPO_4$ Composites for Powder Preparation Methods, *S.-H. Kim, T. Sekino, T. Kusunose, A. Hirvonen, The 8th International Symposium on Eco-Materials Processing and Design (ISEPD 2007), Kitakyushu International Conference Center, Kitakyushu, Japan, Jan.11-14, 2007.

Hot-pressed AlN/BN Composite with Excellent Mechanical and Thermal Properties, *T. Kusunose, M.-J. Cho, T. Sekino, K. Niihara, The 8th International Symposium on Eco-Materials Processing and Design (ISEPD 2007), Kitakyushu International Conference Center, Kitakyushu, Japan, Jan.11-14, 2007.

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Residual Stress Measurement of Plasma Sprayed Coating Layers in ZrO_2, S.-W. Lee, *J. Zhang, H. Chen, J.-S. Song, J.-K. Seo, T. Sekino , The 8th International Symposium on Eco-Materials Processing and Design (ISEPD 2007), Kitakyushu International Conference Center, Kitakyushu, Japan, Jan.11-14, 2007.

Contributions to International Conferences and Journals

T. Sekino	The International Symposium on Eco-Materials Processing and Design (Academic Committee)
T. Sekino	11th International Conferences on Modern Materials and Technologies (CIMTEC 2006) (Advisory Board)
	International Symposium on Hybrid Nano Materials Toward Future Industries (HNM 2006) (Co-Chair)
T. Sekino	The 7th Pacific Rim Conference on Ceramics and Glass Technology (Organizing Committee)

	Nanostructured and Multifunctional Materials Symposium at the 7th Pacific Rim Conference on Ceramic and Glass Technology (Symposium Steering Chair)
T. Sekino	The International Conference on Knowledge Management for Composite Materials, Nanotechnology and Alternate Energy (ACTSEA-2007) (International Advisory Board)
T. Sekino	Key Engineering Materials (Guest Editor)

Publications in Domestic Meetings

The Ceramic Society of Japan	11 papers
Japan Society of Powder and Powder Metallurgy	2 papers

Academic Degrees

Master Degree for Engineering

S. Itano	Synthesis of the TiO_2NT/ZnS Nanocomposites, and Evaluation of Their Structure and Properties
N. Sakayanagi	Fabrication of AlN/BN Composites by Sintering of Nanocomposite Powders Synthesized through Carbothermal Reduction and Nitridation of Complex Oxide

Bachelor Degree for Engineering

H. Hijikata	Fabrication Process of Si_3N_4 Ceramics with Transparency to Visible and Infrared Ray and Its Optimization

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas

T. Sekino	Development of Rare-Earth - Transision Metal Complex Oxide Thermoelectric Materials and Their Mechanisms Elucidation	¥1,800,000

Entrusted Research

T. Sekino	NEDO (Materials Nanotechnology Program, Nanocoating Project)	Development of Nanocomposite Coating by In-situ Structuralization.	¥5,040,000

Contribution to Research

T. Sekino	Otsuka Chemical Co., Ltd.	¥600,000
T. Sekino	Inaba Rubber Co., Ltd.	¥1,000,000
T. Sekino	Nagamine Manufacturing Co., Ltd.	¥300,000
T. Sekino	Nikkato Corporation	¥1,000,000

T. Sekino	A.L.M.T. Corp., Ltd.		¥500,000
T. Kusunose	Nippon Tungsten Co., Ltd.		¥500,000
T. Kusunose	Tosoh Corporation		¥500,000

Cooperative Research

T. Sekino	Tomoe Works Co. Ltd.	Development of Novel Nanocomposites and Their Processing	¥420,000
T. Sekino	Shiga Prefecture	Studies on the Development of Thermoelectric Materials	¥0
T. Kusunose	Sumitomo Electric Industries, Ltd.	Synthesis of Phosphor Exited by Electron or Electric Field	¥300,000
T. Sekino T. Kusunose	Tokuyama Corporatin	Development of AlN/BN Nanocomposites with High Fracture Toughness and High Strength	¥0

Other Research Fund

T. Sekino	NEDO (Industrial Technology Research Grant Program in 2004)	Hyper-functionalization of Oxide Nanotube and Its Application for Environmentally-harmonized Systems	¥6,760,000
T. Kusunose	Izumi Science and Technology Foundation	Fabrication of Electrically Conductive AlN Ceramics with High Thermal Conductivity by Grain Boundary Control	¥1,000,000
T. Kusunose	The Die and Mold Technology Promotion Foundation	Fabrication of SiC/BN Nanocomposite Mold by Carbothermal Reduction and Nitridation of Borosilicate Glass	¥1,000,000

Department of Advanced-Energy Material

Professor:	Katsumi TANIMURA
Associate Professor:	Shin'ichiro TANAKA
Designated Research Assoc.	Ei'ichi INAMI,
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Under Graduate Students:	Kousuke Maeno
Support Staff:	Sachiyo NOZAWA, Masanobu NUNOGAKI

Outline

For fabricating highly functional nano-structured devices in future technology, it is essential to establish the ways to control structures and compositions of materials at the atomic level. In this department, we aim to establish the fundamentals for controlling the ***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 Projects

1. Excitation-Induced Instability on Semiconductor Surfaces

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

2. Ultra-fast surface carrier dynamics on semiconductor surfaces studied by

femtosecond two-photon photoelectron spectroscopy

We have studied the carrier 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 several photoinduced reactions on solid surfaces. Use of femtosecond laser for pump and probe pulses has a strong advantage for resolving the carrier dynamics directly. In particular, the new system based on a tunable OPA laser for pump pulses of 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) and Si(111)-(7x7) surfaces, we have found an ultrafast electron-hole recombination via surface localized states with 1 ps of excitation. Also, the lifetime of the surface D_{down} state is 15 ps, and has an effective surface electron-hole recombination, thus leading to strong density-dependent kinetics of carrier dynamics on this surface. At longer time delays, the transition from bulk-to-surface states is rate-determining of the surface-state population. Consequently, apparent decay of electrons at the surface D_{down} state shows a strong excitation-wavelength dependent feature.

3. 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 have shown a reasonable performance in intensity and in stability.

Publications

Original Papers

Fomation and Clustering of Surface Vacancies under Electronic Excitation on Semiconductor Surfaces, J. Kanasaki, Physica, B376-377 (2006) 834-840.

Two-Hole Localization Mechanism for Electronic Bond Rupture of Surface Atoms by Laser-Induced Valence Excitation of Semiconductors, K. Tanimura, E. Inami, J. Kanasaki, and W. P. Hess, Physical Review, B 74[3] (2006) 035337-1-8.

Excitation-Induced Structural Instability of Semiconductor Surfaces, K. Tanimura and J. Kanasaki, J. Physics: Condensed Matter, 18 [30] (2006) 1479-1516.

International Conferences

Excitation Wavelength and Density Dependent Carrier Dynamics on Si Surfaces

(Invited), K. Tanimura, Dynamik von Elektronentransferprozessen an Grenzflächen, Berlin, Germany, September 24-26, 2006

Graphite-to-Diamond Phase Transformation Induced by Femtosecond-Laser Excitation (Oral), K. Tanimura, *****J. Kanasaki, K. Nasu**,** The 5th International Symposium on Ultrafast Surface Dynamics, Abashiri, Japan, May21-26, 2006.

Density-Dependent Ultrafast Carrier Dynamics on Si surfaces (Oral), *T. Ichibayashi, K. Tanimura, The 5th International Symposium on Ultrafast Surface Dynamics, Abashiri, Japan, May21-26, 2006.

Femtosecond Laser-Induced Phase Transformation on Graphite Surface –Creation of a Novel Crystalline Phase of sp^3-Bonded Carbon－, *K. Kimura, J. Kanasaki, K. Tanimura, K. Nasu, 24th European Conference on Surface Science, Paris, France, September 4-8, 2006.

Structural Instabilities Induced by Injected Tunneling Carriers on Cleaved InP(110)-(1x1) Surfaces, *J. Kanasaki, K. Ichihashi, J. Tsuruta, E. Inami, K. Tanimura, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006.

Photo-Induced Phase Transformation on Graphite Surface, *K. Kimura, J. Kanasaki, K. Tanimura, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006.

Femtosecond Laser-Induced Phase Transformation on Graphite Surfaces, *K. Kimura, J. Kanasaki, K. Tanimura, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9, 2006

Structural Instabilities Induced by Carrier Injection from Scanning Tunneling Microscope Tips on Cleaved InP(110)-(1x1) Surfaces, *E. Inami, J. Kanasaki, K. Tanimura, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9, 2006.

Excitation-Induced Processing for Highly Functional Nano-Structured Materials, E. Inami, *J. Kanasaki, S. Tanaka, and K. Tanimura, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9, 2006.

Structural Instabilities on InP(110)-(1x1) Surfaces Induced by Hole-Injection from the STM Tip, E. Inami, J. Tsuruta, and *J. Kanasaki, 11th International Workshop on Desorption Induced by Electronic Transitions (DIET-XI), Berlin, Germany, March 11-15, 2007.

Excitation-Induced Atomic Desorption and Structural Instability of Semiconductor Surfaces (Invited), K. Tanimura, 11th International Workshop on Desorption Induced by

Electronic Transitions DIET-XI, Berlin, Germany, March 11-15, 2007.

Excitation-Wavelength dependent Ultrafast Carrier Dyniamics on Si Surfaces (Oral), *T. Ichibayashi, K. Tanimura, 11th International Workshop on Desorption Induced by Electronic Transitions DIET-XI, Berlin, Germany, March 11-15, 2007

Contributions to International Conferences and Journals

K. Tanimura International Workshop on Desorption Induced by Electronic Transitions （International Steering Committee member）

Publications in Domestic Meetings

The Physical Society of Japan	8 papers
The Japan Society of Applied Physics	1 paper
The Surface Science Society of Japan	1 paper

Academic Degrees

Master Degree for Engineering

K.Kimura	Photoinduced Structural Phase Transition on Graphite Surfaces
T. Ichihashi	Surface Structural Instability on Hydrogen-Terminated Si(001)-(2x1) Induced by Low-Energy Electron Beams

Sponsorships

Grant-in-Aid for Scientific Research (*)(*)

(A)		¥13,700,000
K. Tanimura	Study of Excited-State Properties of Quasi-Two Dimensional Semiconductor Surfaces	
(C)		
J. Kanasaki	Structural Instability of Semiconductor Surfaces Induced by Low-Energy Electron Beam Excitation	¥500,000

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 molecular glue for DNA
- Photoregulation of RNA-ligand interaction by photoresponsive peptide and its aptamer obtained by in vitro selection
- Detection of single nucleotide polymorphisms by allele specific PCR
- Development of molecules binding to DNA repeat sequence
- 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
Technical staff: Fumie Takei
Post Doctoral Fellows: Jinhua Zhang, He Hanping
Graduate Students: Gosuke Hayashi, Kyong-in Ryu
Under Graduate Students: Shin-nosuke Uno
Research Assistance: Mika Oku, Akiko Seo, Yuka Kubota
Supporting Staff: Miho Ohama

Outlines

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

Current Research Project

Development of Technology for Single Nucleotide Polymorphisms

The technique for promptly detecting the genetic mutation is expected as a basis technology that supports the personalized medicine. In this laboratory, we have proposed the technology for genetic mutation detection that uses a small molecule binding to the mismatch and the bulge structure in the duplex DNA. The practical technology must be handy, accurate, and cheap in cost. To meet this demand, we did not study the chemical modification of DNA, but used the molecule selectively binding to the cytosine bulge. Upon binding to cytosine bulge, the fluorescence wave length shifted the long wave length by 30 nm. By using this characteristic fluorescence, we have succeeded to develop the method detecting single nucleotide polymorphisms

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

The telomeric sequence $d(TTAGGG)_n$ located at the 3’ end of human genomic DNA plays important roles in protecting chromosomal ends from fusion, rearrangement, and translocation. In cancer cells the enzyme telomerase is activated maintains the length of the telomere for achieving the immortality. Therefore, the ligands that bind to telomere and inhibit its elongation are expected to be potential anti-cancer drugs. The single-stranded region of the $d(TTAGGG)_n$ repeat is known to form G-quadruplex structures *in vitro*. We synthesized a novel ligand naphthyridine tetramer (**NT**) and evaluated its specific binding to the human telomeric repeat sequences. The results from enzymatic analyses together with spectroscopic measurements clearly showed that **NT**

did not inhibit telomerase but interfere the telomere elongation by a formation of unique hairpin structure on the template. The novel mode of **NT** binding to the human telomere sequence would be useful for the design of molecules in a next generation.

Development of molecular glue for DNA

Hybridization of single-stranded DNA with its complementary strand is important not only in many biological processes but also in DNA-based bioassays and nanodevices. Modulation and control of the formation of double-stranded DNA is a general strategy to enhance, limit, or trigger these biological processes and functions. We have introduced a new concept of molecular glue for DNA to turn on the hybridization of natural non-modified DNA using a synthetic small molecule. The molecular glue, naphthyridine carbamate (**NC**), can adhere two natural single-stranded DNAs that do not spontaneously hybridize with each other. However, the function of **NC** does not include the dehybridization of duplex once formed and limited to the unidirectional control of DNA hybridization events. To achieve the bidirectional control to turn on and off DNA hybridization, we have developed a novel molecule **TD** representing thermally degradable molecular glue for DNA. Thermal conversion of **TD** irreversibly into the inactive form allows us to run the DNA hybridization/dehybridization cycle by the consumption of **TD**. This new method for turning on and off DNA hybridization has been applied to control the assembly of gold nanoparticles.

Synthesized DNA bearing transition metal chain

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

Publications

Original Papers

Evaluation of Mismatch-binding Ligands as Inhibitors for Rev-RRE Interaction, Nakatani, K.; Horie, S.; Goto, Y.; Kobori, A.; Hagihara, S. Bioorg. Med. Chem. 14 (2006) 5384-5388.

Mismatch Binding Ligands Function as Molecular Glue for DNA, Peng, T.; Dohno, C.; Nakatani, K. Angew. Chem. Int. Ed. 45 (2006) 5623-5626.

International Conferences

Fluorescent Determination of SNPs Using N,N-bis(3-aminopropyl)-2,7-diamino-1,8-naphthyridine, *Fumie Takei, Masaki Hagihara, Jinhua Zhang, Kazuhiko Nakatani, XVII International Roundtable on Nucleosides Nucleotides and Nucleic Acids, Bern, Switzerland, Sep3-7, 2006

Application of L-DNA as Molecular Tag, *Gosuke Hayashi, Kazuhiko Nakatani, XVII International Roundtable on Nucleosides Nucleotides and Nucleic Acids, Bern, Switzerland, Sep3-7, 2006

Mismatch Binding Ligands Function as Molecular Glue of DNA, Tao Peng, Chikara Dohno, *Kazuhiko Nakatani, XVII International Roundtable on Nucleosides Nucleotides and Nucleic Acids, Bern, Switzerland, Sep3-7, 2006

Molecular Design and Applications of Mismatch Binding Ligands, *Kazuhiko Nakatani, The 11th Korea-Japan Joint Symposium on Drug Design and Development, Jedu Island, Korea, May10-12, 2006.

Molecular Glue for DNA, *Kazuhiko Nakatani, 2006 Mini-Symposium on the Frontiers of Organic/Bioorganic Chemistry, POSTECH, Pohan, Korea, Nov30-Dec2, 2006

Publications in Domestic Meetings

Japan Chemical Society Meeting:	4 papers
Symposium on Nucleic Acids Chemistry in Japan:	3 papers
Sanken International Symposium on Nanoscience and Nanotechnology 2006	3 papers
Japanese Society for Chemical Biology Meeting:	1 paper
Symposium on Photochemistry	1 paper

Sponsorship

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

K. Nakatani	Regulation of DNA Structure and Function Based on the Stabilization of DNA Duplex	¥23,800,000
Z. Da-Yang	Synthesis of Novel Cyclic Nucleotides Library by Metal-Catalyst	¥1,900,000
F. Takei	Development of SNP detection method with modified PCR primers	¥2,300,000

Grant-in-Aid for Young Scientists

C. Dohno	Development of Photo-Responsive Mismatch Binding Ligands	¥900,000

Entrusted Research

K. Nakatani	Japan Science and Technology Agency	Fluorescent detection of SNPs by allele specific PCR	¥2,692,000
K. Nakatani	Japan Science and Technology Agency	Development of SNP detection method by allele-specific PCR with tagged primers	¥2,000,000
K. Nakatani	Japan Science and Technology	Investigation of novel functions generated from the	¥3,900,000

	Agency	biomaterials at interfaces	

Other Research Fund

K. Nakatani	KYOWA HAKKO KOGYO CO., LTD	Design of RNA-binding small molecules	¥3,000,000
K. Nakatani	NITTO KASEI CO., LTD	Synthesis of DNA-binding ligands	¥420,000
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	¥39,490,000

Department of Organic Fine Chemicals

Professor:	Nobuo KATO
Associate Professor:	Junko OHKANDA
Research Associates:	Hajime Nitta, Tomikazu KAWANO
Post Doctoral Fellow:	Shuichi MORI (2006.4.1-2006.11.30)
Graduate Students:	Masamitu HIRAOKA, Takatsugu INOUE, Ichiro IMADA, Taro ENOMOTO, Masato HIRANO, Shinnosuke MACHIDA, Yu HARANOSONO, Yusuke HIGUCHI, Toshio MAKI, Shinya MIYAKE
Under Graduate Student:	Yuta FUKAI
Supporting Staff:	Misuzu TANNO

Outlines

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

Current Research Project

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 ISIR-005 that can be regarded as a new lead of anti-cancer agent.

Synthesis of 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 known to be used for inter-species communication. We have designed and synthesized AI-2 antagonists, which can potentially be used as inhibitors for dental plaque formation.

Module Assembly for Protein Surface Recognition: Bivalent Geranylgeranyl-transferase-I Inhibitors for Simultaneous Targeting Interior and Exterior Protein

Surfaces
Modulation of protein-protein interactions by small organic agents still remains a difficult challenge due to the large interfacial areas of buried surface involved in such interactions. As an attempt to improve binding selectivity of the organic agents to targeting protein surface, a series of bivalent enzyme inhibitors consisting two distinct modules, which were designed for complementary recognition of characteristic protein interior and exterior surfaces, was synthesized. The inhibition potency of this family of the compounds against mammalian GGTase-I was evaluated by fluorescent enzyme assay using the fluorogenic substrate, and the results showed that additivity of each module was observed upon the enzyme inhibition. Most importantly, the bivalent compounds were found to be a competitive inhibitor for GGTase-I with high selectivity over a related enzyme, farnesyltransferase.

Combinatorial Library of Asymmetric Metal Complexes and Lead Discovery for Protein Surface Recognition
The goal of this project is to construct a stable assembly of low-molecular-weight modules that consist of appropriate functional groups for complementary binding to the targeting protein surfaces. A series of trisbipyridne ruthenium complexes consisting various functional group at 4, 4'-position of the bipyridine ligands was synthesized, and was screened for inhibition activity against alpha-chymotrypsin using the chromogenic substrate, which allows us to run the kinetic enzyme assay. Among them, the complex bearing phenylalanine residues showed the best inhibition activity (73% inhibition at 50 μM), whereas the one having cationic charged residue derived from lysines showed no activity, suggesting that the complementary electrostatic interaction in between the complex and the protein surface near the active site remarkably dictates the inhibition potency.

Publications

Original Papers
Synthesis and Inclusion Properties of 6,6'-Bi(benzo[*b*]fluoren-5-ol) derivative by cycloaromatization, T. Kawano, M. Suehiro and I. Ueda, Chem. Lett., 35[1] (2006) 58-59.

Structure-Based Design of Imidazole-Containing Peptidomimetic Inhibitors of Protein Farnesyltransferase, J. Ohkanda, C. L. Strickland, M. A. Blaskovich, D. Carrico, J. W. Lockman, A. Vogt, C. J. Bucher, J. Sun, Y. Qian, D. Knowles, E. E. Pusateri, S. M. Sebti and A. D. Hamilton, Org. Biomol. Chem., 4[3], 482-492 (2006).

One-Pot Synthesis of 3-Bromoimidazo[1,2-*a*]pyridine Derivatives Accompanied by Dimethyl Sulfoxide Oxidation, T. Kawano and N. Kato, Chem. Lett., 35[3] (2006) 270-271.

Effect of Water Molecules on the Cycloaromatization of Non-Conjugated Aromatic Tetraynes, T. Kawano, H. Inai, K. Miyawaki and I. Ueda, Bull. Chem. Soc. Jpn., 79[6] (2006) 944-949.

Review Papers

Lipase-Catalyzed Synthesis of Novel Tea Catechin Derivatives and Their Application to Anti-Influenza Agents, K. Kaihatsu, S. Mori, S. Miyake, T. Nakaya, S. D. Fuller and N. Kato, Yakugaku Zasshi, 126 (2006), 57-58.

Patents

12-Deoxyfusicoccins as Differentiation Inducers, N. Kato, Y. Honma, T. Sassa, H. Nitta, T. Yoshino and T. Inoue, JP2006-197482.

12-Deoxyfusicoccins as Differentiation Inducers, N. Kato, Y. Honma, T. Sassa, H. Nitta, T. Yoshino and T. Inoue, PCT/JP2007/051799.

Modulators for the Receptor of Autoinducer-2, N. Kato, M. Hiraoka, J. Ohkanda, T. Kawano, A. Yamaguchi, T. Hirata, K. Nishino, S. Ebisu and B. L. Bassler, JP2007-056450.

A Chimera Fusicoccane Synthase and Its Gene, T. Toyomasu, T. Sassa, T. Dairi and N. Kato, JP2007-094968.

International Conferences

Anti-Cancer Activity of Fusicoccane Diterpene Glycosides (Invited), *N. Kato, 22nd Conference on Combinatorial Chemistry, Japan, Osaka, Japan, Apr. 19-20, 2006.

Synthesis of Fusicoccin Derivative as a Differentiation Inducer, *T. Inoue, T. Yoshino, H. Nitta, T. Kasukabe, Y. Honma, T. Sassa and N. Kato, ICOB-5 & ISCNP-25 IUPAC, Kyoto, Japan, Jul 23-28, 2006.

Hybrid GGTase-I Inhibitors Targeting both Interior and Exterior Protein Surfaces, *J. Ohkanda, S. Machida, N. Kato, K. Harada, The 2nd International Symposium on Bimolecular Chemistry, Kobe, Japan, Aug 7-8, 2006.

Design, Synthesis and Biological Evaluation of Hybrid GGTase-I Inhibitors Targeting both Exterior and Interior Protein Surface, *S. Machida, N. Kato, J. Ohkanda, SANKEN International symposium on Nanoscience and Nanotechnology, Osaka, Japan, Sep 19-20, 2006.

Regulation of DNA Transcription by Infrared Controllable Antigene Peptide Nucleic Acids, *I. Imada, K. Kaihatsu, X. Cai, M. Fujitsuka, T. Majima and N. Kato, SANKEN International Symposium on Nanoscience and Nanotechnology, Osaka, Japan, Sep 19-20, 2006.

Synthesis of Monoester Derivatives of Epigallocatechin Gallate Using Pancreatic Esterase and Their Application to Antiviral Agents, *S. Mori, K. Kaihatsu, S. Miyake, T. Nakaya and N. Kato, SANKEN International Symposium on Nanoscience and Nanotechnology, Osaka, Japan, Sep 19-20 2006.

A New Medicinal Chemical Approach to Target Protein-Protein Interactions, *J. Ohkanda, Japanese-German Frontiers of Science Symposium, Heidelberg, Germany, Nov 3-5, 2006.

Synthesis of Autoinducer-2 Antagonists in Bacterial Quorum-Sensing, *M. Hiraoka, Y. Yano, T. Kawano, H. Hirakawa, A. Kobayashi, T. Hirata, A. Yamaguchi, J. Ohkanda and N. Kato, 5th 21st Century COE "Toward Creating New Industries Based on Inter-Nanoscience", Hyogo, Japan, Dec 8-9, 2006.

Anti-Cancer Activities of Fusicoccane Diterpenoids: Differentiation Inducing Activity vs Cytotoxicity, T. Inoue, H. Nitta, J. Ohkanda, T. Kasukabe, Y. Honma, T. Sassa and *N. Kato, 5th 21st Century COE "Toward Creating New Industries Based on Inter-Nanoscience", Hyogo, Japan, Dec 8-9, 2006.

Regulation of DNA Transcription by Infrared Controllable Antigene Peptide Nucleic Acids, *K. Kaihatsu, X. Cai, M. Fujitsuka, T. Majima and N. Kato, 5th 21st Century COE "Toward Creating New Industries Based on Inter-Nanoscience", Hyogo, Japan, Dec 8-9, 2006.

Synthesis of Monoester Derivatives of Epigallocatechin Gallate Using Pancreatic Esterase and Their Application to Antiviral Agents, *S. Mori, K. Kaihatsu, S. Miyake, T. Nakaya and N. Kato, 5th 21st Century COE "Toward Creating New Industries Based on Inter-Nanoscience", Hyogo, Japan, Dec 8-9, 2006.

Contributions to International Conferences and Journals

N. Kato	ICOB-5 & ISCNP-25 IUPAC (Organizing Committee)
N. Kato	23rd Conference on Combinatorial Chemistry, Japan (Organizing Committee)

Publications in Domestic Meetings

The Chemical Society of Japan	6 papers
The Pharmaceutical Society of Japan	1 paper
Japan Society for Bioscience, Biotechnology, and Agrochemistry	1 paper
The Japanese Society for Chemical Regulation of Plants	1 paper
Symposium on the Chemistry of Natural Products	1 paper
Japanease Society for Chemical Biology	1 paper
Japanese Society of Cathecinology	1 paper
Others	3 papers

Academic Degrees

Master Degree for Science

T. Inoue	Synthesis of Diterpene Glycosides That Have a Differentiation-Inducing Activity and Their Mode of Action

I. Imada	Synthesis of Azobenzene Derivatives That Are Isomerizable by Infrared Two-Photons Excitation and Their Application to the Regulation of DNA Transcription
T. Enomoto	Synthetic Studies of Sordaricin Congeners Having Anti-Fungal Activity
M. Hirano	Isoform-Selective Ras Inhibitors Targeting Poly-Lysine Domain Near the C-Terminus of the Protein
S. Machida	Hybrid GGTase-I Inhibitors for Simultaneous Recognition of Exterior and Interior Protein Surface

Sponsorship

Grant-in-Aid for Scientific Research (C)

J. Ohkanda	Molecular Glue-Driven Module Assembly for Protein Surface Recognition	¥3,700,000

Grant-in-Aid for Scientific Research (A)

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

Grant-in-Aid for Scientific Research in Special Area

N. Kato	Analysis and Control of Intracelluar Signal Transductions by Use of Diterpene Glycosides as Tools	¥2,800,000

Entrusted Research

T. Kato	Program for Promotion of Fundamental Studies in Health Sciences of the National Institute of Biomedical Innovation	Development of the New Anti-Cancer Agent Based on the Differentiation-Inducing Diterpene Glycoside	¥15,000,000

Other Research Fund

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
J. Ohkanda	Suzuken Memorial	Molecular Glue-driven in Vivo Module Assembly and	¥1,000,000

Foundation	Regulation of Protein Surface Function

Department of Organic Molecular Materials

Professor:	Yoshio ASO
Associate Professor:	Takahiro KANEDA
Research Associate:	Yutaka IE
Research Assistant:	Kaori ASANO
Post Doctoral Fellows:	Aihong HAN (-2006.6.30)
	Muhammad Mizanur RAHMAN (2006.9.16-2007.3.15)
Graduate Students:	Nobukazu NEGISHI, Yoshikazu UMEMOTO
	Setsuko ISHIOKA, Masaru ENDO, Liu FENG
	Masashi NITANI, Tomoya HIROSE
Under Graduate Students:	Makoto OKABE, Nobuhiro YAMAMOTO
Supporting Staff:	Misayo IMAI

Outlines

The main subject in the Department of Organic Molecular Materials is the development of novel molecular-based materials with promising electronic and photoelectronic properties for molecular electronics and the development of highly organized supermolecules for supramolecular machines. The research is based on the elucidation of the relationship between molecular structures and physical properties to control and improve the functions. We have been focusing our research on the design, synthesis, and properties of (1) novel extended conjugation systems as active materials for organic electronic and photoelectronic devices, (2) nano-scale conjugated molecules for promising molecular wires, and (3) supermolecules composed of permethylated cyclodextrins and various pi-systems especially azobenzenes, stilbenes, and tolans. These nano-scale molecular materials have potential use as a fundamental framework for molecular machines or electronics.

Current Research Project

Organic Electronics Materials

We have developed organic materials for n-type organic field-effect transistors (FETs). It has been known that the introduction of perfluoroalkyl groups into pi-conjugated systems dramatically increases n-type character. We have newly designed hexafluorocyclopenta[c]thiophene and difluoromethylene-bridged bithiophene monomer units and synthesized their based oligothiophenes. Their electronic absorptions, X-ray analysis, and redox potentials indicated that the ring fusion of fluoroalkylene units to thiophenes not only keeps the planarity between consecutive thiophene rings but also increases n-type character. Preliminary experiments revealed that the bottom-contact FET devices based on the sexithiophenes show n-type response.
In anticipation of self-association properties, we have synthesized the highly branched oligothiophenes with the juncture of 1,3,5-trisubstituted benzene for the development of high carrier-mobility materials in a film. The association constants revealed an increasing association properties with increasing the number of branch points as well as

the length of the central oligothiophenes. The FETs fabricated by spin coating from a solution of the branched oligothiophenes showed reasonably good p-type characteristics. Moreover, we have successfully synthesized the branched oligothiophene/[60]fullerene linkage molecules, which showed ambipolar FET character.

Molecular Electronics Materials

We have synthesized the porphyrin–oligothiophene–fullerene triad bearing a thieno[3,4-d]imidazolium salt in the oligothiophene part A dramatic change of the fluorescence intensity from the zinc-porphyrin unit was observed on displacing the counter anion in the imidazolium salt, indicating that photoinduced intramolecular electron transfer is controllable by the electronic perturbation to this unit, and realizing a new type of the chemical-gate system.

We have been preparing molecular wires for building up nanoelectronic devices with the use of the thiophene 24-mer with ca. 10 nm in length having insulating coverage around the oligomer chain. We firstly prepared the thiophene-monomer unit with bulky t-butyldiphenylsilyl (TBDPS) groups, and then a series of its oligomers up to 12-mer were synthesized by repeated oxidative coupling reactions. The electronic absorption maxima of the oligomers were found to be bathochromically shifted with increasing the number of thiophene rings, clearly indicating that the TBDPS group has little influence on the effective conjugation. 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 nano-gap electrode and we have succeeded in the synthesis of the thiophene 24-mers with terminal thiol anchor groups for gold electrodes as well as with terminal ethynyl anchor groups for silicon electrodes.

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. We have succeeded in the synthesis of the new Janus rotaxane containing photosensitive azobenzene units as a photo-regulated molecular valve where two trans-azobenzene units can undergo two-step photoisomerization to a bis-cis form to open a hole in the center of the molecule. The hole can be closed through thermal isomerization to the bis-trans form on heating. And linear cooligomers, up to pentamer, composed of a photochromically contractible and extendable Janus [2]rotaxane and p-bis(bromomethyl)benzene were synthesized and their positive photochromic behavior was examined. We have also succeeded in the synthesis of th cyclopentameric supermolecule, which include tolan-azobenzene dyads as a guest unit.

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Synthesis and Properties of Perfluoroalkyl-annelated Oligothiophenes (Poster), *Y. Umemoto, Y. Ie, T. Kaneda and Y. Aso, Second SANKWN-CNU Joint symposium on Nanoscience and Nanotechnology, Osaka, Japan, January 25-26, 2007.

Contributions to International Conferences and Journals

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)

Publications in Domestic Meetings

The Chemical Society of Japan	6 papers
The Japan Society of Applied Physics	1 paper
Symposium on Fundamental Organic Chemistry	3 papers
Symposium on Main Element Chemistry	1 paper

Cyclophane Meeting	6 papers
Cyclodextrin Symposium	1 paper

Academic Degrees

Doctor Degree for Engineering

N. Negishi	Studies on Syntheses of Fullerene-Modified and Dendritic Oligothiophenes and Their Application as Organic Electronic Materials

Master Degree for Engineering

S. Ishioka	Molecular Machines Based on Self-Organization of Tolan-Modified Permethylated alpha-Cyclodextrins
M. Endo	Development of Oligothiophene Molecular Wires for the Measurement of Single Molecular Conducting Characteristics
L. Feng	Synthesis and Properties of Conjugated Oligomers Bearing a Triethoxysilyl Group at the Terminal Position and Their Self-assembled Monolayers

Sponsorship

Grant-in-Aid for Scientific Research (B)

Y. Aso	Function-Accumulated Extended-Conjugation Systems Based on Oligothiophenes and Their Novel Functions	¥1,900,000

Grant-in-Aid for Scientific Research on Priority Areas

Y. Aso	Carrier-Transport Materials Based on Extended-Conjugation Systems and Their Novel Functions	¥1,900,000
Y. Aso	Development of Extended Conjugated Oligomers toward Construction of Charge-Transporting Hierarchical Structure	¥1,400,000
Y. Ie	Development of Insulated Oligothiophene Molecular Wires Bearing Tripodal Anchor Units at Terminal Position	¥1,900,000

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

Y. Ie	Development of Perfluoroalkyl-Bridged Oligothiophenes Towards n-Type Semiconductors	¥2,000,000

Entrusted Research

Y. Aso	Japan Science and Technology	Synthesis of Insulated Molecular Wires ¥975,000

	Agency		
Y. Aso	Japan Science and Technology Agency	Development of Novel Conjugated Oligomers with Electron-Transport Properties and Their Application to Organic Electronics	¥2,000,000

Cooperative Research

Y. Aso Y. Ie	Sumitomo Chemical Co., Ltd.	Development of Materials for Organic Electronics	¥4,070,000

Other Research Fund

Y. Aso	CREST, Japan Science and Technology Agency	Construction of Nano-electronic Devices Based on Precise Molecular Design	¥6,700,000
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

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Outlines

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

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

Current Research Project

Multi-beam Chemistry

Multi-beam chemistry has been studied using pulse radiolysis-laser flash photolysis combined method, two-color two-laser photolysis and three-color three-laser photolysis. Photochemistry of reaction intermediates and short-lived chemical species generated from the reaction induced by the first beam excitation of a starting molecule (two-step excitation method), and moreover, photochemistry of other chemical species generated from the reaction of the short-lived intermediate induced by the second beam excitation (three-step excitation method) can be studied. This year, by using the multi-beam method, we have clarified the photo-cleavage of naphthalene dimer radical cation, which was generated during the laser flash photolysis or pulse radiolysis. We also

investigated the excited state properties of ketyl radical of various compounds. Reactivity and properties of excited ketyl radicals were revealed. By utilizing high reducing ability of excited ketyl radical, we have demonstrated the formation of metal nanoparticles. Furthermore, we have successfully observed the fluorescence decay profile of excited radical cations and charge separation process of the S_2-excited Sb porphyrins.

Mechanisms of TiO_2 Photocatalytic Reactions

The photocatalytic one-electron oxidation reaction of an aromatic compound during UV light irradiation of titania nanotubes and nanoparticles was investigated using time-resolved spectroscopies. Remarkably long-lived radical cations of the aromatic compound and trapped electrons were observed for the nanotubes when compared to those for nanoparticles. Airborne singlet oxygen ($^1O_2$) molecules, which are generated during the TiO_2 photocatalytic reactions and diffused from the surface into air, were detected using terrylenediimide (TDI) molecules at the single-molecule level. After UV irradiation to the TiO_2 surface, a spectral blue shift of fluorescence spectrum of TDI arising from the cycloaddition of $^1O_2$ was observed. Using this novel $^1O_2$ nanosensor, the spatial and temporal distributions of $^1O_2$ molecules diffused from the TiO_2 surface have been revealed at the single-molecule level.

Charge transfer through DNA nanoscaled assembly programmable with DNA building blocks

DNA nanostructures based on programmable DNA molecular recognition have been developed, but the nanoelectronics of using DNA is still challenging. A more rapid charge-transfer (CT) process through the DNA nanoassembly is required for further development of programmable DNA nanoelectronics. We succeeded in direct absorption measurements of the long-range CT over a 140-Å DNA assembly based on a GC repetitive sequence constructed by simply mixing DNA building blocks. We show that a CT through DNA nanoscale assembly is possible and programmable with the designed DNA sequence.

Mechanism of Photosensitized One-Electron Oxidation of DNA

To investigate the importance of the reaction rate of radical anion of the photosensitizer with O_2 during the photosensitized DNA damage reactions through the one-electron oxidation pathway, photosensitized DNA damage reactions were compared between two well known DNA damaging photosensitizer, naphthalimide (NI) and napthaldiimide (NDI). NI and NDI have similar photophysical properties but differ in their redox properties, that is, the reaction rates of their radical anion with O_2 are supposed to be somewhat different. NI- and NDI-modified DNA were synthesized and a combination of laser flash photolysis kinetic studies and quantitative HPLC analyses of photosensitized DNA damage reactions were investigated. It was clearly demonstrated that the reaction rate of radical anion of the photosensitizer and O_2 is one of the critically important factors determining the efficiency of photosensitized DNA damage. These results may

provide us with new strategies for the future design of the Sens for therapeutic and biochemical applications.

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 protein supramolecular and nanostructures by designing the building blocks. 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. Also we employed porphyrin derivatives for creation of the light-harvesting system in the TMV supramolecular structure. We observed the energy transfer from Zn-porphyrin to free-base porphyrin and enhancement of emission intensity of free base porphyrin. The TMV supramolecular system described in this report allows the integration of aromatic molecules into the TMV scaffold and serves for creating well-ordered self-assembled materials.

Excited Radicals for Preparation of Nanomaterials

We propose the fabrication method of metal nanoparticles using excited radicals. Radicals in the excited state have a stronger reducing ability than those in the ground state and are favorable reducing agents for metal ion. A variety of excited radicals can be conveniently generated by using two-color two-laser flash photolysis. The specific three-dimensional resolution of two-color two-laser makes the construction of three-dimensional arrays of metal nanoparticles possible. In this year, we tried to fabricate AuNps using the excited benzophenone ketyl radical as a reducing agent. The formation of AuNp was significantly enhanced by the two-color two-laser irradiation. The efficient electron transfer from the excited radical enhanced the formation of AuNps.

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Fujitsuka No. 2007-28166

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International Conferences

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T. Majima, XXIst IUPAC Symposium on Photochemistry in Kyoto, Japan, April 2-7, 2006.

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Charge Separation in Diphenylacetylene-Modified DNA, T. Takada, K. Kawai, M. Fujitsuka, and *T. Majima, SANKEN International Symposium on Nanoscience and Nanotechnology 2006. Perspective on Interdsciplinary Nanobiology and Industrial

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Rapid Hole Transfer through Consective Adenine Sequences (Invited), * T. Takada, K. Kawai, M. Fujitsuka, and T. Majima, 2006 Korea-Japan Symposium on Frontier Photoscience (2006KJFP), Sogang Univercity, Seoul, Nov 3-6, 2006.

Detection of the Local Structural Changes in the Dimer Interface of *Bam*HI Initiated by DNA Binding and Dissociation Using a Solvatochromic Fluorophore (Invited), *K. Nakayama, M. Endo, M. Fujitsuka, and T. Majima, 2006 Korea-Japan Symposium on Frontier Photoscience (2006KJFP), Sogang Univercity, Seoul, Nov 3-6, 2006.

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Laser-induced Molecular Chemistry and its Application (Invited), *T. Majima, International Symposium on “Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

DNA Supramolecular Structures for the Creation of Functional Nannomaterials (Invited), *M. Endo and T. Majima, International Symposium on “Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

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Photochemical Formation of Gold Nanoparticles in a PVA Film during Two-color Two-laser irradiation (Invited), *M. Sakamoto and T. Majima, International Symposium on “Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

Monitoring G-Quadruplex Structures and G-Quadruplex-Ligand Complex by 2-Aminopurine Modified Oligonucleotides (Oral), *T, Kimura, K, Kawai, M. Fujitsuka, and T. Majima, International Symposium on “Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

High Yield Generation of Long-Lived Charge-Separated State in Diphenylacetylene-Modified DNA (Oral), *T. Takada, K. Kawai, M. Fujitsuka, and T. Majima, International Symposium on “Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

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Emission from Charge Recombination during the Pulse Radiolysis of Arylethynylpyrenes (Oral), *S. Samori, S. Tojo, M. Fujitsuka, S.-W. Yang, T.-I. Ho, J.-S. Yang, and T. Majima, International Symposium on “Recent Progress of Laser Chemistry,

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Single-Molecule Detection of Airbone Singlet Oxygen (Oral), *K. Naito, T. Tachikawa, S.C. Cui, A. Sugimoto, M. Fujitsuka, and T. Majima, International Symposium on "Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

Charge Transfer through DNA Nanoscaled Assembly Programmable with DNA Building Blocks (Oral), *Y. Osakada, K. Kawai, M. Fujitsuka, and T. Majima, International Symposium on "Recent Progress of Laser Chemistry, SANKEN, Japan, Nov 28-29, 2006.

Laser Chemistry of Nanomaterials and its Application (Invited), *T. Majima, International Symposium on "Photochemistry of Nanomaerials, SANKEN, Dec 7, 2006.

DNA Supramolecular Structures for the Creation of Functional Nannomaterials (Invited), *M. Endo and T. Majima, International Symposium on "Photochemistry of Nanomaerials, SANKEN, Dec 7, 2006.

Photochemistry of Short-lived Species using Multi-beam Irradiation (Invited), *M. Fujitsuka and T. Majima, International Symposium on "Photochemistry of Nanomaerials, SANKEN, Dec 7, 2006.

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Beam-Induced Molecular Chemistry (Oral), *T. Majima, International Symposium of Fifth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Yumebutai International Conference, Japan, Dec. 8-9, 2006.

One-Electron Oxidation Pathways during β-Cyclodextrin-Modified TiO_2 Photocatalytic Reaction, Takashi Tachikawa, Sachiko Tojo, Mamoru Fujitsuka, and *T. Majima, International Symposium of Fifth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Yumebutai International Conference, Japan, Dec. 8-9, 2006.

Long-Distance Hole Transfer through Consecutive Adenine Sequence, T. Takada, K. Kawai, M. Fujitsuka, and *T. Majima, International Symposium of Fifth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Yumebutai International Conference, Japan, Dec. 8-9, 2006.

Solvent Effect on Benzophenone Ketyl Radicals in the Excited State, S. S. Kim, M. Sakamoto, X. Cai, M. Fujitsuka, and *T. Majima, International Symposium of Fifth 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Yumebutai International Conference, Japan, Dec. 8-9, 2006.

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Energy Levels of Oligothiophenes in the Higher Excited Triplet States, Y. Oseki, M. Fujitsuka, M. Sakamoto, X. Cai, and *T. Majima, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience”, Yumebutai International Conference, Japan, Dec. 8-9, 2006.

Effects of Reaction Rate of Radical Anion of a Photosensitizer with Molecular Oxygen on the Photosensitized DNA Damage, *Y. Osakada, K. Kawai, M. Fujitsuka and T. Majima, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience”, Yumebutai International Conference, Japan, Dec. 8-9, 2006.

Single-Molecule Detection of Airborne Singlet Oxygen, K. Naito, T. Tachikawa, S. C. Cui, A. Sugimoto, M. Fujitsuka, and *T. Majima, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience”, Yumebutai International Conference, Japan, Dec. 8-9, 2006.

Emission from Charge Recombination during the Pulse Radiolysis of Organic Electrochemiluminescent Compounds, S. Samori, S. Tojo, M. Fujitsuka and *T. Majima, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience”, Yumebutai International Conference, Japan, Dec. 8-9, 2006.

Charge Transfer in DNA (Oral), *T. Majima, Commemorative Workshop of Opening SANKEN USA Branch, San Francisco, Dec 15-16, 2006.

Development of New TiO_2 Photocatalysts (Invited), *T. Majima, The 8th International Conference on ECOMATERIALS, Kitakyusyu International Conference Center, Jan 11-14, 2007.

Single Molecule Fluorescence Imaging of TiO_2 Photocatalytic Reaction (Oral), *T. Majima, Second SANKEN- CNU Joint Symposium on Nanoscience and Nanotechnology, Icho-Kaikan, SANKEN, Japan, Jan 25-26, 2007.

Energy Levels of Oligothiophenes in the Higher Excited Triplet States, *Y. Oseki, M. Fujitsuka, M. Sakamoto, X. Cai, and T. Majima, Second SANKEN- CNU Joint Symposium on Nanoscience and Nanotechnology, Icho-Kaikan, SANKEN, Japan, Jan 25-26, 2007.

Emission from Charge Recombination during the Pulse Radiolysis of Organic Electrochemiluminescent Compounds, *S. Samori, S. Tojo, M. Fujitsuka and T. Majima, Second SANKEN- CNU Joint Symposium on Nanoscience and Nanotechnology, Icho-Kaikan, SANKEN, Japan, Jan 25-26, 2007.

Effects of Reaction Rate of Radical Anion of a Photosensitizer with Molecular Oxygen on the Photosensitized DNA Damage, *Y. Osakada, K. Kawai, M. Fujitsuka and T. Majima, Second SANKEN- CNU Joint Symposium on Nanoscience and Nanotechnology, Icho-Kaikan, SANKEN, Japan, Jan 25-26, 2007.

Single-Molecule Detection of Airborne Singlet Oxygen, *K. Naito, T. Tachikawa, S. -C. Cui,
A. Sugimoto, M. Fujitsuka, and T. Majima, Second SANKEN- CNU Joint Symposium on Nanoscience and Nanotechnology, Icho-Kaikan, SANKEN, Japan, Jan 25-26, 2007.

Charge Transport in DNA (Invited), *T. Majima, International Conference on Frontiers of Radiation and Photochemistry, PhotoRadChem-2007, KOTTAYAM, Feb 8-9, 2007.

Rapid Energy Migration along Photofunctional Polymers, M. Fujitsuka and *T. Majima, International Conference on Frontiers of Radiation and Photochemistry, PhotoRadChem-2007, KOTTAYAM, Feb 8-9, 2007.

Charge Separation via Rapid Hole Transfer through Consective Adenine Sequences, T. Takada, K. Kawai, M. Fujitsuka, and *T. Majima, International Conference on Frontiers of Radiation and Photochemistry, PhotoRadChem-2007, KOTTAYAM, Feb 8-9, 2007.

Two-color Two-laser Fabrication of Gold Nanoparticles in a PVA Film, M. Sakamoto, S. S. Kim, Takashi Tachikawa, Mamoru Fujitsuka, and *Tetsuro Majima, International Conference on Frontiers of Radiation and Photochemistry, PhotoRadChem-2007, KOTTAYAM, Feb 8-9, 2007.

Single-Molecule Fluorescence Imaging of the Remote TiO_2; Photocatalytic Reaction, *T. Tachikawa, M. Fujitsuka, and T. Majima, 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007.

Energy Levels of Oligothiophenes in the Higher Excited Triplet States, *Y. Oseki, M. Fujitsuka, and T. Majima, 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007.

Contributions to International Conferences and Journals

T. Majima	2006 International Symposium on Frontier Photoscience (Conference Chair)
T. Majima	Langmuir (Editor)

Publications in Domestic Meetings

Photochemistry Meeting	12 papers
Radiation Chemistry Meeting	3 papers
85th Japan Chemical Society Meeting	10 papers

Academic Degrees

Doctor Degree of Engineering

Y. Oseki	Studies on Oligomers of Aromatic Compounds in the Higher Excited States

Master Degree of Engineering

Y. Asanoi	Photochemistry of TiO_2-DNA Nanocomposites
M. Okada	Photochemical Control of Apoptosis-Inducible Enzymes

Sponsorship

Grand-in-Aid for Scientific Research (S)

T. Majima	Nanoscience of Photofuctionalized DNA	¥19,240,000

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

T. Majima	Fundamental Science and Technology of Photofunctional Interfaces	¥10,200,000

Grand-in-Aid for Basic Scientific Research

T. Majima	Formation of Carbon Nanotubes Arrays based on DNA Self-assembly	¥1,000,000

Grand-in-Aid for Scientific Research (C)

S. Tojo	Development of novel TiO_2 catalysts modified by polyacids and its multi-excitation effect	¥2,500,000

Grand-in-Aid for Encouragement of Young Scientists

T. Tachikawa	Development of TiO_2-DNA nano composites towards photodynamic therapy	¥1,310,000

Grand-in-Aid for Scientific Research for Young Scientist

T. Kimura	Hydration of DNA Structure Studied by Dynamic Stokes Shift	¥900,000

Grand-in-Aid for Scientific Research for Young Scientist

Y. Oseki	Study on charge transfer via higher triplet state and ultra fast photo-switching molecular devices	¥1,000,000

Grand-in-Aid for Scientific Research for Young Scientist

Y. Osakada	Study on photoinduced DNA damage caused by charge transfer in DNA toward application to photo dynamic therapy	¥1,000,000

Grand-in-Aid for Scientific Research for Young Scientist

K. Naito	Characterization and application of photo-functionalized carbon nanotube by single molecular fluorescence spectroscopy		¥1,000,000

Entrusted Research

T. Majima	IDEC Co. Satake Co.	Selection of plastic by laser light	¥4,510,000

Other Research Fund

T. Majima	Matsushita Electric Industrial Co.	Study of highly reactive TiO_2 nanotuve photocatalysts	¥1,155,000
T. Majima	Mitsubishi Chemical Co.	Basic research on chemical reaction via higher excited states	¥1,000,000
T. Majima	Asahi Glass Co.		¥1,000,000

Department of Synthetic Organic Chemistry

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Under Graduate Students:	Kaori TANAKA
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Outlines

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

Current Research Project

Development of Multifunctional Asymmetric Catalysts

Chiral dinuclear vanadium(V) 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.

Development of 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.

New Asymmetric Spiro-type Ligands

So far we have developed a new type of chiral bis(isoxazoline) ligands with spiro[4.4]nonane skeleton (SPRIXs). Pd(II)-SPRIX catalysts are 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 isoxazoline and isoxazole ring with spiro[4.5]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.

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.

Stereoselective Reactions with Planar-Chiral Cyclopentadienyl Complexes

We reported the first example of ruthenium-catalyzed asymmetric allylic amination and alkylation of symmetrically substituted allyl carbonates by using planar-chiral cyclopentadienyl-Ru complexes. These planar-chiral cyclopentadienyl-Ru complexes have been found to be highly efficient catalysts for asymmetric *O*-allylation of phenol derivatives with unsymmetrically substituted allyl halides.

Precise Polymerization with Transition-Metal Complexes

Organorhodium complexes effectively initiated a living polymerization of aryl isocyanides possessing bulky substituents at the *ortho* position. Addition of excess amounts of phosphine led to the acceralation of the polymerization and the enhancement of living nature. Polymerization of aryl isocyanides possessing *tert*-butyl groups at the *ortho* position and chiral ester and or amide groups at the *para* position produced single-handed helical polymers predominantly.

Efficient Solvent-free Catalytic Oxidation System Using Green Solid Disperse Phase

We have developed a new approach to solvent-free catalytic oxidation system using ‘green solid disperse phase’. The solvent-free catalytic epoxidation system was carried out at powdery solid-state by using dodecatungstate catalyst ($(CetylPy)_{10}[H_2W_{12}O_{42}]$) /solid disperse phase (fluorapatite (FAp)) with a solid hydrogen peroxide (urea-H_2O_2). The solid catalyst/FAp was reusable and retained its high catalytic activity, although the

catalyst was not fixed on the solid-phase. The high efficiency in the system was found to be due to a new peroxo species that retains the framework of the parent cluster with site-specific peroxo group. The system enable to make use the structural diversity of polyoxometalates as a catalyst.
As a new green catalytic reaction system, we developed a O_2-oxidation-system using Keggin vanadomolybdophosphoric acid ($H_{3+n}PVnMo_{12-n}O_{40}$:PVn)/FAp. The solid-phase-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

Design and Synthesis of Novel Chiral Spiro Ionic Liquids, M. L. Patil, C. V. L. Rao, K. Yonezawa, S. Takizawa, K. Onitsuka and H. Sasai, Org. Lett., 8[2] (2006) 227-230.

Conformational Lock in Brønsted Acid - Lewis Base Organocatalyst for the Aza-Morita-Baylis-Hillman Reaction, K. Matsui, K. Tanaka, A. Horii, S. Takizawa and H. Sasai, Tetrahedron: Asymmetry, 17[4] (2006) 578-583.

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Development of Efficient Methods for the Immobilisation of Multicomponent Asymmetric Catalysts, D. Jayaprakash, S. Takizawa, T. Arai and H. Sasai, Journal of

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Review Papers

Precise Synthesis and Functionalities of Helical Polyisocyanides (in Japanese), K. Onitsuka and F. Takei, Kobunshi Ronbunshu, 63[7] (2006) 458-467.

Helical Conformational Change in Polyisocyanides Induced by External Stimuli (in Japanese), K. Onitsuka and F. Takei, Jasco Report, 48[2] (2006) 26-30.

Solvent-free Epoxidation and Oxidation Using Solid Disperse Phase (in Japanese), Y. Sasaki and J. Ichihara, Kagaku Kogyo, 57[6] (2006) 431-436.

Books

New Development of Organocatalyst, H. Sasai, S. Takizawa, K. Matsui, CMC Publishing, (2006) 231-242.

Patents

Novel Vanadium Compounds, S. Takizawa, H. Sasai, T. Katayama, JP2006-240632

International Conferences

Design and Synthesis of Novel Chiral Spiro Ionic Liquids, *M. L. Patil, C. V. L. Rao, K. Yonezawa, S. Takizawa, K. Onitsuka, H. Sasai, 8th International Symposium on Organic Reactions, Kobe, Japan, Apr. 23-26, 2006.

Development of Effective Enzyme Mimic for Urease, *D. Jayaprakash, R. N. Nadaf, H. Sasai, 8th International Symposium on Organic Reactions, Kobe, Japan, Apr. 23-26, 2006.

Development and Applications of Novel Spiro-type Ligands, *P. Koranne, T. Tsujihara, K. Takenaka, K. Onitsuka, H. Sasai, 8th International Symposium on Organic Reactions, Kobe, Japan, Apr. 23-26, 2006.

Development of Catalytic Enantioselective Reaction Utilizing Chiral Spiro-type Ligands (Oral), *T. Tsujihara, P. Koranne, J. Yogo, K. Wakita, T. Shinohara, S. Takizawa, K. Onitsuka, H. Sasai, International Molecular Chirality Conference, Toyama, Japan, May 18-19, 2006.

Design and Synthesis of Novel Chiral Spiro Ionic Liquids, *M. L. Patil, C. V. L. Rao, K.

Yonezawa, S. Takizawa, K. Onitsuka, H. Sasai, International Molecular Chirality Conference, Toyama, Japan, May 18-19, 2006.

A Novel Bifunctional Asymmetric Organocatalysts for Aza-Morita-Baylis-Hillman (Aza-MBH) Reaction, *K. Matsui, S. Takizawa, H. Sasai, 7th Tetrahedron Symposium Challenges in Organic Chemistry, Kyoto, Japan, May 25-26, 2006.

Enantioselective Catalyses Using Novel Spiro-type Ligands, *P. Koranne, T. Tsujihara, S. Takizawa, J. Yogo, K. Onitsuka, H. Sasai, 7th Tetrahedron Symposium Challenges in Organic Chemistry, Kyoto, Japan, May 25-26, 2006.

Development of Novel Chiral Isoxazoline/Isoxazole Hybrid-type Ligands (Oral), P. S. Koranne, T. Tsujihara, S. Takizawa, K. Onitsuka, *H. Sasai, 18th International Symposium on Chirality, Busan, Korea, Jun. 25-28, 2006.

Development of New Methods towards the Synthesis of Novel Chiral Spiro Ionic Liquids, *M. L. Patil, C. V. L. Rao, K. Yonezawa, S. Takizawa, K. Onitsuka, H. Sasai, 18th International Symposium on Chirality, Busan, Korea, Jun. 25-28, 2006.

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Bifunctional Organocatalysts for Enantioselective Aza-Morita-Baylis-Hillman Reaction, K. Matsui, K. Tanaka, A. Horii, S. Takizawa, *H. Sasai, International Symposium on Organocatalysis in Organic Synthesis, Glasgow, UK, Jul. 5-7, 2006.

Development of Metal-bridged Polymers as Enantioselective Catalysts, S. Takizawa, *N. Inoue, H. Sasai, XXII International Conference on Organometallic Chemistry, Zaragoza, Spain, Jul. 23-28, 2006.

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Precise Synthesis and Properties of Helical Polyisocyanides (Invited), *K. Onitsuka, S. Takahashi, 16th International Symposium on Fine Chemistry and Functional Polymers & IUPAC 2nd International Symposium on Novel Materials and Synthesis, Lanzhou, China, Jul. 24-27, 2006.

Enantioselective Catalysis Using Novel Spiro-type Ligands and Novel Spiro Isoxazoline-Isoxazole Hybrid Ligands (Oral), *P. S. Koranne, T. Tsujihara, S. Takizawa, K. Onitsuka, H. Sasai, 232nd ACS National Meeting, San Francisco, USA, Sep. 10-14, 2006.

Asymmetric Catalysis of Planar-Chiral Cyclopentadienyl-Ruthenium Complexes in Allylic Substitutions, *K. Onitsuka, H. Okuda, H. Sasai, 1st International Conference of Cutting-Edge Organic Chemistry in Asia, Naha, Okinawa, Japan, Oct.16-20, 2006.

Bifunctional Organocatalysts for Enantioselective Aza-Morita-Baylis-Hillman (Aza-MBH) Reaction, *K. Matsui, K. Tanaka, A. Horii, S. Takizawa, H. Sasai, 1st International Conference of Cutting-Edge Organic Chemistry in Asia, Naha, Okinawa, Japan, October16-20, 2006.

Bifunctional Organocatalysts for Enantioselective Aza-Morita-Baylis-Hillman (Aza-MBH) Reaction, *K. Matsui, K. Tanaka, A. Horii, S. Takizawa, H. Sasai, 10th International Kyoto Conference on New Aspects of Organic Chemistry, Kyoto, Japan, Nov. 13-17, 2006.

Asymmetric Allylation Catalyzed by Planar-Chiral Cyclopentadienyl-Ruthenium Complexes, *K. Onitsuka, H. Okuda, H. Sasai, 10th International Kyoto Conference on New Aspects of Organic Chemistry, Kyoto, Japan, Nov. 13-17, 2006.

Dual Activation in an Enantioselective Homolytic Coupling Reaction, *T. Katayama, C. Kameyama, S. Takizawa, K, Onitsuka, H, Sasai, 10th International Kyoto Conference on New Aspects of Organic Chemistry, Kyoto, Japan, Nov. 13-17, 2006.

Enantioselective Synthesis of Heterocyclic Compounds Utilizing Pd(II)-SPRIX Catalyst, *G. B. Bajracharya, P. Koranne, T. Tsujihara, K. Takenaka, S. Takizawa, K. Onitsuka, H, Sasai, 10th International Kyoto Conference on New Aspects of Organic Chemistry, Kyoto, Japan, Nov. 13-17, 2006.

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Applications of Novel Chiral Spiro Isoxazoline/Isoxazole, P. Koranne, G. B. Bajracharya, K. Onitsuka, *H, Sasai, 5th 21st Century COE Towards Creating New Industries Based on Inter-Nanosience International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Development of Chiral Isoxazoline/Isoxazole Ligands and Their Application in Enantioselective Catalysis, *P. Koranne, G. B. Bajracharya, M. L. Patil, T. Tsujihara, C. V. L. Rao, S. Takizawa, K. Onitsuka, H, Sasai, 5th 21st Century COE Towards Creating New Industries Based on Inter-Nanosience International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Development of Novel Asymmetric Cascade Reaction Catalyzed by Pd-SPRIX, *T. Tsujihara, K. Takenaka, S. Takizawa, K. Onitsuka, H, Sasai, 5th 21st Century COE Towards Creating New Industries Based on Inter-Nanosience International Symposium,

Awaji, Japan, Dec. 8-9, 2006.

Development of Artificial Enzyme Utilizing Multiple Interactions in Catalytic Site, *T. Kawase, R. N. Nadaf. G. R. Kassem, D. Jayaprakash, S. Takizawa, H, Sasai, 5th 21st Century COE Towards Creating New Industries Based on Inter-Nanosience International Symposium, Awaji, Japan, Dec. 8-9, 2006.

Living Polymerization of Bulky Aryl Isocyanide with Arylrhodium Complexes and Application to Precise Synthesis of Helical Polymers, *K. Onitsuka, M. Yamamoto, T. Mori, F. Takei, S. Takahashi, Osaka University Macromolecular Symposium on Chemistry, Physics, and Biology in Macromolecular Science, Osaka, Japan, Feb. 19-21, 2007.

Utility of Cetylpyridinium Dodecatungstate As a Green Solid Catalyst for Epoxidation, Y. Sasaki, K. Momoi, K. Iteya, *J. Ichihara, GSC-AON 2007 (JOINT MEETING OF THE 1st Asian-Oceanian Conference on Green and Sustainable Chemistry AND THE 7th Annual Green and Sustainable Chemistry Symposium), Tokyo, Japan, March 6-9, 2007.

Contributions to International Conferences and Journals

H. Sasai	ICOB-5 & ISCNP-25 IUPAC International Conference on Biodiversity and Natural Product (Organizing Committee)

Publications in Domestic Meetings

Symposium on Organic Synthesis	1 paper
Symposium on Organic Reaction	2 papers
Symposium on Organometallic Chemistry	3 papers
The Electrochemical Society of Japan	1 paper
The Society of Polymer Science, Japan	1 paper
The Chemical Society of Japan	12 papers

Academic Degrees

Doctor Degree for Science

T. Kawase	Development of Artificial Enzyme Utilizing Multiple Interactions in Catalytic Site
C. V. L. Rao	Design, Synthesis and Applications of Novel Chiral Spiro Heterocyclic Compounds
P. S. Koranne	Design of Novel Hybrid Spiro Isoxazoline-isoxazole Ligands and Applications to Pd-catalyzed Enantioselective Reactions

Master Degree for Science

H. Okuda	Regio- and Enantioselective *O*-Allylation of Phenol and Alcohol Catalyzed by Planar-Chiral Cyclopentadienyl-Ruthenium Complex

T. Katayama	Asymmetric Oxidative Homocoupling of 2-Naphthol Derivatives Catalyzed by Chiral Dinuclear Vanadium(V) Complexes
T. Shiromoto	Development of Helical Polyisocyanide Catalysts Possessing Lewis Base Pendants
A. Horii	Acid - Base Type of Organocatalyst for Enantioselective Aza-Morita-Baylis-Hillman (Aza-MBH) Reaction

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

H. Sasai	Development of Chiral Organocatalyst with Synergistic Effect	¥2,100,000
K. Onitsuka	Synthesis and Properties of Hybrid-type of Organometallic Conjugated Polymers	¥1,300,000

Grant-in-Aid for Scientific Research (C)

J. Ichihara	Solvent-free catalytic oxidation system on environmentally benign solid-disperse-phase	¥700,000

Grant-in-Aid for JSPS Fellows

H. Sasai	Polymer-Supported Artificial Enzyme with Dendritic Systems	¥1,200,000
H. Sasai	Development and Application of Novel Asymmetric Spiro Catalytst	¥1,500,000

Grant-in-Aid for Scientific Research on Exploratory Research

N/A

Entrusted Research

H. Sasai	Japan Science and Technology Agency	Preparation of Novel Medicinal Intermediates Based on Enantioselective Reactions Using Chiral Spiro Ligands	¥3,250,000

Other Research Fund

K. Onitsuka	The Japan Securities Scholarship Foundation	Synthesis of Functional Nano-scale Organometallic Molecules Directed Toward Organic-Inorganic Hybrid Materials	¥1,200,000
K. Onitsuka	Mukai Science and Technology Foundation	Development of Helical Polyisocyanide Materials for Separation of Chiral Compounds	¥1,500,000

Department of Analytical Molecular Chemistry

Professor: Nobuo KATO
Research Associates: Yoshio TAKAI, Kunihiro KAIHATSU
Post Doctoral Fellow: Shuichi MORI (2006.12.1-)

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 Project

Studied by Electron-Spray Ionization MS Spectrometry

Using the enantiomer-labeled host method based on the host-metal-guest complexation system, enantiomeric excess (ee) detection of a chiral carboxylic acid (guset) has been determined by ESI mass spectrometry. The ee of the chiral carboxylic acid is detected based on the correlation with the peak intensities of the diastereomeric host-metal-guest complex ions.

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 TiO_2 surface and the TiO_2 photocatalytic reaction mechanism.

Regulation of DNA Transcription by Infrared Two-photon Controllable Antisense Peptide Nucleic Acids (PNAs)

Technologies that regulate the gene expression at a specific tissue with a desired timing can be utilized to investigate the life systems and/or to develop novel therapeutic agents. We set our goal to remote control the gene expression by azobenzenes that respond to none harmful infrared (IR) laser irradiation. By collaborating with the Department of Organic Fine Chemicals and the Department of Molecular Excitation Chemistry, we succeeded to synthesize a series of azobenzenes that switch their geometrical (trans-cis) configuration by IR two-photon absorption. Their azobenzenes were introduced into antisense peptide nucleic acid (PNA), a DNA/RNA analogue. So far, we succeeded to regulate the association between PNA-AZO and duplex DNA by IR two-photon laser irradiation system.

Synthesis of Novel Catechin Derivatives as Anti-Influenza Virus Agents

Epigallocatechin gallate (EGCG), a major green tea extract, has been known to have anti-inflenza effects. However, it isn't utilized for therapeutic applications due to its poor chemical stability and cellular membrane permeability. By collaborating with

Department of Organic Fine Chemicals, we developed a method to prepare fatty acid monoesters of EGCG by lipase-catalyzed esterification. The antiviral effect of EGCG-monoester derivatives on influenza virus A/PR8/34/H1N1 was examined by plaque formation assay with Madin-Derby canine kidney (MDCK) cells. The viral inhibitory effect of EGCG monoesters was enhanced as a function of alkyl chain length. Further, EGCG-mono palmitoyl ester was appeared to possess about 30-fold potent antiviral effect compare to EGCG.

Publications

Original Papers

Enantiomeric Excess Determination of a Chiral Carboxylic Acid Using the Enantiomer-Labeled Host Method by Electrospray Ionization Mass Spectrometry, Y. Takai, K. Iguchi, H. Yamada, M. Shizuma, R. Arakawa and M. Sawada, JMS Letters, J. Mass Spectrometry, 41[2] (2006) 266-268.

Visible Light-Induced Degradation of Ethylene Glycol on Nitrogen-Doped TiO_2 Powders, T. Tachikawa, Y. Takai, S. Tojo, M. Fujitsuka, H. Irie, K. Hashimoto and T. Majima, J. Phys. Chem. B, 110[26] (2006) 13158-13165.

Probing the Surface Adsorption and Photocatalytic Degradation of Catechols on TiO2 by Solid-State NMR Spectroscopy, T. Tachikawa, Y. Takai, S. Tojo, M. Fujitsuka and T. Majima, Langmuir, 22[3] (2006) 893-896.

Review Papers

Lipase-Catalyzed Synthesis of Novel Tea Catechin Derivatives and Their Application to Anti-Influenza Agents, K. Kaihatsu, S. Mori, S. Miyake, T. Nakaya, S. D. Fuller and N. Kato, Yakugaku Zasshi, 126 (2006), 57-58.

International Conferences

Evidence for Ring-size Controlled Competitive Channels in α vs. ω-Hydrogen Migration in *N*-(5-Phenylvaleryl)azacycloalkan-2-thiones Probed by Isotope Labeling and Charge Inversion, *H. Yamaoka, K. Shiono, S. Hayakawa, K. Isa, N. Dougawa, Y. Takai; N. M. M. Nibbering: The 54th ASMS Conference, Seatle, USA, May 28-Jun 1, 2006.

Unimolecular Dissociation for *N,N'*-(Di)acylimidazolidin(e)-2-(thi)ones, *H. Yamaoka, K. Okada, K. Isa, N. Dougawa, K. Kuzuno, Y. Kawabata, Y. Takai, M. Sawada, N. M. M. Nibbering, 17th International Mass Spectrometry Conference, Prague, Czech Republic, Aug 27–Sep 1, 2006.

Regulation of DNA Transcription by Infrared Controllable Antigene Peptide Nucleic Acids, *I. Imada, K. Kaihatsu, X. Cai, M. Fujitsuka, T. Majima and N. Kato, Sanken International Symposium on Nanoscience and Nanotechnology 2006 [SISNN-2006], Osaka, Japan, Sep 19-20, 2006.

Synthesis of Monoester Derivatives of Epigallocatechin Gallate Using Pancreatic Esterase and Their Application to Antiviral Agents, *S. Mori, K. Kaihatsu, S. Miyake, T. Nakaya and N. Kato, Sanken International Symposium on Nanoscience and Nanotechnology 2006 [SISNN-2006], Osaka, Japan, Sep 19-20 2006.

Regulation of DNA Transcription by Infrared Controllable Antigene Peptide Nucleic Acids, *K. Kaihatsu, X. Cai, M. Fujitsuka, T. Majima and N. Kato, 5th 21st Century COE "Toward Creating New Industries Based on Inter-Nanoscience", Hyogo, Japan, Dec 8-9, 2006.

Synthesis of Monoester Derivatives of Epigallocatechin Gallate Using Pancreatic Esterase and Their Application to Antiviral Agents, *S. Mori, K. Kaihatsu, S. Miyake, T. Nakaya and N. Kato, 5th 21st Century COE "Toward Creating New Industries Based on Inter-Nanoscience", Hyogo, Japan, Dec 8-9, 2006.

Publications in Domestic Meetings

The Chemical Society of Japan	6 paper
The Mass Spectrometry of Japan	4 papers
The Pharmaceutical Society of Japan	1 paper
Japanese Society of Cathecinology	1 paper
Symposium on Pharmaceutical Food Science	1 paper
Bio-Optics Research Meeting	1 paper
Others	4 papers

Sponsorship

Entrusted Research

K. Kaihatsu	NEDO (Industrial technology research and development projects)	Development of Screening Systems for Anti-RNA Virus Drugs Using Novel Tea Catechin Derivatives	¥14,300,000

Other Research Fund

K. Kaihatsu	Taiyo Kagaku Co., Ltd	Developing functional materials with food components by electrolytic spinning technology	¥1,000,000

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 distributed ontology development environment
- Systematization of functional knowledge using ontological engineering and its deployment
- Release of OMNIBUS: Ontology of learning/instructional theories and theory- and standards-aware authoring system
- Analysis of collaborative learning interaction and meta-cognitive skill modeling
- Enhancement of the methodology of mobile user models for task-oriented mobile service navigation
- Creation of novel sensors
- 3D modeling and visualization
- Medical image analysis
- Omnidirectiomal surveillance system and human behavior analysis
- Predicate Invention
- Introducing sensors to constructive adaptive user interfaces
- Adaptive agents
- Adaptive Intelligent Tutoring Systems
- Web summarization
- Construction of sensor networks
- Knowledge discovery from extremely high dimensional data
- Knowledge discovery from graph structured data
- Data mining of comprehensive knowledge
- Discovery of time-dependent law equations from data

Department of Knowledge Systems

Professor:	Riichiro MIZOGUCHI
Associate Professor:	Yoshinobu KITAMURA
Research Associate:	Munehiko SASAJIMA
Specially Appointed Research Associates:	Yusuke HAYASHI
Post Doctoral Fellow:	Daniele Allard
Graduate Students:	Eiichi SUNAGAWA, Masataka TAKEUCHI, Yusuke KOJI, Shinya TARUMI, Seiji ISOTANI, Mesbahy HOUDA, Naoya WASHIO, Masanori OOKUBO
Under Graduate Students:	Satoshi ENDO, Koichiro FURUTANI
Supporting Staff:	Naomi BANO

Outline

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 Projects

1. Ontology: Theoretical Foundation of Knowledge Engineering

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

is badly needed in knowledge engineering fields. The research on ontology engineering is one of the most promising approaches to establishment of the foundation. We theorized about the fundamental issues on ontology from both scientific and engineering viewpoints. As a result, we published three enlightening papers which describe drawbacks of the current research, importance of ontological engineering, definitions of an ontology, its functions and roles, its classification and research topics. We further published some research results based on ontological engineering to show concrete examples of a new research direction. One of the most remarkable achievements is a book on “Ontological Engineering” has been published from Ohm-sha Ltd. In January, 2005 which is the first book on the topic in Japan. HOZO, an environment for ontology building/utilization, has been augmented to make it a usable tool by revising its GUI and reimplementation of some functions. It has been extended to cope with distributed development of a large ontology. In 2006, in order to maintain consistency of ontologies built in a distributed manner, we have developed two functionalities to manage the dependencies between component ontologies and to help users keep and restore consistencies among them when they are changed. Furthermore, API functionality and compliance with WWW standard has been augmented. Concerning theoretical issues, further refinement of Role theory has been done from the point of view of instance management.

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 2006, we developed a framework for functional metadata for technical documents on intra-network, which enables engineers to retrieve documents using ontological concepts about functionality of products in semantic relations. Next, aiming at contributing to interoperability of technical knowledge, we extended our ontology to include upper-categories of the concepts of function and physical processes related to products as well as functional processes.

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 the following; 1) development of a comprehensive ontology of Education of Informatics in high school and a prototype of an intelligent and dynamic authoring support multi-agent system based on the ontology, 2) design of paper-writing training system based on our innovative model of meta-cognitive skills, 3) the public release of a learning and instructional theory ontology and development of a prototype of theory- and standard-compliant authoring tool named SMARTIES based on the ontology, and 4) development of a collaborative learning process model using the modified version of our collaborative learning theory ontology and a visualization system of the theories based on the model.

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’ profound 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 an integrated system of *Kfarm* and our functional modeling

system. This integration helps users store a wide range of the design rationale of artifacts and facilitates the growth and sharing of design knowledge.

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. You seek for information when you face a trouble, which is difficult to get over with knowledge at hand, on your way of achieving a task. Such a situation is the context and origin of the necessity for the information. In this research project, we have been developing a task ontology-based modeling framework for mobile service navigation. We applied our modeling framework to more general domain, and modified ontologies behind the model. Furthermore, we carried out several experiments and proved effectiveness of our modeling method.

Publications

Original Papers

An Ontological Model of Device Function: Industrial Deployment and Lessons Learned, Y. Kitamura, Y. Koji and R. Mizoguchi: Applied Ontology, 1 [3-4] (2006) 237-262.

Building an Ontology of IT Education Goals, T. Kasai, H. Yamaguchi, K. Nagano and R. Mizoguchi: Int. J. Cont. Engineering Education and Lifelong Learning, 16[1/2] (2006) 1-17.

An Ontological Approach to Support Design of Collaborative Workplace Blended of Practice and Education, M. Takeuchi, Y. Hayashi, M. Ikeda and R. Mizoguchi: The Transactions of the Japanese Society for Artificial Intelligence, 21[6] (2006) 184-194.

Review Papers

Knowledge Representation in Ontology Engineering and the Semantic Web, R. Mizoguchi: Journal of JSAI, 21[6] (2006) 699-705.

Books

A Primer of Ontology Development, K. Kozaki, Y. Kitamura, M. Sasajima and R. Mizoguchi: Ohmsya, (2006).

International Conferences

Towards Ontologies of Functionality and Semantic Annotation for Technical Knowledge Management (Oral), *Y. Kitamura, N. Washio, Y. Koji, and R. Mizoguchi, New Frontiers in Artificial Intelligence: Joint JSAI 2005 Workshop Post-Proceedings, LNCS 4012, Springer Berlin / Heidelberg (2006) 17-28.

A Collaborative Learning Design Environment to Integrate Practice and Learning based on Collaborative Space Ontology and Patterns (Oral), *M. Takeuchi, Y. Hayashi, M. Ikeda, R. Mizoguchi, the 8th International Conference on Intelligent Tutoring Systems(ITS2006), Jhongli, Taiwan, June 26-30, 2006.

Mobile User Behavior Modeling for Task-Oriented Navigation Based on Ontological Engineering (Invited), *R. Mizoguchi and *M.Sasajima, International Workshop on Mobile Services and Ontologies, Nara, Japan, May 9, 2006.

Fundamental Consideration of Role Concepts for Ontology Evaluation (Oral), *K. Kozaki, E. Sunagawa, Y. Kitamura and R. Mizoguchi, Evaluation of Ontologies for the Web (EON2006) 4th EON Workshop, Edinburgh, United Kingdom, May 22, 2006.

Ontology Engineering and Its Applications (Plenary), *R. Mizoguchi, KICSS2006, Ayutthaya, Thailand, August, 2006.

Role Organization Model in Hozo (Oral), E. Sunagawa, K. Kozaki, Y. Kitamura, *R. Mizoguchi, EKAW 2006 - 15th International Conference on Knowledge Engineering and Knowledge Management Managing Knowledge in a World of Networks, Podebrady, Czech Republic, Oct. 2-6, 2006.

An Ontology-Based Annotation Framework for Representing the Functionality of Engineering Devices (Oral), *Y. Kitamura, *N. Washio, Y. Koji, M. Sasajima, S. Takafuji, R. Mizoguchi, ASME 2006 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference (ASME IDETC/CIE 2006), Philadelphia, Pennsylvania, USA, September 10-13, 2006.

Roles of Ontologies of Engineering Artifacts for Design Knowledge Modeling (Invited), *Y. Kitamura, the 5th International Seminar and Workshop Engineering Design in Integrated Product Development (EDIProD 2006), Gronow, Poland, 21-23 September 2006.

Some Ontological Distinctions of Functions of Technical Artefacts (Invited), *Y. Kitamura, R. Mizoguchi, The 15th Altenberg Workshop in Theoretical Biology “Comparative Philosophy of Technical Artefacts and Biological Organisms”, Altenberg, Austria, September 21-24, 2006.

Towards a Reference Ontology of Functionality for Interoperable Annotation for Engineering Documents, *Y. Kitamura, N. Washio, M. Ookubo, Y. Koji, M. Sasajima, S.

Takafuji, R. Mizoguchi. ESWC 2006, Budva, Montenegro, 11-14 June 2006.

Task Ontology-Based Framework for Modeling Users' Activities for Mobile Service Navigation, *M. Sasajima, Y. Kitamura, T. Naganuma, S. Kurakake, R. Mizoguchi, ESWC 2006, Budva, Montenegro, 11-14 June 2006.

Ontological Support for a Theory-Eclectic Approach to Instructional and Learning Design (Oral), *Y. Hayashi, J. Bourdeau and R. Mizoguchi, First European Conference on Technology Enhanced Learning, EC-TEL2006, Crete, Greece, Oct. 1-4, 2006.

Ontological Modeling Approach to Blending Theories for Instructional and Learning Design (Oral), *Y. Hayashi, J. Bourdeau and R. Mizoguchi. The 14th International Conference on Computers in Education (ICCE2006), Beijing, China, Nov.30-Dec. 4, 2006.

An Integrated Framework for Fine-Grained Analysis and Design of Group Learning (Oral), *S. Isotani and R. Mizoguchi. The 14th International Conference on Computers in Education (ICCE2006), Beijing, China, Nov.30-Dec. 4, 2006.

Building and Evaluation of a Semantic Web System that Provides Teachers with Lesson Plans (Oral), *T. Kasai, H. Yamaguchi, K. Nagano, R. Mizoguchi, The 14th International Conference on Computers in Education (ICCE2006), Beijing, China, Nov.30-Dec. 4, 2006.

Surmonter l'interference Culturelle et Linguistique a l'aide de CALL (Oral), *A. Daniele, R. Mizoguchi, J. Bourdeau, Actes de colloque de la Journee Scientifique Francophone (JSF) 2006, Tokyo, Japan, Dec. 1, 2006.

Task Ontology-Based Modeling Framework for Navigation of Mobile Internet Services (Oral), *M. Sasajima, Y. Kitamura, T. Naganuma, K. Fujii, S. Kurakake and R. Mizoguchi, Internet and Multimedia Systems and Applications- EuroIMSA2007, Chamonix, France, March 13-15, 2007.

Ontological Engineering and Its Deployment (Plenary), *R. Mizoguchi, Third International Conference on Intelligent Computing and Information Systems, Cairo, Egypt, March 15-18, 2007.

Industrial Impact of Ontology Engineering (Plenary), *R. Mizoguchi, Semantic Technology Annual Conference 2007, Seoul, Korea, March 28, 2007.

Development of Contents Management System Based on Light-Weight Ontology (Oral), *K. Kozaki, Y. Kitamura and R. Mizoguchi, Proc. of the 2007 IAENG International Conference on Internet Computing and Web Services, Hong Kong, March 21-23, 2007.

Contributions to International Conferences and Journals

R.Mizoguchi	European Project on SEKT (Steering committee member)
R.Mizoguchi	Semantic Web Science Association (Vice-president)
R.Mizoguchi	International Artificial Intelligence in Education Society (Executive Committee member)
R.Mizoguchi	Asia-Pacific Society for Computers in Education(APSCE) (Board member)
R.Mizoguchi	The 1st Asian Semantic Web Conference (ASWC2006) (PC Chair)
R.Mizoguchi	The 14th International Conference on Computers in Education (ICCE2006) (PC Chair)
R.Mizoguchi	The 3rd European Semantic Web Conference (ESWC2006) (PC member)
R.Mizoguchi	Fifth international semantic web conference (ISWC2006) (PC member)
R.Mizoguchi	The 15th International Conference on Knowledge Engineering and Knowledge Management (EKAW2006) (PC member)
R.Mizoguchi	The 15th International World Wide Web Conference Semantic Web Track (PC member)
R.Mizoguchi	The 8th International Conference on Intelligent Tutoring Systems (ITS2006) (PC member)
R.Mizoguchi	The First European Conference on Technology Enhanced Learning (EC-TEL 2006) (PC member)
R.Mizoguchi	The 12th International Conference on Artificial Intelligence: Methodology, Systems, Applications (AIMSA 2006) (PC member)
R.Mizoguchi	2006 IEEE International Conference on Information Reuse and Integration (IEEE-IRI 06) (PC member)
R.Mizoguchi	The First International Conference on Knowledge, Information and Creativity Support Systems (KICSS 2006) (Technical Committee and International Advisory Committee)
R.Mizoguchi	IFIP AI 2006: Artificial Intelligence in Theory And Practice (PC member)
R.Mizoguchi	The Ninth Pacific Rim International Conference on Artificial Intelligence (PRICAI2006) (Workshop Chair)
R.Mizoguchi	The Sixth International Symposium on Tools and Methods of Competitive Engineering (TMCE 2006)(PC member)
R.Mizoguchi	International Workshop on Applications of Semantic Web Technologies for E-Learning (SW-EL) (PC member)
R.Mizoguchi	LORNET Conference I2LOR 2006 (PC member)
R.Mizoguchi	International Journal of Applied Ontology(Editorial board)
R.Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
R.Mizoguchi	International Journal of Artificial Intelligence in Education

	(Editorial board)
R.Mizoguchi	International Journal of Web Semantics (Editorial board)
R.Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)
Y.Kitamura	The 1st Asian Semantic Web Conference (ASWC2006) (PC member)
Y.Kitamura	The Sixth International Symposium on Tools and Methods of Competitive Engineering (TMCE 2006) (PC member)
Y.Kitamura	Canadian Semantic Web Working Symposium 2006 (PC member)
Y.Kitamura	2006 IEEE International Conference on Information Reuse and Integration (IEEE-IRI 06) (PC member)
Y.Kitamura	The 5th International Seminar and Workshop Engineering Design in Integrated Product Development (EDIProD 2006) (PC member)
Y.Hayashi	The 14th International Conference on Computers in Education (ICCE2006) (PC member)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	8 papers
The institute of Electronics, information and communication engineers	1 paper
The Japan society of mechanical engineers	3 papers
Japan Reserch Group for Medical Ontology	2 papers

Academic Degrees

Doctor Degree of Engineering

Y. Koji	Function-oriented knowledge management of physical processes of artifacts
E. Sunagawa	A Development of Ontology Development System Based on a Framework for Distributed Construction and Role Organization Theories
M. Takeuchi	Building a Collaborative Learning Environment for Creation and Inheritance of Organizational Knowledge

Master Degree of Engineering

Mesbahy Houda	A Design of Ontology-based Architecture to Support Description of Functional Decomposition Tree
N. Washio	Function-oriented metadata schema and development of a semantic search system for technical documents.

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas

R. Mizoguchi	Technical documents integration based on an	¥5,400,000

	artifact ontology		

Grant-in-Aid for Encouragement of Young Scientists (A)

Y. Kitamura	Development of an open interoperable platform for function-oriented technical knowledge based on an upper functional ontology	¥3,600,000

Grant-in-Aid for JSPS Fellow

R. Mizoguchi	Ontological Modeling of Second Language Learning Interferences and an Experimental Computer Application	¥700,000

Entrusted Research

R. Mizoguchi	The Society of Chemical Engineers, Japan	Surveillance Study for Development of Structued 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	¥3,150,000

Donation

R. Mizoguchi	Justsystem Corporation	¥5,000,000
R. Mizoguchi	Y.M.P-International Corporation	¥650,000
R. Mizoguchi	Y.M.P-International Corporation	¥650,000
R. Mizoguchi	Y.M.P-International Corporation	¥650,000
R. Mizoguchi	Y.M.P-International Corporation	¥650,000
R. Mizoguchi	ENEGATE co. ltd.	¥1,000,000

Cooperative Research

R. Mizoguchi	NTT DoCoMo, Inc.	Research on an ontology for users in mobile environment to understand the real world context	¥3,000,000
R. Mizoguchi	Justsystem Corporation	Information sharing for safety-first manufacturing based on the unification of ontological engineering and natural language processing	¥20,000,000

Department of Intelligent Media

Professor:	Yasushi YAGI
Associate Professor:	Yasuhiro MUKAIGAWA
Research Associate:	Ryusuke SAGAWA, Yasushi MAKIHARA
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Outline

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 Projects

1. Research about Catadioptric Camera Systems Considering with Space Resolution

Catadioptric omnidirectional imaging systems have been applied to many applications such as virtual reality, mobile robots and surveillance, since these can capture omnidirectional scene at video rate. But in some case, optical property of conventionals are not enough to satisfy requirements of real tasks. We need to develop an imaging system taking account into optical characteristics such as field of view and blur. In this papar, I take into both of field of view and resolution about omnidirectional imaging systems. Specifically, two omnidirectional imaging systems based on each different type of spatial division are proposed shown as follows.

One is an omnidirecitonal imaging system constructed by a curved mirror and a camera. It can observe a omnidirectional scene with its observation density changed according to the azimuth angle. A basic ideas of designing are stretching a rotational symmetry mirror about an axis that is perpendicular to the rotational axis, and deforming it again in order to it been able to observe a horizontal plane. I applied above designing to a conventional isotropic omnidirectional camera to develop an anisotropic

omnidireciontal imaging system: Horizontal fixed-viewpoints Biconical Paraboloidal(HBP) mirror system.

Second is another omnidirectional imagings system constructed by multiple mirrors and cameras. Units consisting of a camera and a curved mirror for spreading out a its filed of view are mounted at height of a person can cover an omnidirecional scene. And the curved mirrors also control projections between image planes and the scene in order to realize uniform resolution at whole of the scene. By adjusting parameters of the mirror defined as a smoothly changing function, a projection error is minimized.

Furthermore, I evaluated the HBP mirror system through several analyses and experiments. The analyses are about blur, resolution distribution, detection sensibility about optical flows, and multi viewpoint problems. In order to evaluate effectiveness of the HBP mirror system when it is used for a vision of a mobile robot, I also did surveillance experiments in a devastated area with a virtual remote surveillance system. All results from the analyses and the experiments indicated that the HBP mirror system effectively works.

2. Narrow Baseline Omnidirectional Stereo using Disparity Detection Filter

We propose a disparity detection filter which is a novel method to detect disparity for narrow baseline system. Although the method to detect near objects, which we previously proposed, has low computational cost, but it can only determine whether objects are close enough or not. The disparity detection filter can be applied to our omnidirectional sensor and it can detect disparity of objects through hierarchically-smoothed images with various window sizes. This method does not need finding correspondences along epipolar lines and the computational cost is low, because the disparity of each hierarchically-smoothed image is detected by intensity gradient. In addition, the method is better adapted to detect small disparity. Applying the method, we can detect disparity at high speed with narrow base line stereo cameras and our omnidirectional sensor.

3. Development of Rapid Measuring System of Reflectance Property Using an Ellipsoidal Mirror and a Projector

Measuring BRDF (Bi-directional Reflectance Distribution Function) requires huge amounts of time because a target object must be illuminated from all incident angles and the reflected lights must be measured from all reflected angles. In this paper, we present a high-speed method to measure BRDFs using an ellipsoidal mirror and a projector. Our method makes it possible to change incident angles without a mechanical drive. Moreover, the omni-directional reflected lights from the object can be measured by one static camera at once. In addition we use multiplexed illumination using a projector for improving a quality. We made two prototypes which have a different layout method of an object and evaluated their performances.

4. A Probabilistic Method for Aligning Range Images by Using Sensor Characteristics

This paper describes a probabilistic method of aligning range images. To align range images, it is generally needed to search for correspondences. However, it is difficult to find correct corresponding points in aligning range images with large noises. Therefore,

we utilize sensor characteristics to align them. First, we formulate this issue as problems of estimating the maximum likelihood. Next, our method estimates parameters based on the Expectation Maximization (EM) approach. By examining an error distribution of a range finder, we model it as a normal distribution along the line of sight. Due to the error model, the algorithm is implemented as an extension of the Iterative Closest Point (ICP) method. Since our proposed method uses multiple correspondences for each vertex of range images, the error after aligning range images are smaller than that of earlier methods that use one-to-one correspondences. Finally, we tested our method by simulation and real range images and validated efficiency of our method.

5. Construction of a Multi-view Gait Measurement System

This paper describes a multi-view synchronized capturing system to construct a large-scale gait database. First, the system equips 25 multi-view synchronized cameras: 2 layers of 12 surrounding cameras, and one top-view camera to treat pan and tilt view changes. Then, to observe changes of walking speeds and surface inclines efficiently, we capture a mode sequence composed of a combination of multiple speeds and inclines at once, which is controlled by treadmill. Moreover, we control the background color to extract clear silhouettes by using multiple surrounding screens and projectors. Finally, we correct lens distortions and subsequently calibrate camera parameters including camera pose, position, and focal length. Experiments show that these two calibrations are performed accurately.

6. Gait Identification based on Multi-view Observations using Omnidirectional Camera

We propose a method of gait identification based on multi-view gait images using an omnidirectional camera. We first transform omnidirectional silhouette images into panoramic ones and obtain a spatio-temporal gait silhouette volume (GSV). Next, we extract frequency-domain features by Fourier analysis based on gait periods estimated by autocorrelation of the GSVs. Because the omnidirectional camera provides a change of observation views, multi-view features can be extracted from parts of GSV corresponding to basis views. In an identification phase, distance between a probe and a gallery feature of the same view is calculated, and then these for all views are integrated for matching. Experiments of gait identification including 15 subjects from 5 views demonstrate the effectiveness of the proposed method.

7. Real-time Synchronic Measuring Range Image and Texture

Real-time measuring range image and texture of the target moving object can be applied for the field of real-world robot control or object recognition. The difficulty in the measuring is to capture range image and texture in same time and real-time. The range measuring method with color structured lignt can capture range image with 1shot. This method resolve real-time range measuring but the color structured light is disturbance for texture. In our method, we project multi band IR structured Light and measure the target object range using the projected light. Optical light is using for capturing texture. IR light is using for measuring range image. To divide wavelength for each using make measuring range image and texture in same time possible. Setting color camera for texture and W/B cameras for range image on coaxial position resolve

texture mapping occlusion.

8. Toward Omni-directional Surveillance System: A Detection of Moving Objects and a Design of a Small Sensor

In this paper, a surveillance system using a wearable omni-directional sensor is presented. Detecting moving objects is one of the main functions of the system. In this method, feature points which have a similar motion are classified into one group. This method leads to a simple calculation because only feature points are used to estimate the difference between two frames. In addition, a look-up table of translation is made in advance to improve the calculation speed. The effectiveness of this method is confirmed in the experiments using simulated images. We also present a small sensor, which is composed of a hyperbolic mirror and multiple paraboloidal mirrors. We can take images of all-around view from the multiple mirrors, which enable us to know the distance to objects.

Publications

Original Papers

Super Wide Field of View Head Mounted Display Using Catadioptrical Optics, H. Nagahara, Y. Yagi, M. Yachida, Presence: Teleoperators & Virtual Environments, 15[5] (2006) 588-598.

International Conferences

Gait Recognition Using a View Transformation Model in the Frequency Domain, *Y. Makihara, R. Sagawa, Y. Mukaigawa, T. Echigo, Y. Yagi, the 9th European Conf. on Computer Vision, Graz, Austria, May 7-13, 2006.

A Probabilistic Method for Aligning and Merging Range Images with Anisotropic Error Distribution, *R. Sagawa, N. Osawa, Y. Yagi, Third International Symposium on 3D Data Processing, Visualization and Transmission, Chapel Hill, USA, June 14-16, 2006.

Which Reference View is Effective for Gait Identification Using a View Transformation Model?, *Y. Makihara, R. Sagawa, Y. Mukaigawa, T. Echigo, Y. Yagi, the IEEE Computer Society Workshop on Biometrics 2006, New York, USA, Jun. 17-18, 2006.

Adaptation to Walking Direction Changes for Gait Identification, *Y. Makihara, R. Sagawa, Y. Mukaigawa, T. Echigo, Y. Yagi, the 18th Int. Conf. on Pattern Recognition, Hong Kong, China, Aug. 20-24, 2006.

Adaptive Control of Video Display for Diagnostic Assistance by Analysis of Capsule Endoscopic Images, *H. Vu , T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, Y. Yagi, the 18th Int. Conf. on Pattern Recognition, Hong Kong, China, Aug. 20-24, 2006.

A Fast Compensation Method of Inter-reflection for Pattern Projection onto a Non-planar Surface, *Y . Mukaigawa, T. Kakinuma, Y. Ohta, IEEE International

Workshop on Projector-Camera Systems (PROCAMS2006), New York, USA, June 17, 2006.

Diagnosis Supporting System for Capsule Endoscopy, *Y. Yagi, H. Vu, T. Echigo, R. Sagawa, K. Yagi, M. Shiba, K. Higuchi, T. Arakawa, International Conference on Ulcer Research (ICUR), Jul. 7-9, 2006.

Evaluation of a HBP mirror system for remote surveillance, *K. Kondo, Y. Mukaigawa, T. Suzuki, Y. Yagi, IEEE/RSJ International Conference on Intelligent Robots and Systems, Beijing, China, October 11-13, 2006.

Analytical Compensation of Inter-reflection for Pattern Projection, *Y.Mukaigawa,T.Kakinuma, Y.Ohta, ACM Symposium on Virtual Reality Software and Technology (VRST2006), Limassol, Cyprus, Nov. 1-3, 2006.

Integrating Shape and Color Features for Adaptive Real-time Object Tracking, *J. Wang, Y. Yagi, The 2006 IEEE International Conference on Robotics and Biomimetics, Kunming, China, December 17-20, 2006.

Contributions to International Conferences and Journals

Y. Yagi	IEEE International Conference on Robotics&Biomimetics 2006 (Program Co-Chair)
Y. Yagi	International Journal of Automation and Computing (Associate Editor)
Y. Yagi	8th Asian Conference on Computer Vision (Program Chair)
Y. Yagi	IEEE International Conference on Robotics and Automation (Associate Editor)
Y. Yagi	International Conference On Smart homes and health Telematics (Organizing Committee)
Y. Yagi	IEEE International Conference on Computer Vision (Program Committee)
Y. Yagi	The Korea-Japan joint workshop on Frontiers of Computer Vision2007 (Organizing Committee)
Y. Yagi	The Seventh Workshop on Omnidirectional Vision, Camera Networks and Non-classical Cameras (Program Committee)
Y. Yagi	Computer Vision and Pattern Recognition 2006 (Program Committee)
Y. Yagi	9th European Conference on Computer Vision ECCV 2006 (Program Committee)
Y. Yagi	2006 IEEE/RSJ International Conference on Intelligent Robots and Systems (Program Committee)
Y. Yagi	2007 IEEE Conference on Computer Vision and Pattern Recognition (Reviewer)
Y. Mukaigawa	Computer Vision and Pattern Recognition 2006 (Program Committee)

Y. Mukaigawa	IEEE International Conference on Computer Vision (Program Committee)
Y. Mukaigawa	8th Asian Conference on Computer Vision (Area Chair)
R. Sagawa	8th Asian Conference on Computer Vision (Technical Staff)
R. Sagawa	The 6th International Conference on 3-D Digital Imaging and Modeling (Program Committee)
Y. Makihara	8th Asian Conference on Computer Vision (Technical Staff)

Publications in Domestic Meetings

Information Processing Society of Japan	10 papers
The Institute of Electronics, Information and Communication Engineers	9 papers
The Japan Society of Naval Architects and Ocean Engineers	1 paper
The Society of Instrument and Control Engineers	1 paper

Academic Degrees

Doctor Degree for Information Science

K. Kondo	Research about Catadioptric Camera Systems Considering with Space Resolution

Master Degree for Information Science

Y. Kojima	Narrow Baseline Omnidirectional Stereo using Disparity Detection Filter
K. Sumino	Development of Rapid Measuring System of Reflectance Property Using an Ellipsoidal Mirror and a Projector
N. Ohsawa	A Probabilistic Method for Aligning Range Images by Using Sensor Characteristics

Sponsorships

Grant-in-Aid for Scientific Research (S)

Y. Yagi	Wearable Omnidirectional Stereo Surveillance System	¥28,210,000

Grant-in-Aid for Young Scientists (A)

Y. Mukaigawa	Full measurement of spatially varying BRDF and its advanced application	¥10,790,000

Other Research Funds

Y. Yagi	Japan Science and Technology Agency, Special Coordination Funds for Promoting Science and Technology	Dive Into the Movie Project	¥61,212,000
Y. Yagi	Ministry of Internal Affairs	Multimedia Information	¥1,950,000

and Communications, Strategic Information and Communications R&D Promotion Programme	Search by Teleoperated Robot Network in a Disaster Site

Department of Architecture for Intelligence

Professor:	Masayuki NUMAO
Associate Professor:	Satoshi KURIHARA
Research Associate:	Koichi MORIYAMA
Research Associate:	Ken-ichi FUKUI
Post Doctoral Fellows:	Roberto LEGASPI
Graduate Students:	Kazushi NAKAMURA, Minoru KAWANO, Ryozo KIYOHARA, Md. Nazmul HUDA(-2006.7.30), Nagayoshi YAMASHITA, Norihiro IMANAKA, Toshinori KAWASAKI, Motoki KONISHI, Akihiro OTA, Hidenori FUKUI, Seiichi HONDA, Mitsuhiro MATSUMOTO, Naofumi YASUBA
Under Graduate Students:	Toshihito SUGIMOTO, Hiroshi TAMAKI, Takayuki NISHIKAWA
Supporting Staff:	Fumie NAKAO, Kana KOYAGI(2006.4.1-2006.9.30), Sumiko SUGITA(2006.9.1-)

Outline

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 Projects

Constructive Adaptive User Interfaces

This department is developing a computer with learning ability, for which it researches efficient learning algorithms, acquisition of background knowledge for learning, application to Intelligent Tutoring Systems. These are applied to adaptive user interfaces. The conventional adaptive user interfaces only select a good response out of some previously given ones. Although this helps to use interfaces, such as a navigation system, it is not sufficient to stimulate human intelligence or creativity. The department has developed a method to compose a new content adaptively. This technology enables automatic acquisition of human feelings, and automatic music composition system adapted to personality and emotion of its user.

Intelligent Tutoring System

To have an instructional plan guide the learning process is significant to various

teaching styles and an important task in an ITS. Though various approaches have been used to tackle this task, the compelling need is for an ITS to improve on its own the plans established in a dynamic way. We hypothesize that the use of knowledge derived from student categories can significantly support the improvement of plans on the part of the ITS. This means that category knowledge can become effectors of effective plans. We have conceived a Category-based Self-improving Planning Module (CSPM) for an ITS tutor agent that utilizes the knowledge learned from learner categories to support self-improvement. The learning framework of CSPM employs unsupervised machine learning and knowledge acquisition heuristics for learning from experience. We have experimented on the feasibility of CSPM using recorded teaching scenarios.

Intelligent Ubiquitous Sensor-Networks

In recent years, progress in computer technology, the appearance of IPv6, the development of various radio technology including IEEE802.11, and the practical use of radio-tags like RFID have greatly activated studies of ubiquitous computing like sensor-networks. But, the purpose of many proposed ubiquitous systems is to present information of the virtual-world like the Internet to humans living in the real-world by using physical properties like monitors and loudspeakers, etc. On the other hand, our purpose is to construct a framework to enable flexible and real-time interaction between humans and the real-world. Keyword is resonance. Each human has his own natural frequency, which is a metaphor for personality or daily habitual behaviors. In the proposed framework, each human behavior reacts with the environment and the environment performs sensor-data mining and extracts each human's natural frequency.
The real-world that we assume in this study is homes and offices, etc., where daily habitual behaviors of humans are easy to extract. So, we call the real-world “the environment.” The environment learns the daily habitual behaviors of each human, and performs the most suitable interaction to whoever should receive it. To embody this interaction framework, the environment must be an autonomous action entity, and it is necessary to construct this entity as a massively multi-agent system to enable management and control of various broadly dispersed sensors and physical properties for interaction and to enable real-time interaction with humans. To begin with, we have set up several interaction devices between humans and the environment as well as various kinds of many sensors.

Publications

Original Papers

A Category-Based Framework of a Self-Improving Instructional Planner, R. Legaspi, R. Sison, and M. Numao: Transactions of Japanese Society for Artificial Intelligence, 21 [1] (2006) 94-102.

An Emotion-Driven Musical Piece Generator for a Constructive Adaptive User Interface, R. Legaspi, Y. Hashimoto, and M. Numao: Lecture Notes in Artificial Intelligence, 4099 (2006) 890-894.

Adaptive Agent Selection in Large-Scale Multi-Agent Systems, T Sugawara, K. Fukuda,

T. Hirotsu, S. Sato and S. Kurihara: Lecture Notes in Computer Science, 4099 (2006) 818-822.

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Music Compositional Intelligence with an Affective Flavor, *R. Legaspi, Y. Hashimoto, K. Moriyama, S. Kurihara, and M. Numao. ACM International Conference on Intelligent User Interfaces, Hawaii, U.S.A., Jan.28-31, 2007.

Contributions to International Conferences and Journals

M. Numao	New Generation Computing (Area Editor)
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S. Kurihara	Second International Workshop on Massively Multi Agent Systems (MMAS'06) (Program Committee)
S. Kurihara	Seventh International Workshop on Multi-Agent-Based Simulation (MABS'06) (Program Committee)
K. Moriyama	PAKDD08: 12th Pacific Asia Conference on Knowledge Discovery and Data Mining (Local Arrangement Committee)

Publications in Domestic Meetings

Japanese Society of Artificial Intelligence	6 papers
Information Processing Society of Japan	6 papers
Institute of Electronics, Information and Communication Engineers	2 papers
The Society of Instrument and Control Engineers	1 paper
Japanese Society for Software Science and Technology	2 papers
The Electrochemical Society of Japan	1 paper

Academic Degrees

Master Degree for Information Science

N. Imanaka	Evaluation of AE signals in SOFC utilizing SOM
T. Kawasaki	Adaptive Choreography System for Street Dancing

Sponsorships

Grant-in-Aid for Young Scientists (B)

K. Moriyama	Deriving Appropriate Utility in Agent Learning	¥800,000

Entrusted Research

M. Numao	Japanese Society for the Promotion of Science	Investigation of science trend in artificial intelligence field	¥14,500,000

Cooperative Research

S. Kurihara	NTT Corporation	Multi agent algorithm for ubiquitous environment and application	¥800,000

Other Research Fund

S. Kurihara	Artificial Intelligence Research Promotion Foundation	Planning technique for active interaction from real environment to human	¥500,000

Department of Architecture for Intelligence

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Outline

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 Projects

Constructive Adaptive User Interfaces

This department is developing a computer with learning ability, for which it researches efficient learning algorithms, acquisition of background knowledge for learning, application to Intelligent Tutoring Systems. These are applied to adaptive user interfaces. The conventional adaptive user interfaces only select a good response out of some previously given ones. Although this helps to use interfaces, such as a navigation system, it is not sufficient to stimulate human intelligence or creativity. The department has developed a method to compose a new content adaptively. This technology enables automatic acquisition of human feelings, and automatic music composition system adapted to personality and emotion of its user.

Intelligent Tutoring System

To have an instructional plan guide the learning process is significant to various

teaching styles and an important task in an ITS. Though various approaches have been used to tackle this task, the compelling need is for an ITS to improve on its own the plans established in a dynamic way. We hypothesize that the use of knowledge derived from student categories can significantly support the improvement of plans on the part of the ITS. This means that category knowledge can become effectors of effective plans. We have conceived a Category-based Self-improving Planning Module (CSPM) for an ITS tutor agent that utilizes the knowledge learned from learner categories to support self-improvement. The learning framework of CSPM employs unsupervised machine learning and knowledge acquisition heuristics for learning from experience. We have experimented on the feasibility of CSPM using recorded teaching scenarios.

Intelligent Ubiquitous Sensor-Networks

In recent years, progress in computer technology, the appearance of IPv6, the development of various radio technology including IEEE802.11, and the practical use of radio-tags like RFID have greatly activated studies of ubiquitous computing like sensor-networks. But, the purpose of many proposed ubiquitous systems is to present information of the virtual-world like the Internet to humans living in the real-world by using physical properties like monitors and loudspeakers, etc. On the other hand, our purpose is to construct a framework to enable flexible and real-time interaction between humans and the real-world. Keyword is resonance. Each human has his own natural frequency, which is a metaphor for personality or daily habitual behaviors. In the proposed framework, each human behavior reacts with the environment and the environment performs sensor-data mining and extracts each human's natural frequency.
The real-world that we assume in this study is homes and offices, etc., where daily habitual behaviors of humans are easy to extract. So, we call the real-world “the environment.” The environment learns the daily habitual behaviors of each human, and performs the most suitable interaction to whoever should receive it. To embody this interaction framework, the environment must be an autonomous action entity, and it is necessary to construct this entity as a massively multi-agent system to enable management and control of various broadly dispersed sensors and physical properties for interaction and to enable real-time interaction with humans. To begin with, we have set up several interaction devices between humans and the environment as well as various kinds of many sensors.

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Department of Advanced Reasoning

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Outline

We, humans, can extract variety of knowledge from given data by the full use of our reasoning. However, such reasoning ability of humans is so limited that most of the massive and complex data acquired through computer network are wasted without any humans' inspection. To provide efficient remedies to this difficulty, our department studies novel reasoning approaches to extract knowledge from the massive and complex data by using computers. These techniques are named data mining and knowledge discovery. We also study the application of these techniques to variety of fields such as science, information network, quality/risk management, medicine, security, marketing and finance. In this year, we obtained significant outcomes in the research topics of knowledge discovery from massively high dimensional data, knowledge discovery from graph structured data, data mining of comprehensive knowledge and discovery of time dependent law equations from data.

Current Research Projects

Knowledge discovery from extremely high dimensional data

Measurement data consisting of massive variables (extremely high dimensional data), which represent many events simultaneously occurred, became available by the development of computer network, ubiquitous sensing and scientific measurement technologies. Examples are the sales data of a large scale shopping center under various conditions and the profile data of thousands of gene expressions in biological systems. Our department started a new research topic to discover temporal dynamics and variable relations from such data acquired from large scale and complex systems.

The first attempt made in this year is the development of an approach to derive a complete set of event groups embedded in a given time series data where the events in each group co-occur in an objective system. Moreover, the approach seeks a complete set of conditional relations between two event groups. This approach is named HISC (High-order Substate Chain) modeling method. This method enabled to identify the regularity of event occurrences from extremely high dimensional time series data such as the rule to predict popular sales items in a shop upon the popular sales in the other shops at a certain past time in the shopping center.

Another attempt is to efficiently derive correlation coefficients among thousands of variables from a given extremely high dimensional data. As massive computation power is required to compute correlation coefficients among huge number of variables, the efficient algorithm of this computation is highly important for causal reasoning among variables. This approach, which estimates objective correlation coefficients from the other known correlation coefficients, enabled to compute large number of correlation coefficients far more efficiently than their direct computation by using the given data.

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 ten 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. Moreover, we have developed CL-GBI which is an approach to search the patterns without chunking, B-GBI which is to use beam search for efficiency and DT-GBI which is a classification approach with searching and generating features in form of the characteristic patterns. Significant results have been obtained in their applications to command prediction for friendly user-computer interface and preliminary study of hepatitis data analysis.
2. We have developed Apriori-based Graph Mining (AGM) algorithm based on the idea to represent graphs by adjacency matrices and to efficiently disambiguate the representation of isomorphic structures by introducing a notion of canonical form. This algorithm derives a complete set of induced subgraphs including disconnected subgraphs and a complete set of association rules among the subgraphs by introducing the principle of Apriori-based basket analysis. Moreover, we have extended this approach and obtained AcGM which limits its searching patterns to induced or general connected subgraphs for the efficiency and B-AGM which derives frequent sub-ordered trees, frequent sub-unordered trees, frequent subpathes and frequent subsequences not limited to frequent subgraphs by introducing constraint biases. The application fields of AGM have been significantly extended by these developments. These approaches have been applied to the analysis of the subgraph co-occurrences in the molecular substructures of chemical compounds having mutagenesis and carcinogenesis. Furthermore, AGM and AcGM have been applied to graph mining based statistical causal inference to analyse highly massive and complicated causal structures among gene expressions embedded in gene micro array data.
3. AGM was made to be a public software to return the benefit resulted from our research to the public society.

4. Based on a standard PMML (Predictive Model Markup Language) which is a subset of XML, a new language to represent graph, GML(Graph Markup Language) has been designed. The current graph mining tools in public support a graph representation only dedicated to each tool. This causes a strong difficulty to share the graph data and their mined results. With our proposal, a powerful environment becomes available for flexibly combining and using many tools and system in graph mining.
5. A set of open software tools for the graph representation, the data conversion, and the AGM analysis by using the aforementioned GML was developed to return the benefit resulted from our research to the public society.
6. We developed tree mining approaches named Dryade and Dryade-Parent which searches a complete set of frequent embedded/induced subtrees in tree structured data. These approaches can mine all frequent subtree patterns very efficiently while the patterns are limited to graphs without any loops.

In this year, Dryade-DAG has been developed where frequent subgraphs embedded in DAG (Directed Acyclic Graph) data are searched efficiently. This approach has been applied to causal network data of gene expressions, and a graph mining based framework of large scale statistical causal inference has been established to efficiently analyze large scale gene expression process. Furthermore, from the viewpoint of practical use, CL-GBI has been extended so that one can specify subgraphs which should or should not be included in the discovered subgraphs as constraints, and it has been experimentally confirmed that the extended CL-GBI can efficiently discover the subgraphs satisfying given constraints. In addition, we extended the search algorithm of CL-GBI by introducing a pruning mechanism based on information gain, and confirmed its ability to efficiently discover the subgraphs as good features to classify given graph data.

Data mining of comprehensive knowledge

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 department has worked on this topic in the last several years and obtained the following achievements.

1. We established monotonic interval density measure to mine quantitative association rules in the framework of Basket Analysis. This measure has been implemented into a tool program named QFIMiner for quantitative frequent itemset mining. The tool program achieved the world top level performance 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.
2. Moreover, a new classification approach named LSC-CAEP based on the quantitative frequent itemset mining has been developed. The performance of this

classification approach demonstrated significant practicality in both efficiency and accuracy.

In this year, the applicability of this quantitative basket analysis method and its tool QFIMiner to the aforementioned temporal dynamics modeling based on extremely high dimensional data has been investigated.

Discovery of time dependent law equations from data

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 law equations under both experimental and observation environments. 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. An approach to discover a complex law equation model consisting of simultaneous equations was developed. 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.
3. 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. 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.

In this year, we assessed the applicability of the time dependent law equation discovery to the aforementioned temporal dynamics modeling for extremely high dimensional data.

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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New Frontiers in Artificial Intelligence: Proceedings of the 19th Annual Conferences of the Japanese Society for Artificial Intelligence, LNAI 4012, T. Washio, A. Sakurai, K. Nakajima, H. Takeda, S. Tojo and M. Yokoo Ed.: Springer-Verlag, (2006)

Mining Graph Data (L. B. Holder and D. J. Cook Ed.), K. Ohara, P. C. Nguyen, A. Mogi, H. Motoda and T. Washio: Wiley-Interscience, (2006) 203-226

Patents

Program, Memory Media and Instrument to Estimate Positive Semi-Definite Similarity Measure for Massive Instances, T. Washio, K. Nakanishi, H. Kuwajima: No.2007-34905

International Conferences

Constructing Decision Trees for Graph-Structured Data by Chunkingless Graph-Based Induction (Oral), *P. C. Nguyen, K. Ohara, A. Mogi, H. Motoda and T. Washio, The 10th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2006), Singapore Hilton Hotel, Singapore, Apr. 9-12, 2006.

Analysis on a Relation between Enterprise Profit and Financial Sate by Using Data Mining Techniques (Oral), *T. Washio, Y. Shinnou, K. Yada, H. Motoda and T. Okada, Workshop on Risk Mining (RM2006), Collocated with the 20th National Meeting of JSAI, Tower Hall Funahori, Tokyo, Japan, Jun. 6, 2006.

Extracting Discriminative Patterns from Graph Structured Data using Constrained Search (Oral), *K. Takabayashi, P. C. Nguyen, K. Ohara, H. Motoda and T. Washio, The 2006 Pacific Rim Knowledge Acquisition Workshop (PKAW 2006), Workshop held in conjunction with the 9th Pacific Rim International Conference on Artificial Intelligence (PRICAI 2006), Guilin Park Hotel, Guilin, China, Aug 7-8, 2006.

Mining Discriminative Patterns from Graph Structured Data with Constrained Search (Oral), *K. Takabayashi, P. C. Nguyen, K. Ohara, H. Motoda and T. Washio, The Workshop on Mining and Learning with Graphs (MLG), Workshop held in conjunction with the 17th European Conference on Machine Learning (ECML) and the 10th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD), Humboldt-University, Berlin, Germany, Sep. 18, 2006.

High-Order Substate Chain Prediction Based on Massive Sensor Outputs (Oral), *V. P. Nguyen and T. Washio, The 4th International Workshop on Knowledge Discovery from Data Streams, Workshop held in conjunction with the 17th European Conference on Machine Learning (ECML) and the 10th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD), Humboldt-University, Berlin, Germany, Sep. 18, 2006.

Model Trawling : Modeling Dynamics of Massive Dimensional and Complex Systems (Invited), *T. Washio and V. P. Nguyen, Joint 3rd International Conference on Soft Computing and Intelligent Systems and 7th International Symposium on Advanced Intelligent Systems (The IEEE SCIS & ISIS 2006), Tokyo Institute of Technology, Tokyo, Japan, Sep. 20-24, 2006.

From Closed Tree Mining to Closed DAG Mining (Invited), *A. Termier, Y. Tamada, S. Imoto, T. Washio, and T. Higuchi, The International Workshop on Data-Mining and Statistical Science (DMSS2006), Century Royal Hotel, Sapporo, Japan, Sep. 25-26, 2006.

Modeling Dynamics of Massive Dimensional and Complex Systems (Oral), *V. P. Nguyen and T. Washio, The International Workshop on Data-Mining and Statistical Science (DMSS2006), Century Royal Hotel, Sapporo, Japan, Sep. 25-26, 2006.

Modeling Dynamic Substate Chains among Massive States for Prediction (Oral), *V. P. Nguyen and T. Washio, Foundations of Data Mining and Novel Techniques in High Dimensional Structural and Unstructured Data, Workshop held in conjunction with the 6th IEEE International Conference on Data Mining (ICDM 2006), Hong Kong Convention and Exhibition Centre, Hong Kong, Dec. 18, 2006.

A Method to Search ARX Model Orders and Its Application to Sales Dynamics Analysis (Oral), *K. Fukata, T. Washio, and H. Motoda, International Workshop on Data Mining for Design and Marketing 2006 (DMDM2006), Workshop held in conjunction with the 6th IEEE International Conference on Data Mining (ICDM 2006), Hong Kong Convention and Exhibition Centre, Hong Kong, Dec. 18, 2006.

Contributions to International Conferences and Journals

T.Washio	Special Issue on Applications Eligible for Data Mining, Journal of Advanced Engineering Informatics (Editor)
T.Washio	New Frontiers in Artificial Intelligence: Proceeding of the 19th Annual Conferences of the Japanese Society for Artificial Intelligence (Volume Editor)
T.Washio	The 9th Pacific Rim International Conference on Artificial Intelligence (PRICAI2006) (Program Committee)
T.Washio	The 11th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2007) (Workshop Chair)
T.Washio	The 23rd International Conference on Machine Learning (ICML2006) (Program Committee)
T.Washio	The 16th International Conference on Inductive Logic Programming (ILP2006) (Program Committee)
T.Washio	European Conference on Machine Learning/European Conference on Principles and Practice of Knowledge Discovery in Database (ECML/PKDD2006) (Program Committee)
T.Washio	Knowledge Management (KM) track of the ACM 15th Conference on Information and Knowledge Management (CIKM2006) (Program Committee)
T.Washio	New Frontiers in Artificial Intelligence: Proceeding of the 20th Annual Conferences of the Japanese Society for Artificial Intelligence (Volume Editor)
T.Washio	The 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008) (Program Chair)
T.Washio	The 9th International Conference on Discovery Science (DS2006) (Program Committee)
T.Washio	International Workshop on Knowledge Discovery in Inductive Databases (KDID2006) (Program Committee)
T.Washio	The IEEE International Conference on Data Mining2006: Workshop on Risk Mining 2006 (ICDM2006/RM2006) (Program Committee Chair)
T.Washio	The 2006 Pacific Rim Knowledge Acquisition Workshop (Program Committee)
T.Washio	The 6th IEEE International Conference on Data Mining (ICDM2006) (Program Committee)
T.Washio	The 2007 IEEE Congress on Evolutionary Computation (CEC2007) (Program Committee)
T.Washio	New Frontiers in Artificial Intelligence: Proceeding of the 19th Annual Conferences of the Japanese Society for Artificial Intelligence (Editor)
T.Washio	International Conference on Mining and Learning with Graphs (Steering Committee)
T.Washio	IADIS European First International Conference on Data Mining

	(Program Committee)
T.Washio	The 10th International Conference on Discovery Science (DS2007) (Program Committee)
T.Washio	International Conference on Large-scale Knowledge Resources (ILKR2008) (Program Committee)
T.Washio	The 24th International Conference on Machine Learning (ICML2007) (Program Committee)
T.Washio	The 20th International Conference on Industrial, Engineering & Other Applications of Applied Intelligent Systems (IEA/AIE2007) (Program Committee)
T.Washio	The 6th European Conference on Computational Biology (ECCB) (Program Committee)
T.Washio	The 15th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) (Program Committee)
T.Washio	The 18th European Conference on Machine Learning (ECML) (Program Committee)
T.Washio	The 11th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD2007) (Program Committee)
T.Washio	The 24th International Conference on Mining and Learning 2007 Workshop on the Induction of Process Models(ICML2007) (Program Committee)
T.Washio	The ACM 16th Conference on Information and Knowledge Management (CIKM2007)(Program Committee)
T.Washio	Data Mining and Knowledge Discovery (Editorial Board)
K.Ohara	The 12th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD2008)(Local arrangement Committee Co-Chair)
K.Ohara	The 9th Australian Joint Conference on Artificial Intelligence (AI2006)(Program Committee)
K.Ohara	The 17th Annual International Conference on Inductive Logic Programming (ILP2007)(Program Committee)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	10 paper
Japan Statistical Society	1 papers
Transdisciplinary Federation of Science and Technology	1 papers

Academic Degrees

Master Degree for Engineering

K. Nakanishi	Study on Fast Derivation of Highly Correlated Variable Sets based on Geometrical Constraints
H. T. Lu	Study on Supporting Mining Algorithm Selection based on Data Analysis Histories

V. P. Nguyen	Study on Dynamic Chain Modeling of Massive States

Sponsorships

Grant-in Aid for Scientific Research(B)

T. Washio	Development of Data Mining Method for 3-dimentional Graph Structured Data and Its Application to Identification System of Bioactive Molecules	¥3,200,000

Grant-in Aid for Scientific Research on Priority Area

T. Washio	Establishment of Knowledge Mining and Modeling Principles for Large Scale Dimensional Time Series and Its Application to Commercial Ubiquitous Data	¥2,900,000

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	¥900,000

Entrusted Research

T. Washio	Japan Science and Technology Agency	Technology Development to Enhance Semi-Conductor Manufacturing Yield by Using Large Scale Dimensional Data Mining	¥3,382,000

Division of Biological Science

Outline

The Division of Biological Sciences is composed of three departments: Dept. of Single-Molecule Biophysics, Dept. of Cell Membrane Biology, and Dept. of Structural Molecular Biology. These departments are engaged in researches in various fields of biological sciences including molecular enzymology, signal transduction, energy transformation, membrane transport, and mechanism of gene expression. The research projects covered by this division are as follows:

1. Single-molecule studies on the mechanochemical coupling of F- and V-type H^+ ATPases.
2. Single-molecule imaging of membrane proteins reconstituted in an artificial planner 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 quinohemoproteins
8. Identification of novel protein kinase C-interacting proteins and elucidation of their roles in signal transduction
9. Development of a new method of the gene delivery system using hepatitis B virus surface antigen particles

Achievements

- Cellular Function of Fasciculation and Elongation Protein Zeta-1 in Rat Embryo Hippocampal Neuron
- Pinpoint Drug and Gene Delivery System Using ZZ tag-Displaying Bio-Nanocapsule and Targeting Molecule-fused IgG Fc Protein
- Reaction Mechanism of Bacterial Copper Amine Oxidase: Conformational Changes of the TPQ Cofactor during the Catalytic Cycle
- ENH1 Scaffolds the PKCε-PKD1 Signaling Complex at the Z-Discs of Cardiomyocytes
- Real-time controlling of F1-ATPase rotation using a micro heater system.
- Studies on the mechanical modulation of catalytic reactions of F1-ATPase by single-molecule manipulation.
- Single-molecule studies on the chemomechanical coupling ratio of F1-ATPase
- Single-molecule imaging of vesicle formation and budding catalyzed by COP II

proteins.

- Single DNA molecule analysis with a femtoliter chamber array.
- Single cell analysis on xenobiotic extruding activity with a femtoliter chamber array.
- Determination of the crystal structure of the substrate-bound form of bacterial major multidrug exporter AcrB
- Indole-sensing mechanism on the up-regulation of drug exporter genes in *E. coli*
- Catabolite control mechanism of the expression of bacterial multidrug exporter gene *mdtEF*.
- Growth phase-dependent expression of bacterial xenobiotic exporters.
- Analysis of ABCA5 knock-out mice, a novel ABCA subfamily transporter
- Studies on the sphingosine-1-phosphate export mechanism from platelet
- Construction of ABCA7-knockout mice

Department of Structural Molecular Biology

Professor:	Katsuyuki TANIZAWA
Associate Professor:	Shun'ichi KURODA
Research Associate:	Kenji TATEMATSU
Post Doctoral Fellows:	Andrés D. MATURANA (2006.4.1-2006.10.31), Joo-Hee JUNG, Hiroyasu KADOYA, Nobuo YOSHIMOTO, Kazutoshi ONO (2006.7.1-2007.3.31)
Research Assistants:	Yoko MATSUSHITA, Kumiko HAZAMA (2006.4.1-2006.6.30), Takae TOYOSHIMA (2006.4.1-2006.4.30), Noriko MATSUNAGA (2006.4.1-2006.7.31), Noriko SHIKAKU, Kazuyo SADAMOTO (2006.9.1-2006.12.20), Nobuyuki BOKUI (2007.1.1-2007.3.31), Masumi IIJIMA (2007.1.16-2007.3.31)
Graduate Students:	Nobuyuki BOKUI (2006.4.1-2006.12.31), Junko IKUTA, Takeshi KASUYA, Hiroyuki TONOI, Hiroshi SANPEI, Shota NAKANISHI, Atsushi NAGAMI, Mayumi NIIYAMA, Yasuo SASAKI
Supporting Staff:	Mayumi MURATA (2006.4.1-2006.6.30), Ai OKUBO (2006.7.1-2007.3.31), Mayuko MURAI (2006.9.1-2007.3.31)

Outline

The research of this laboratory is focused on the biochemical and molecular biological studies on various enzymes. Their active-site structures and catalytic mechanisms are being investigated by site-directed mutagenesis, various spectroscopies, and X-ray crystallography. A previous conspicuous finding is the copper ion-dependent, post-translational modification mechanism for the biogenesis of the topa quinone cofactor in copper amine oxidase. Furthermore, we investigate the intracellular mechanisms involving protein kinase C family, which play important roles in the cell proliferation, differentiation, oncogenesis, and apoptosis by cross talking with other molecules. Recently, we have succeeded to identify several protein kinase C-interacting proteins and characterized them as regulatory proteins for the protein kinase activities and/or their subcellular localization and also as effectors of kinase signaling. In addition, we have developed 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 Projects

Cellular Function of Fasciculation and Elongation Protein Zeta-1 in Rat Embryo Hippocampal Neuron

The fasciculation and elongation protein zeta-1 (FEZ1), a mammalian orthologue of *Caenorhabditis elegans* UNC-76 protein, is a 45-kDa protein with four coiled-coiled domains and efficiently promotes the neurite elongation in the rat phaeochromocytoma

PC12 cells. UNC-76 proteins of *C. elegans* and *Drosophila* have been genetically demonstrated to be involved in the axonal guidance. We have shown that FEZ1 RNA interference (RNAi) represses the formation of axon in rat embryo hippocampal neurons. An anterograde mitochondrial movement is also retarded in neurites of the RNAi-treated hippocampal neurons. Moreover, the size of mitochondria is considerably elongated by the RNAi treatment. The transport of mitochondria from soma to axon or dendrites is essential for the neuronal differentiation. Therefore, our results strongly suggest that FEZ1 participates in the establishment of neuronal polarity by controlling the mitochondrial motility along axon.

Pinpoint Drug and Gene Delivery System Using ZZ tag-Displaying Bio-Nanocapsule and Targeting Molecule-fused IgG Fc Protein

We have recently developed a novel pinpoint drug and gene delivery system using bio-nanocapsules (BNCs), which is made of hepatitis B virus surface antigen protein. BNC is overproduced in the recombinant yeast cells as a hollow particle with about 100 nm in diameter and is able to incorporate genes, proteins, drugs, and polystyrene beads. Its surface is modifiable with various bio-recognition molecules, facilitating delivering various materials to cells and tissues of interest at will. Particularly, the immunoglobulin Fc-binding domain of *Staphylococcus aureus* protein A (ZZ-tag) has been displayed on the surface of BNC, which is useful for binding full-length antibodies specifically recognizing cells and tissues. In this study, we have constructed a bacterial expression system for periplasmic signal peptide (pelB)- and Fc-fused forms of various targeting molecules such as ligands, receptors, and homing peptides. They are expected to be overproduced in *Escherichia coli* and secreted into the periplasmic fraction, if possible, and also purified readily using a protein A-conjugated affinity column. We report the *ex vivo* and *in vivo* pinpoint targeting data using the combination of ZZ-tag displaying BNC and Fc-fused targeting protein. This system will facilitate the simultaneous examination of various targeting molecules and increase the efficiency of selecting the optimal targeting molecule for BNC.

Reaction Mechanism of Bacterial Copper Amine Oxidase: Conformational Changes of the TPQ Cofactor during the Catalytic Cycle

The catalytic reaction of copper amine oxidase comprises the reductive and oxidative half-reactions, divided on the basis of the redox state of the covalently-bound organic cofactor, topaquinone (TPQ). A substrate amine reduces TPQ to an aminoresorcinol form in the reductive half-reaction. The reduced TPQ is then re-oxidized by dioxygen in the following oxidative half-reaction. It has been proposed that the TPQ cofactor changes its conformation during the catalytic cycle, serving as a mediator of $2H^+$- and $2e^-$-transfers from substrate to dioxygen. To unravel the dynamic movement of TPQ directly associated with these $2H^+/2e^-$-transferring processes, we have determined X-ray crystal structures of catalytic intermediates formed in the enzyme from *Arthrobacter globiformis* (AGAO) and its variants, including a mutant enzyme lacking the catalytic base and those with the bound Cu^{2+} ion being replaced by other metal ions. The structures of Schiff-base intermediates formed in the base-less mutant have revealed a ‘wedge-shaped’ movement of the TPQ ring, which appears to be advantageous for

abstraction of substrate α-proton and also for the following hydrolysis. Furthermore, the structures of Cu-AGAO (wild type) and Ni-AGAO with TPQ in the substrate-reduced form have revealed that TPQ is in an 'on-copper' conformation in Cu-AGAO, which is probably a facile conformation for $1e^-$-transfer to Cu^{2+}, but branching off the normal reaction path. On the other hand, the reduced TPQ in Ni-AGAO is in a catalytically active 'off-copper' conformation without forming a semiquinone radical of TPQ.

ENH1 Scaffolds the PKCε-PKD1 Signaling Complex at the Z-Discs of Cardiomyocytes

Enigma homologue 1 (ENH1) is a heart and skeletal muscle-specific protein, which binds α-actinin through its PDZ domain and some PKC (Protein Kinase C) isoforms through its 3 LIM domains (LIM1-3). Upon treatment of hypertrophic agents (*e.g.*, norepinephrine, angiotensin II, endothelin 1, phorbol ester), neonatal rat cardiomyocytes (NRC) form sarcomere structures, and ENH1 was translocated from cytosol to the Z-discs in NRC. Recently, several lines of evidence demonstrated that the PKD1 (Protein Kinase D1) activated by direct phosphorylation with PKCε plays a pivotal role for inducing cardiac hypertrophy. In this study, we investigated if ENH1 is involved in the PKCε-PKD1 signaling complex at the Z-discs of NRC. Two hybrid analyses showed that the LIM1-3 domains strongly interact with the C-terminal half of PKD1 (catalytic domain). The interaction of PKD1 with ENH1 was not affected by the phosphorylation activity of PKD1 in the immunoprecipitation assay; however, the phosphorylation activity of PKD1 was repressed by the interaction with ENH1. In addition, the interaction of PKCε with ENH1 was observed only in the presence of PKD1. In NRC, the cardiac hypertrophic signaling was significantly repressed by the ENH1 RNAi (RNA interference). Taken together, ENH1 functions as a scaffold protein for PKCε-PKD1 signaling complex at the Z-discs of NRC, which may prevent cardiomyocytes from improper cardiac hypertrophy by mediating the PKD1 phosphorylation activity.

Publications

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Engineered Bio-nanocapsules, the Selective Vector for Drug Delivery System, D. Yu, T. Fukuda, Tuoya, S. Kuroda, K. Tanizawa, A. Kondo, M. Ueda, T. Yamada, H. Tada, and

M. Seno: IUBMB Life, 58 (2006) 1–6.

Kinetic and Structural Studies on the Catalytic Role of the Aspartic Acid Residue Conserved in Copper Amine Oxidase, Y.-C. Chiu, T. Okajima, T. Murakawa, M. Uchida, M. Taki, S. Hirota, M. Kim, H. Hayashi, Y. Yamamoto, and K. Tanizawa: Biochemistry, 45 (2006) 4105–4120.

Involvement of a Putative [Fe-S]-Cluster-Binding Protein in the Biogenesis of Quinohemoprotein Amine Dehydrogenase, K. Ono, T. Okajima, M. Tani, S. Kuroda, D. Sun, V. L. Davidson, and K. Tanizawa: J. Biol. Chem., 281 (2006) 13672–13684.

Secretory Production System of Bionanocapsules Using a Stably Transfected Insect Cell Line, T. Shishido, M. Muraoka, M. Ueda, M. Seno, K. Tanizawa, S. Kuroda, H. Fukuda, and A. Kondo: Appl. Microbiol. Biotechnol., 73 (2006) 505–511.

Quantitative and Dynamic Analyses of G Protein-Coupled Receptor Signaling in Yeast using Fus1, Enhanced Green Fluorescence Protein (EGFP), and His3 Fusion Protein, J. Ishii, S. Matsumura, S. Kimura, K. Tatematsu, and S. Kuroda, H. Fukuda, and A. Kondo: Biotechnol. Prog., 22 (2006) 954–960.

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Nell-1 Induces Acrania-like Cranioskeletal Deformities during Mouse Embryonic Development, X. Zhang, C. M. Cowan, X. Jiang, C. Soo, S. Miao, D. Carpenter, B. Wu, S. Kuroda, and K. Ting: Lab. Invest., 86 (2006) 633–44.

Nell-1-Induced Bone Regeneration in Calvarial Defects, T. Aghaloo, C. M. Cowan, Y. F. Chou, X. Zhang, H. Lee, S. Miao, N. Hong, S. Kuroda, B. Wu, K. Ting, and C. Soo: Am. J. Pathol., 169 (2006) 903–15.

Review Papers

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Development of New HPV Vaccine by Surface Display Method on Lactic Acid Bacteria (in Japanese), T. Sewaki, K. R. Pu, T. C. Kim, M. H. Sung, and S. Kuroda: Saibo, 38 (2006) 36–39.

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Bionanocapsules for *In Vivo* Pinpoint Gene and Drug Delivery System, T. Yamada, J. H. Jung, M. Seno, M. Ueda, A. Kondo, K. Tanizawa, and S. Kuroda: A Manual on Gene Transfer Vector and Genetic Modification Technology (John Rossi & Ted Friedmann, Eds.), Cold Spring Harbor Press (2006).

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Patents

"Method and Material for Introduction of Genes into Hollow Bionanoparticles" S. Kuroda, J. H. Jung, K. Tanizawa, J. Ohishi, Y. Katayama, T. Kang, and T. Yamada: JP2006-205698.

"Efficient Method of Purification of Bionanocapsules" S. Kuroda, Y. Maekawa, and M. Nagita: JP2006-35666.

"Efficient Method of Introduction of Materials inside Bionanocapsules" S. Kuroda, J. Ueda, and M. Nagita: JP2006-240746.

"Basal Plate and Method of Preparation" S. Hiramatsu, G. M. Jung, T. Hatahira, D. Kanamori, S. Kuroda, and K. Tanizawa: JP2006-257829.

"Nanoparticles for Immunological Measurement" S. Hiramatsu, G. M. Jung, T. Hatahira, D. Kanamori, S. Kuroda, and K. Tanizawa: JP2006-258398.

"Biotinylated or Homing Peptide-Displaying Bionanocapsules" S. Kuroda, J. Ueda, M. Nagita, and H. Tonoi: JP2006-356378.

“Biotinylated Nanoparticles for Immunological Measurement” S. Hiramatsu, G. M. Jung, T. Hatahira, D. Kanamori, H. Kadoya, S. Kuroda, and K. Tanizawa: JP2007-3677.

“Composite Particles Used for Drug Delivery System” N. Shimizu, C. Ogino, and S. Kuroda: JP2007-32765.

International Conferences

Reaction Mechanism of Bacterial Copper Amine Oxidase: Conformational Changes of the TPQ Cofactor during the Catalytic Cycle, *T. Okajima, T. Murakawa, Y.-C. Chiu, S. Kuroda, and K. Tanizawa, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto International Conference Hall, Kyoto, Japan, June 18–23, 2006.

Quantum Mechanical Hydrogen Tunneling in Bacterial Copper Amine Oxidase Reaction, *T. Murakawa, T. Okajima, S. Kuroda, M. Taki, Y. Yamamoto, H. Hayashi, and K. Tanizawa, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto International Conference Hall, Kyoto, Japan, June 18–23, 2006.

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Pinpoint Drug and Gene Delivery System Using ZZ tag-Displaying Bio-nanocapsule and Targeting Molecule-fused IgG Fc Protein, *H. Tonoi, H. Tada, A. Ueda, A. Kondo, M. Seno, M. Ueda, K. Tanizawa, and S. Kuroda, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto International Conference Hall, Kyoto, Japan, June 18–23, 2006.

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Improvement of *In Vivo* Pinpoint Drug Delivery System Using Bio-nanocapsules, *J.-H. Jung, T. Yamada, A. Kondo, M. Seno, M. Ueda, K. Tanizawa, and S. Kuroda, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto International Conference Hall, Kyoto, Japan, June 18–23, 2006.

Hepatitis B Virus Envelope Pre-S Peptide Applicable for the Human Liver-specific Protein Delivering System, *T. Kasuya, A. Uyeda, K. Tanizawa, and S. Kuroda, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto International Conference Hall, Kyoto, Japan, June 18–23, 2006.

PDZ-LIM Protein, ENH1 Scaffolds Protein Kinase D1 to Modulate the Activity of L-Type Calcium Channels in Neonatal Rat Cardiomyocytes (Oral), A. D. Maturana, Sanken International Symposium on Nanoscience and Nanotechnology 2006 – Perspective on Interdisciplinary Nanobiology and Industrial Nanotechnology, Icho Kaikan, Suita, Osaka, Japan, September 19–20, 2006.

Mechanism of Reductive Half-reaction Catalyzed by Topa Quinone-containing Copper Amine Oxidase (Invited), K. Tanizawa, Japan-China Crossover Science Symposium 2006, Mito, Ibaraki, Japan, October 13–18, 2006.

Involvement of a Hypothetical [Fe-S]-Binding Protein in the Biosynthesis of Quinohemoprotein Amine Dehydrogenase (Invited), K. Tanizawa, Japan-Italy Symposium of New Trends in Enzyme Science and Technology, Nagoya, Japan, November 15–17, 2006.

Fasciculation and Elongation Protein Zeta-1 (FEZ1) Participates in the Polarization of Hippocampal Neuron by Controlling the Mitochondrial Motility, *J. Ikuta, A. D. Maturana, T. Fujita, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 5th 21st Century COE International Symposium “Towards Creating New Industries Based on Inter-Nanoscience”, Awaji, Hyogo, Japan, December 8–9, 2006.

Improvement of *In Vivo* Pinpoint Drug Delivery System Using Bio-nanocapsules, J.-H. Jung, T. Yamada, A. Kondo, M. Seno, M. Ueda, *K. Tanizawa, and S. Kuroda, 5th 21st Century COE International Symposium “Towards Creating New Industries Based on Inter-Nanoscience”, Awaji, Hyogo, Japan, December 8–9, 2006.

Hepatitis B Virus Envelope Pre-S Peptide Applicable for the Human Liver-specific

Protein Delivering System, T. Kasuya, A. Uyeda, *K. Tanizawa, and S. Kuroda, 5th 21st Century COE International Symposium “Towards Creating New Industries Based on Inter-Nanoscience”, Awaji, Hyogo, Japan, December 8–9, 2006.

Contributions to International Conferences and Journals

K. Tanizawa	The 20th IUBMB International Congress of Biochemistry and Molecular Biology and the 11th FAOBMB Congress (Member of Program Committee, Reviewer for Young Scientist Award)
K. Tanizawa	Federation of Asian and Oceanian Biochemists and Molecular Biologists (Delegate of Japan)
S. Kuroda	Human Science Forum (Kinki Bio-industry Association) (Member of Organizing Committee)

Publications in Domestic Meetings

Japanese Agricultural Biochemical Society, Kansai Branch Meeting	1 paper
The Molecular Biology Society of Japan	1 paper
Bimonthly Meeting of Vitamin B Committee	2 papers

Academic Degrees

Doctor Degree for Science

K. Ono	Biochemical and Molecular Biological Studies on the Role of an Iron-Sulfur Protein in Posttranslational Modification of Quinohemoprotein Amine Dehydrogenase
J. Ikuta	Cellular Function of Fasciculation and Elongation Protein Zeta-1 in Rat Embryo Hippocampal Neuron

Master Degree for Frontier Bioscience

H. Tonoi	Pinpoint Drug and Gene Delivery System Using ZZ Tag-Displaying Bio-Nanocapsule and Targeting Molecule-fused IgG Fc Protein

Sponsorships

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	¥6,300,000

Grant-in-Aid for Scientific Research (B)

K. Tanizawa	Mechanisms of Biosynthesis and Catalysis of Built-in Type Quinone Cofactor	¥9,200,000

Grant-in-Aid for Scientific Research (21st Century COE)

K. Tatematsu	Development of Targeted Drug Delivery System	¥1,000,000

		by Chemical Modification of Harmless Metal Clusters	

Health and Labour Sciences Research Grants

S. Kuroda		Development of Bio-Nanocarriers for Pinpoint Drug Delivery System and Its Application for Cancer Therapy	¥4,000,000

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	¥3,675,000
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	¥1,300,000
K. Tanizawa	Bio-oriented Technology Research Advancement Institution (BRAIN)	Development of Innovative and Hypersensitive Bio-sensing Technology Using Yeast-derived Bio-nanocapsule	¥20,000,000
S. Kuroda	Ministry of Education, Culture, Sports, Science, and Technology	Protein 3000 Project	¥2,500,000
S. Kuroda	Osaka Science and Technology Center (Ministry of Economy, Trade and Technology)	Development of Proteome-based High Throughput Screening System Using Combinatorial Biochemistry.	¥500,000

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.	¥10,000,000
S. Kuroda	Japan Science and Technology Agency (Promotion Program of Utilization of Regional Research and Development)	Development of Bio-nanoparticles for Pinpoint Drug Delivery System in Medical Field.	¥44,910,000

Cooperative Research

S. Kuroda	As One Corp.	Development of Screening Method for Agonists and Receptors Using Combinatorial Biochemistry	¥16,000,000
S. Kuroda	Beacle Inc.	Development of Hollow Bio-nanocapsule Applicable to Tissue/Cell-specific Targeting and Imaging	¥2,180,000
K. Tatematsu	GenoLac BL Corp.	Production and Development of New Live Bacterial Vaccines	¥406,000
K. Tatematsu	Toyobo Co., Ltd.	Preparation of Cell-free Extract and Establishment of Stable Storage	¥320,000

Other Research Fund

K. Tanizawa	Vitamin B Committee	¥250,000

Department of Single Molecule Biophysics

Professor:	Hiroyuki NOJI
Associate Professor:	Yoh WADA
Research Associate:	Kazuhito TABATA, Ryota IINO
Post Doctoral Fellows:	Daichi OKUNO, Hiromi IMAMURA, Hiroshi UENO, Liza LAM, Sawako ENOKI
Research Technician:	Yuko IKO, Masahiro NAKANO, Rie HASEGAWA
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Under Graduate Students:	Mahito MATSUNO, Mariko NAKAMURA, Yoshihito KOMORIYA, Yoshihiro NISHIKAWA,
Supporting Staff:	Miki WALSH and Lisa DATE

Outline

Our main research objective is to reveal energy-conversion mechanism of biomolecular motors using single-molecule imaging and single-molecule manipulation techniques. Currently, we launched research projects of micro- and bio-devices to realize high sensitive and high throughput detection of biological reactions using micro/nano technology. We conduct quite interdisciplinary researches crossing biophysics, biochemistry, nanotechnology, and micro/nano fabrication.

Current Research Projects

Single-molecule studies on a rotary molecular motor, F_1-ATPase

Rotational direction and speed of F_1-ATPase, a biological rotary motor, was manipulated by magnetic tweezers, and chemical reaction catalyzed by this enzyme was regulated by external force for the first time. Affinity of ATP strongly depended on the angle of the rotor subunit γ, and drastically changed (about 1000 times!). In contrast, the equilibrium for ATP hydrolysis/synthesis did not depend on the angle of the γ.

Imaging of COPII vesicle formation and budding from artificial membrane

COPII system is responsible for the vesicle formation from endoplasmic reticulum in eukaryotic cells. We have succeeded in the real time observation of the process of COPII vesicle formation in the reconstituted system.

Single cell measurement of drug efflux from bacteria

Multidrug resistance of bacteria is a serious problem in antibiotic treatment of infection. Multidrug resistance often results from expression of efflux transporters located in the cell membrane. By applying femtoliter chamber array, we developed rapid and direct method assessing drug efflux at the single cell level.

Single molecule analysis of DNA

Single DNA Molecules are enclosed in femtoliter chamber array, and digestion by

restriction enzyme was directly imaged under a microscope. Furthermore, DNA fragment was stretched by applying oscillating voltage and the size was measured directly under a microscope.

Publications

Original Papers

Single Molecule Energetics of F_1-ATPase Motor, E. Muneyuki, T. Watanabe-Nakayama, T. Suzuki, M. Yoshida, T. Nishizaka. and H. Noji, 92. (2006) 1806-1812.

Temperature Distribution Measurement on Microfabricated Thermodevice for Single Biomolecular Observation Using Fluorescent Dye, H. F. Arata, P. Low, K. Ishizuka, C. Bergaud, B. Kim, H. Noji and H. Fujita, Sensors and Actuators, B: Chemical 117 (2) (2006) 339-345.

Chemical Delivery Microsystem for Single-Molecule Analysis Using Multilaminar Continuous Flow, S. W. Lee, T. Yamamoto, H. Noji and T. Fujii, Enzyme and Microbial Technology 39 (3) (2006) 519-525.

Electrophysiological Recordings of Single Ion Channels in Planar Lipid Bilayers Using Apolymethyl Methacrylate Microfluidic Chip, H. Suzuki, K. V. Tabata, H. Noji and S. Takeuchi, Biosens Bioelectro 22 (6) (2006) 1111-1115.

Motion Control of Single F_1-ATPase Rotary Biomolecular Motor Using Microfabricated Local Heating Devices, H. F. Arata, H. Noji and Fujita, H., APPLIED PHYSICS LETTERS 88, (2006) 083902

Highly Reproducible Method of Planar Lipid Bilayer Reconstitution in Polymethyl Methacrylate Microfluidic Chip, H. Suzuki, K. V. Tabata, H. Noji and S. Takeuchi, Langmuir 22 (2006) 1937-1942.

Review Papers

F_1-ATPase: a highly coupled reversible rotary motor, R. Iino, H. Noji. Biochem Soc Trans. 34 (2006) 993-996.

International Conferences

Single-Molecule Studies on the Mechanism of ATP Synthesis by F_1-ATPase (Invited), H. Noji, Gordon Research Conference of The Molecular & Cellular Bioenergetics, USA. June 12, 2006

Femtolitre Chamber Array for Single Molecule Analysis of F_1-Motor Protein (Invited), H. Noji, Bioscience2006, United Kingdom, July 27, 2006

Mechanochemical Coupling of F_1-ATPase (Invited), H. Noji, The 20th Symposium of The Protein Society and 20th Anniversary Celebration, USA, August 6, 2006

Rotary Motors (Invited), H. Noji, 2006 Biophysical Society Discussions, USA. October 20, 2006

Femtoliter Chamber for Single-Molecule Analysis (Invited), H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Chemomechanical coupling of F_1-ATPase motor protein (Invited), H. Noji, SANKEN Workshop on Nano-Bioscience at Berkeley, USA, March 21, 2007

Micron-Sized Reaction Chamber Array for Highly Sensitive Detection of Biological Reaction (Invited), R. Iino, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Highly Sensitive Measurement of Biological Reaction in Femtoliter Chamber Array (Invited), R. Iino, SANKEN WORKSHOP on Nano-Bioscience at Berkeley, USA, March 21, 2007

Rotation Mechanism of V_1-ATPase Is Distinct from That of F_1-ATPase, *H. Imamura, M. Takeda, S. Funamoto, M. Yoshida, K.Yokoyama, 20TH IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, June 19, 2006

Does Forcible Rotation of F_1 motor Enhance ATP Hydrolysis?, *Y. Iko, T. Akamatsu, S. Sakakihara, K. V. Tabata, H. Noji, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Pausing of F_1 by 5'-(β, γ-imido)triphosphate (AMPPNP), *R. Fujisawa, D. Okuno, H. Noji, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Observation of Single-Molecule Restriction Enzyme Reaction in Microchamber Made from Acrylamide Gel, *L. Lam, K. Ishizuka, S. Sakakihara, H. Noji, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Mechanical Modulation of ATP Binding Affinity and ATP Hydrolysis / Synthesis Equilibrium of F_1-ATPase, *D. Okuno, R. Watanabe, S. Sakakihara, K. Shimabukuro, M. Yoshida, H. Noji, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Development of The Single Molecule Imaging System of The F_o motor, *H. Ueno, K. V. Tabata, T. Suzuki, T. Ide, M. Yoshida, H. Noji, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Pathway for Assembly of V_1 Complex of Thermus Thermophilus V-ATPase, *H. Imamura, S. Funamoto, M. Yoshida, K. Yokoyama, SANKEN International Symposium

on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

Imaging of COPII Vesicle Formation and Budding from Artificial Membrane, *K. V. Tabata, K. Sato, T. Ide, H. Noji, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19, 2006

ε Subunit Stops Rotation of Thermophilic F_1-ATPase; Single Molecular Analysis of The Inhibition by The ε Subunit, *T. Haruyama, Y. Hirono-Hara, H. Noji, Y. Kato-Yamada, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Membrane Transport Assay System for Transporter Proteins Using Artificial Lipid Bilayers, *H. Suzuki, K. V. Tabata, H. Noji, S. Takeuchi, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Imaging of COPII Vesicle Formation and Budding from Artificial Membrane, *K. V. Tabata, K. Sato, T. Ide, H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Designing a Mutant F_1-ATPase for Easy and Rapid Single Molecule Analysis, *M. Nakamura, H. Ueno, H. Imamura, H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Single-Molecule Analysis of F_1-Motor Loaded with Nonhydrolyzable Substrate, *R. Fujisawa, D. Okuno, H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Does Forcible Rotation of F_1 Motor Enhance ATP Hydrolysis?, *Y. Iko, T. Akamatsu, S. Sakakihara, K. V. Tabata, H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Development of the single molecule imaging system of the F_o motor, H. Ueno, K. V. Tabata, T. Suzuki, T. Ide, M. Yoshida, H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Mechanical Modulation of ATP Binding Affinity and ATP Hydrolysis / Synthesis Equilibrium of F_1-ATPase, *D. Okuno, R. Watanabe, S. Sakakihara, K. Shimabukuro, M. Yoshida, H. Noji, EABS & BSJ 2006, Okinawa, Japan, November 13, 2006

Single Cell Measurement of Drug Efflux by RND Family Transporter in Femtoliter Chamber Array, *R. Iino, M. Nakata, K. Nishino, S. Sakakihara, S. Takeuchi, A. Yamaguchi, H. Noji, 5th 21th Century COE International Symposium “Towards creating new industries based on inter-nanoscience”, Osaka, Japan, December 8, 2006

Mechanical Twisting of Single Green Fluorescent Protein Molecules, *S. Enoki, R. Iino, H. Noji, 5th 21th Century COE International Symposium “Towards creating new industries based on inter-nanoscience”, Osaka, Japan, December 8, 2006

Lipid Bilayer Microchambers: An Pptical Detection System for Membrane Transport, *H. Suzuki, K. V. Tabata, H. Noji and S. Takeuchi, (2006) Proceedings of the IEEE International Conference on Micro Electro Mechanical Systems (MEMS) 1627841, pp.482-485

Restriction Enzyme Assay in Femtoliter Microchamber, *L. Lam, K. Ishizuka, S. Sakakihara and H. Noji, (2006) Proc. 10th International Conference on Miniaturized Systems for Chemistry and Life Sciences (μTAS), Tokyo, Vol. 1, pp.1429-1431

Development of an Assay System for ABC Transporters Reconstituted in an Artificial Lipid Bilayer. *H. Suzuki, K. V. Tabata, H. Noji and S. Takeuchi, (2006) Proceedings of 10th International Conference on Miniaturized Systems for Chemistry and Life Sciences (μTAS), Tokyo, Vol. 2, pp. 1363-1365

Publications in Domestic Meetings

Protein Science Society of Japan	1 paper
Institute of Electrical Engineers, Sensor Micro-machine Subdivision, Bio-micro System Workshop	2 papers
Japan Bioenergetics Group Workshop	5 papers

Sponsorships

Grants-in-Aid for Scientific Research from the ministry of Health, Labour and Welfare

H. Noji	Development of single molecule PCR device	¥5,000,000

Grants-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (MEXT)

H. Noji	Rotational mechanism of F_oF_1-ATP synthase	¥49,800,000

Grants-in-Aid for Scientific Research from Japan Society for the Promotion of Science (JSPS)

H. Noji	Development of novel single molecule measurement method using ultra-small reaction chamber array	¥15,600,000

Grants-in-Aid for Scientific Research from JSPS

R. Iino	Single molecule measurement of rotation of ATP synthase driven by proton motive force	¥2,000,000

Grants-in-Aid for Scientific Research from JSPS

R. Iino	Screening of novel xenobiotic transporter genes by femtoliter reaction chamber array	¥1,000,000

Grants-in-Aid for Scientific Research from JSPS

K. Tabata	Protein patterning using a photoeliminative GFP and the method of single protein fluorescence imaging on lipid bilayer membrane	¥1,000,000

Grants-in-Aid for Scientific Research from JSPS

L. Lam	Micro-device development for single molecule DNA analysis	¥1,200,000

Grants-in-Aid for Scientific Research from JSPS

H. Imamura	Rotational mechanism of V_1-motor analyzed by single molecule technique and X-ray crystallography	¥1,200,000

Grants-in-Aid for Scientific Research from JSPS

H. Ueno	Single molecule rotational observation of F_o-motor reconstituted into planar membrane	¥1,200,000

Entrusted Research

H. Noji	Bio-oriented Technology Research Advancement Institution	Preparation of Membrane Protein and single molecule observation	¥30,760,000

Department of Cell Membrane Biology

Professor:	Akihito YAMAGUCHI
Associate Professor:	Satoshi MURAKAMI
Guest Associate Professor:	Yoshimi MATSUMOTO(2007.1.1- 2007.3.31)
Research Associate:	Takahiro HIRATA
Specially Appointed Research Associate:	Syoko NISHI
Post Doctoral Fellows:	Takashi MATSUMOTO, Yoshimi MATSUMOTO(2006.11.1-2006.12.31), Hidetada HIRAKAWA(2007.2.1-2007.3.31)
Graduate Students:	Naoki KOBAYASHI, Satofumi HASHIMOTO, Ayumi IWATA, Megumi OHIGASHI, Yasuko SENDA, Yu HISANO, Eiji NIKAIDO, Li-Yuan WANG, Kosuke MIYATA, Mamiko ONOE
Under Graduate Students:	Hiroki SAKATA, Yasunobu YOSHIDA
Supporting Staff:	Kotoko ISE, Reiko SATO, Mari NISHIDA

Outline

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. This was published in *Nature* 2006. 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 PTS sugars induce *mdtEF* gene expression through catabolite control.

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. Finally, we succeeded to construct ABCA7-knockout mice.

Current Research Projects

Crystallographic and protein engineering analysis of xenobiotic exporters.
We have succeeded to determine the first crystal structure of bacterial multidrug efflux transporter AcrB in 2002. This is the first crystal structure for transporter proteins. 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 reveled that drugs are exported by three-step functionally rotating orderd 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 cystein mutants was co-expressed in *E. coli*. Our observation indicates that the AcrB can directly interact to TolC.

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 catabolite control system.

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 thyrogrobulin that is essential for thyroid hormone biosynthesis. This result suggested the possible contribution of ABCA5 protein in thyroid hormone synthesis. In addition, we constructed the ABCA7-knockout mice

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

Crystal Structure of the DsbB-DsbA Complex Reveals a Mechanism of Disulfide Bond Generation, K. Inaba, S. Murakami, M. Suzuki, A. Nakagawa, E. Yamashita, K. Okada and K. Ito: Cell, 127 (2006) 789-801.

Application of Femtosecond Laser Ablation for Detaching Grown Protein Crystals from Glass Capillary Tube, M. Kashii, R. Fujisawa, H. Adachi, Y. Mori, T. Sasaki, Y. Koga, K. Takano, S. Kanaya, H. Matsumura, T. Inoue, S. Murakami, K. Sugamoto and H. Yoshikawa: J. Biosci. Bioeng., 102 (2006) 372-374.

Crystal Structures of a Multidrug Transporter Reveal a Functionally Rotating Mechanism, S. Murakami, R. Nakashima, E. Yamashita, T. Matsumoto and A. Yamaguchi: Nature, 443 (2006) 173-179.

N-Acetyl-D-Glucosamine Induces the Expression of Multidrug Exporter Genes, *mdtEF*, via Catabolite Activation in *Escherichia coli*, H. Hirakawa, Y. Inazumi, Y. Senda, A. Kobayashi, T. Hirata, K. Nishino and A. Yamaguchi: J. Bacteriol., 188 (2006) 5851–5858.

Growth Phase-Dependent Expression of Drug Exporters in *Escherichia coli* and Its Contribution to Drug Tolerance, A. Kobayashi, H. Hirakawa, T. Hirata, K. Nishino and A. Yamaguchi: J. Bacteriol., 188 (2006) 5693–5703.

Effect of Drug Transporter Genes on Cysteine Export and Overproduction in *Escherichia coli*., S. Yamada, N. Awano, K. Inubushi, E. Maeda, S. Nakamori, K. Nishino, A. Yamaguchi and H. Takagi: Appl. Environ. Microbiol., 72 (2006) 4735-4742.

Crystallization and Preliminary Crystallographic Analysis of Orotidine 5’-Monophosphate Decarboxylase from the Human Malaria Parasite *Plasmodium falciparum*, S. R Krungkrai, K. Tokuoka, Y. Kusakari, T. Inoue, H. Adachi, H. Matsumura, K. Takano, S. Murakami, Y. Mori, Y. Kai, J. Krungkrai and T. Horii: Acta Crystallogr., F62 (2006) 542-545.

Purification, Crystallization and Preliminary X-ray Diffraction of SecDF, a Translocon-Associated Membrane Protein, from *Thermus thermophilus*, T. Tsukazaki, H. Mori, S. Fukai, T. Numata, A. Perederina, H. Adachi, H. Matsumura, K. Takano, S. Murakami, T. Inoue, Y. Mori, T. Sasaki D. G Vassylyev, O. Nureki and K. Ito: Acta Crystallogr., F62 (2006) 376-380.

Crystallization and Preliminary X-ray Analysis of the tRNA Thiolation Enzyme MnmA from *Escherichia coli* Complexed with $tRNA^{Glu}$, T. Numata, Y. Ikeuchi, S. Fukai, H. Adachi, H. Matsumura, K. Takano, S. Murakami, T. Inoue, Y. Mori, T. Sasaki, T. Suzuki and O. Nureki: Acta Crystallogr., F62 (2006) 368-371.

Sphingosine 1-Phosphate is Released from the Cytosol of Rat Platelets in a

Carrier-Mediated Manner, N. Kobayashi, T. Nishi, T. Hirata, A. Kihara, T. Sano, Y. Igarashi and A. Yamaguchi: J. Lipid Res., 47 (2006) 614-621.

Solution-Stirring Method Improves Crystal Quality of Human Triosephosphate Isomerase, H. Adachi, A. Niino, T. Kinoshita, M. Warizaya, R. Maruki, K. Takano, H. Matsumura, T. Inoue, S. Murakami, Y. Mori and T. Sasaki: J. Biosci. Bioeng., 101 (2006) 83-86.

Review Papers

Protein Crystallography, Phase Improvement and Density Modification, S. Murakami: Journal of the Crystallographic Society of Japan, 48 (2006) 381-386.

A Riddle of Bacterial Drug Resistance, Substrate Recognition and Efflux Mechanisms of Multidrug Transporter, S. Murakami: Bionics, 3 (2006) 38-43.

Crystallization of Protein and Small Organic Molecules using Femtosecond Laser Irradiation, H. Adachi, Y. Mori, T. Sasaki, K. Takano, H. Matsumura, T. Inoue and S. Murakami: Kouso Kougaku News, 56 (2006) 9-13.

A Major Reason Confers Drug Resistance on Bacteria, S. Murakami: Newton, 26 (2006) 109.

Protein Crystallization by Combining Femtsecond Laser Irradiation and Solution-stirring Techniques, Y. Mori, H. Adachi, K. Takano, T. Inoue, S. Murakami, H. Matsumura and T. Sasaki: OPTRONICS, 25 (2006) 201-207.

SOSHO Project and Biogrid Partnership in Drug Development, T. Inoue, Y. Kado, K. Aritake, H. Matsumura, Y. Kai, Y. Fukunishi, H. Nakamura, T. Kinoshita, I. Nakanishi, S. Minakata, M. Komatsu, H. Adachi, Y. Mori, K. Takano, S. Murakami, T. Sasaki, M. Miyano and Y. Urade: SAR News, 10 (2006) 2-6.

Patents

Measurement Method of Efflux Activity from Single Cell and Its Utilization, R. Iino, K. Nishino, M. Nakata, S. Sakakibara, A. Yamaguchi and H. Noji, Tokugan2006-294558

International Conferences

Crystal Structure of Multi-Drug Transporter Reveal a Functionally Rotating Mechanism (Invited), *S. Murakami, Seminar, Department of Physiology, UCLA, Mar.23, 2007.

Crystal Structure of Multi-Drug Transporter AcrB Reveal a Functionally Rotating Mechanism (Oral), *S. Murakami, SANKEN Workshop on Nano-Bioscience at Berkeley, University of California Berkeley, USA, Mar.21-22, 2007.

Crystal Structure of a Bacterial Multidrug Transporter Reveal a Functionally Rotating Mechanism (Invited), *S. Murakami, Seminar, University of Cambridge, UK, Feb.8, 2007.

Structure and Function of Bacterial Xenobiotic Exporters (Oral), *A. Yamaguchi, Second SANKEN- CNU Joint Symposium on Nanoscience and Nanotechnology SANKEN and SANKEN 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience", Osaka Univ., Japan, Jan.25-26, 2007.

Crystal Structure of a Bacterial Multidrug Transporter Reveal a Functionally Rotating Mechanism (Invited), *S. Murakami, Seminar, BOSE INSTITUTE, Kolkata, India, Jan.10, 2007.

Crystal Structure of a Bacterial Multidrug Transporter Reveal a Functionally Rotating Mechanism (Invited), *S. Murakami, Seminar, Dept. of Crystallography and Biophisics Univ. of Madras, Chennai, India, Jan.8, 2007.

Crystal Structure of a Bacterial Multidrug Transporter Reveal a Functionally Rotating Mechanism (Invited), *S. Murakami, 94th Indian science congress, Symposium IV: Structure and Functional Relationship of Macromolecules, Chidambaram, Tamilnadu, India, Annamalai Univ., Jan.4-7, 2007.

Synthesis of Autoinducer-2 Antagonists in Bacterial Quorum-Sensing, *M. Hiraoka, Y. Yano, T. Kawano, H. Hirakawa, A. Kobayashi, T. Hirata, A. Yamaguchi, J. Ohkanda and N. Kato, 5th 21COE International Symposium, Towards Creating New Industries Based on Inter-Nanoscience, Awaji Yumebutai International Conference Center, Japan, Dec.8-9, 2006.

Single Cell Measurement of Drug Efflux by RND Family Transporter in Femtoliter Chamber Array, *R. Iino, M. Nakata, K. Nishino, S. Sakakihara, S. Takeuchi, A. Yamaguchi and H. Noji, 5th 21COE International Symposium, Towards Creating New Industries Based on Inter-Nanoscience, Awaji Yumebutai International Conference Center, Japan, Dec.8-9, 2006.

Characterization of Mouse ABCA5 Protein, *M. Ohigashi, T. Nishi and A. Yamaguchi, 5th 21COE International Symposium, Towards Creating New Industries Based on Inter-Nanoscience, Awaji Yumebutai International Conference Center, Japan, Dec.8-9, 2006.

A Biological Function of Multidrug Transporters in Iron Homeostasis, *K. Nishino, T. Hirata and A. Yamaguchi, 5th 21COE International Symposium, Towards Creating New Industries Based on Inter-Nanoscience, Awaji Yumebutai International Conference Center, Japan, Dec.8-9, 2006.

Tissue Specific Expression of the Splicing Variants of the Mouse Vacuolar Proton Translocating ATPase a4 Subunit, *S. Kawasaki-Nishi, A. Yamaguchi, M. Forgac and T. Nishi, 5th 21COE International Symposium, Towards Creating New Industries Based on Inter-Nanoscience, Awaji Yumebutai International Conference Center, Japan, Dec.8-9, 2006.

Intracellular Localization and Tissue Distribution of Novel RND-Type Proteins in Mice, *S. Hashimoto, Y. Kubo, T. Nishi, T. Hirata and A. Yamaguchi, 5th 21COE International Symposium, Towards Creating New Industries Based on Inter-Nanoscience, Awaji Yumebutai International Conference Center, Japan, Dec.8-9, 2006.

A Functionally Rotating Mechanism Revealed in Crystal Structures of the Multidrug Transporter, AcrB, with Bound Substrates (invited), *S. Murakami, AsCA'06/CrSJ:Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Tsukuba, Japan, Nov.20-23, 2006.

The Crystal Structure of Orotidine 5'-Monophosphate Decarboxylase from the Human Malaria Parasite *Plasmodium falciparum*, *K. Tokuoka, S. Krungkrai, Y. Kusakari, T. Inoue, H. Adachi, H. Matsumura, K. Takano, S. Murakami, Y. Mori, Y. Kai, K. Jerapan and T. Horii, AsCA'06/CrSJ:Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Tsukuba, Japan, Nov.20-23, 2006

The Crystallization and X-ray Diffraction of the Exo-Arabinanase from *Penicillium Chrysogenum*, *Y. Sogabe, T. Kinoshita, A. Yamaguchi, T. Kitatani, T. Sakamoto, H. Ihara, H. Matsumura, K. Takano, S. Murakami, T. Inoue, Y. Mori and T. Tada, AsCA'06/CrSJ:Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Tsukuba, Japan, Nov.20-23, 2006.

Membrane Protein Crystallization under High Pressure, *H. Yoshikawa, S. Nakata, R. Murai, T. Kitatani, M. Syou, H. Adachi, T. Inoue, H. Matsumura, K. Takano, S. Murakami, Y. Mori and T. Sasaki, AsCA'06/CrSJ:Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Tsukuba, Japan, Nov.20-23, 2006.

Crystal Structure of a Multidrug Transporter Reveal a Functionally Rotating Mechanism (Oral), *S. Murakami, EABS & BSJ 2006:Fifth East Asian Biophysics Symposium & Forty-Fourth Annual Meeting of the Biophysical Society of Japan, Okinawa, Japan, Nov.12-16, 2006.

Improvement and Analysis of ATP Synthase Crystals, *Y. Shirakihara, A. Shiratori, S. Murakami, T. Suzuki and M. Yoshida, EABS & BSJ 2006:Fifth East Asian Biophysics Symposium & Forty-Fourth Annual Meeting of the Biophysical Society of Japan, Okinawa, Japan, Nov.12-16, 2006.

A Functionally Rotating Mechanism Revealed in Crystal Structures of the Multidrug Transporter, AcrB, with Bound Substrates (Invited), *S. Murakami, SLS seminar, Swiss, Sep.20, 2006.

A Functionally Rotating Mechanism Revealed in Crystal Structures of the Multidrug Transporter, AcrB, with Bound Substrates (Invited), *S. Murakami, Switzerland-Japan Symposium on Structural Biology 2006 , Brunnen, Switzerland, Sep.17-19, 2006.

A Functionally Rotating Mechanism Revealed in Crystal Structures of the Multidrug Transporter, AcrB, with Bound Substrates (Invited), *S. Murakami, Astbury Seminar, University of Leeds, UK, Sep.12, 2006.

Bacterial Multidrug Exporters -From the Molecular Structure to the Biological Funciton (Oral), *A. Yamaguchi, The 6th Awaji International Forum on Infection and Immunity, The Hyogo Prefectual Awaji Yumebutai International Conference Center, Japan, Sep.4-8, 2006.

Effect of Solution Stirring on Protein Crystallization, *R. Murai, S. Nakata, M. Kashii, H. Adachi, K. Takano, H. Matsumura, S. Murakami, T. Inoue, Y. Mori and T. Sasaki, American Crystallographic Association, 2006 Annual Meeting, Honolulu, Hawaii, Jul.22-27, 2006.

Protein Crystal Processing Using Ultraviolet Laser Irradiation, *K. Takano, H. Kitano, H. Adachi, M. Kashii, H. Matsumura, S. Murakami, T. Inoue, Y. Mori, M. Doi and T. Sasaki, American Crystallographic Association, 2006 Annual Meeting, Honolulu, Hawaii, Jul.22-27, 2006.

Plasma Membrane Transporters Participate the Sphingosine 1-Phosphate Secretion from the Rat Platelet, *T. Nishi, N. Kobayashi, T. Hirata and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, Jun.18-23, 2006.

Cellular Localization of Mouse ABCA5 Proteins in Mouse Tissues, *M. Ohigashi, T. Nishi and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, Jun.18-23, 2006.

Membrane Topology of EmrB, an Outer Membrane Channel-Coupled Multidrug Efflux Transporter, in *Escherichia coli*, *Y. Hisano, N. Tamura, S. Murakami and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, Jun.18-23, 2006.

Lipopolysaccharide Modifications Mediating Bacterial Resistance to Fe(III) and Al(III), *K. Nishino, E. Groisman and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, Jun.18-23, 2006.

The Induction of Bacterial Xenobiotic Exporter, MdtEF, by N-Acetyl-D-Glucosamine is Mediated via PTS System in *Escherichia coli*, *Y. Senda, A. Kobayashi, Y. Inazumi, H. Hirakawa, T. Hirata, K. Nishino and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, Jun.18-23, 2006.

mdtABC and *acrD* Drug-Exporter Genes are Suppressed by a Ferric Uptake Regulator, Fur, in *Escherichia coli*, T. Masaki, H. Hirakawa, K. Nishino, *T. Hirata and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular

Biology, Kyoto, Japan, Jun.18-23, 2006.

Fur Negatively Regulates Drug-Exporter Genes of *mdtABC* and *acrD* in *Escherichia coli*, T. Masaki, H. Hirakawa, *T. Hirata and A. Yamaguchi, American Society of Microbiology, 106th General Meeting,, Orlando, Florida, May21-25, 2006.

Studies on the Substrate-Recognition Site of AcrB Using Chimeric and Site-Directed Mutagenesis, *N. Kobayashi, S. Murakami and A. Yamaguchi, American Society of Microbiology, 106th General Meeting,, Orlando, Florida, May21-25, 2006.

Topological Analysis of EmrB, a TolC-Coupled Multidrug Efflux Protein in *Escherichia coli*, *Y. Hisano, N. Tamura, S. Murakami and A. Yamaguchi, American Society of Microbiology, 106th General Meeting,, Orlando, Florida, May21-25, 2006.

Contributions to International Conferences and Journals

A. Yamaguchi Journal of Bacteriology (Editorial Board Member)

Publications in Domestic Meetings

127th The Pharmaceutical Society of Japan	4 papers
5th Infectious Diseases Okinawa Forum	1 paper
The Molecular Biology Society of Japan 2006 Forum	4 papers
1st KG-Spring-8 Symposium	1 paper
21st Century COE nano-bio group symposium	2 papers
32th Japanese Bioenergetics Group	4 papers
National Project on Protein Structural and Functional Analyses "Brain and Nervous System" 5th Workshop	1 paper
28th Membrane-Drug Interaction Symposium	2 papers
10th Spring-8 Symposium	1 paper
Sakigake Live 2006	2 papers
18th Symposium on Microbial Sciences	2 papers
The 54th Japanese Society of Chemotherapy	2 papers
6th Protein Science Society of Japan	3 papers
3nd 21st Century research conference on Escherichia coli	2 papers
5th BIO EXPO JAPAN	1 paper
80th Japanese Society for Bacteriology	5 papers

Academic Degrees

Master Degree for Pharmaceutical Sciences

Y. Senda	The Induction of Bacterial Xenobiotic Exporter, MdtEF, is Mediated via PTS System in *Escherichia coli*
Y. Hisano	Membrane Topology of EmrB, an Outer Membrane Channel Coupled Multidrug Efflux Transporter, in *Escherichia coli*

Sponsorships

Grant-in-Aid for Scientific Research (C)

T. Hirata	Clarification of biological function of multidrug transporters	¥700,000

Grant-in-Aid for Young Scientists (B)

S. Murakami	Identification of Intrinsic Substrates of Multidrug transporters	¥1,200,000
S. Nishi	Investigation of novel role of V-ATPase isoforms on formation of intercellular environment	¥1,800,000

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.	¥6,240,000
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	¥936,320
S. Murakami	Japan Science and Technology Agency (CREST)	Creation of perfect protein crystals	¥11,050,000
S. Murakami	Japan Science and Technology Agency Strategic international cooperative program/England	Clarification of multidrug efflux mechanism based on crystal structure of multidrug toransporter	¥3,250,000
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	¥1,000,000

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.	¥43,400,000

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

- For pursuing higher performance of the L-band electron linac, conducted are studies on development of a high-performance 216 MHz RF cavity for the SHB system, on stabilization of the amplitude and the phase of the RF power from the klystron by the feed forward method, and on upgrade of the computer control system for faster response by modifying the control program for DC power supplies connected with RS422.
- As part of studies to produce and measure highly brilliant electron beams, degradation of spatial resolution of a fluorescent monitor due to blurring is quantitatively evaluated with a wire scanner and a new phase space monitor is begun to develop for simultaneously measuring the RF phase and the energy of

accelerated electrons.

- The relation is studied between the energy spectrum of a high-intensity single-bunch electron beam and the wake field induced in the accelerating tube of the L-band linac.
- SASE experiments are conducted in the far-infrared region with the strong focusing wiggler and the second and the third harmonic peaks due to non-linear harmonic generation of SASE as well as the fundamental peak are observed as strong as or stronger than the peak intensities observed before remodeling of the L-band linac.
- As a part of development of high performance wiggler for SASE, a highly precise magnetic field measurement system is commissioned.
- Analysis of primary process in interactions between beams and molecular/polymer materials.
- Development of ultrafast measurement system using electron and photon pulse.
- Electronic structure and physical properties of σ-and π-conjugated polymer materials.
- Reaction mechanisms in polymeric materials for microelectronics.
- Formation of size-controlled nano-wires along particle trajectories in polymeric materials.
- Electrodeless measurement of conductivity in organic semiconductors by microwave technique.
- Ionizing radiation induced damages in DNA.

Department of Accelerator Science

Professor:	Goro ISOYAMA
Associate Professor:	Ryukou KATO, Ravi Kumar ANAKARA VADAKATH (Special Mission, 2007.1.1-2007.3.31)
Research Associate:	Toshiji IKEDA, Shigeru KASHIWAGI
Graduate Students:	Yukiyoshi KON

Outline

Particle accelerators are widely used from basic science to industrial applications. In this department, we conduct research on accelerators and quantum beams such as a free electron laser (FEL). Although accelerators are artificial things, fundamental aspects of physics such as non-linearity and the collective effect become apparent when extreme performance is pursued. Because new kinds of quantum beams extend the world we can see with, they are expected to be used in a large variety of fields extending from basic research to applications. To put it concretely, we conduct researches on production of a highly brilliant electron beam with a linear accelerator and related beam dynamics, development of an infrared FEL for user experiments and SASE (Self-Amplified Spontaneous Emission) in the infrared region.

Current Research Projects

Upgrade of the L-band Linac

For highly stable operation of the linac in the single-bunch and multi-bunch modes, we have started project to renew the sub-harmonic buncher (SHB) system consisting of three RF cavities. As the first step, a 216 MHz quarter wavelength cavity is designed and fabricated. Since temperature stability of the RF cavity is essential to stabilization of the electron beam, the RF cavity is made only of oxygen-free copper, which has higher thermal conductivity than the clad plate of stainless steel and copper previously used, and the special design is adopted to cool main parts effectively with water. The effective and highly stable cooling system is realized so that several long holes of 5 mm in diameter are drilled along the beam axis in the outer and the inner conductors made of oxygen-free copper and that cooling water with temperature stability of 0.01 ºC is run through the holes. After a high-power test, the cavity will be install on the L-band linac.

The amplitude and the phase of the pulsed RF power provided to the pre-buncher, the buncher, and the accelerating tube of the linac have to be constant over the pulse duration of 4 μs. For the purpose, ripples of the flat-top in the high voltage square pulse applied to the klystron, which generates the RF power for the linac, are reduced to 0.1 %, but the amplitude varies by 8.6 % and the phase by 27 degrees for 4.9 μs in the RF pulse. These variations of the amplitude and the phase affect the energy spectrum of the accelerated electron beam and hence it is not possible to accelerate electron beams with uniform energy in the multi-bunch and the steady modes, which have longer pulse durations. In order to solve this problem, we have attempted to stabilize the amplitude and the phase by the feed-forward method. Although the time response of the power

amplifier for driving the klystron and a phase shifter used for control are both close to 1 μs, the amplitude variation is decreased to less than 1 % and the phase variation is maintained within 1 degree by controlling them also in differential mode taking the response times into account.

As a part of the upgrade of the computer control system for the L-band linac, the control system is modified to make the cycle frequency higher for reading statuses and output currents of the DC power supplies, which are connected with RS422 to the PLSs for control system. BASIC modules in the PLCs were used in the previous system to control the RS422 line and BASIC limits the speed of the control system so that the response was slow. Instead of the BASIC modules, conventional CPU modules and RS422 modules for them are used and the control program is re-written in the ladder language, so that the reading cycle is made twice faster.

Production and Measurement of Highly Brilliant Electron Beams

The characteristics of the electron beam accelerated with the L-band electron linac are measured with the wire scanner monitor, which was fabricated and installed in last fiscal year. The relation between the thickness of a fluorescent monitor and its image resolution are measured as a function of the thickness of the fluorescent plate from 50 μm to 2 mm with the wire scanner that has the position resolution higher than 50 μm. It is demonstrated for the first time that degradation of the position resolution of the fluorescent monitor due to blurring cannot be neglected even for the 50 μm thick fluorescent plate, which was believed to be negligible.

We have started research and development of a phase space monitor, with which the electron distribution can be directly measured on the phase space defined by the accelerating energy and the time of the L-band linac. The energy of the electron beam is dispersed after passing through a bending magnet. Cherenkov light is emitted when the electron beam goes through the material called aerogel, which has the refractive index slightly higher than that of the air, and the emitted light is measured with a streak camera. If the streak axis is taken perpendicular to the energy axis, the phase space distribution of the electron beam is reconstructed on the display screen of the streak camera. Although the experiment is preliminary, it is found that the method makes it possible to measure the time spectrum with the higher resolution because Cherenkov light emitted in the aerojel is much more stronger that transition radiation emitted on the surface of a metal plate or Cherenkov light emitted in the air.

Study of the Short-Range Longitudinal Wake Field and the Energy Spectrum

The electromagnetic field, called as the wake field, produced in the accelerating tube of the L-band linac by the high-intensity single-bunch beam affects the electron beam being accelerated and hence it is crucial to understand the wake field and its influences for generation and applications of the highly bright electron beam. We measure the energy spectrum of the high-intensity single-bunch beam with charge approximately 30 nC/bunch as a function of the accelerating phase of the electron bunch. The energy spectrum of the high-intensity beam changes significantly and asymmetrically with respect to the crest of the sinusoidal accelerating field. In order to understand these behaviors, we numerically calculate the wake potential produced by the electron bunch and its energy spectrum. The wake function is necessary to calculate the wake potential

but the empirical SLAC wake function does not agree with the wake function estimated from the energy spectrum of the electron beam accelerated at an RF phase near the RF crest. We calculate the wake potential using the electromagnet simulation code ABCI and parameters of the wake function are modified to reproduce the calculated wake potential. As a result, we demonstrate that the calculation with the modified wake function agrees with the results of measurement.

Basic Study on SASE in the Far-Infrared Region

We conduct SASE experiments with the strong focusing wiggler innovated last fiscal year. In order to focus the electron beam and to reduce the beam size as designed in the strong focusing wiggler, the betatron functions in the FEL beam line have to be smoothly matched to specific values of the wiggler at the entrance. We measure the betatron functions in the FEL beam line by the quadrupole scan method and the model of the beam line is made on the computer using the measured betatron functions so that optimum conditions for the FEL beam line can be found by beam dynamics calculation. We conduct SASE experiments with single bunch beam of 10.3 MeV energy and observe the fundamental peak at 218 μm wavelength and the second and the third harmonic peaks due to non-linear harmonic generation of SASE respectively at 110 and 74 μm. The measured intensities of these peaks are comparable or higher than those observed with the conventional wiggler.

Development of a High Performance Wiggler for SASE

We are conducting experiments to measure and evaluate characteristics of permanent magnet materials, which are one of the bases for realizing high performance wigglers for SASE and FEL. The permanent magnet material we use is the compound of neodymium, iron, and boron. Powdery raw materials are compressed and shaped under the strong magnetic field to be raw blocks. They are sintered and then machined down to specified dimensions. The finished blocks are magnetized again in the magnetic field and permanent magnet blocks are completed. The main characteristics of permanent magnet such as the magnetic field strength, the direction of the magnetization axis, and the uniformity of magnetization depend not on the final magnetization but on the first process for compression and shaping under the magnetic field. In order to investigate how the first process is made, it is necessary to measure the magnetic field distribution on the surface of magnetized raw blocks. We have set up the magnetic field measurement system at ISIR, Osaka University, which is as accurate as the original device developed at KEK, and we are arranging for measuring surface magnetic field distributions of many permanent magnet blocks. In the course, we calibrate the Hole probe for the measurement system using the calibration system of the Hole probe against NMR at KEK.

Publications

Original Papers

Comparison of Electrical Properties of Ceramic Insulators under Gamma Ray and Ion Irradiation, T. Tanaka, R. Nagayasu, F. Sato, T. Muroga, T. Ikeda, and T. Iida, Fusion Engineering and Design 81 (2006) 1027-1031.

Coherent Radiation from High-Current Electron Beams of Linear Accelerators and its Applications, S. Okuda, M. Takanaka, M. Nakamura, R. Kato, T. Takahashi, S-K Nam, R. Taniguchi, T. Kojima, Radiation Physics and Chemistry 75 (2006) 903-907.

Review Papers

The Fourth Generation Light Source SASE Currently being Watched with Keen Interest – Novel Laser to Make Rapid Progress in Biological Research – (in Japanese), G. Isoyama, Chemistry Vol. 61, No. 11 (2006) 30-35.

International Conferences

Study of Focusing Properties of a New Type Wiggler on the ISIR FEL at Osaka University, *S. Kashiwagi, G. Isoyama, R. Kato, N. Noda, K. Tsuchiya, S. Yamamoto, Proc. of the 28th International Free Electron Laser Conference, Berlin, Germany, August 27 - September 1, 2006 (THPPH040).

Longitudinal Phase-space Measurements of a High-brightness Single-bunch Beam, *R. Kato, T. Igo, G. Isoyama, S. Kashiwagi, Y. Kon, Proc. of the 28th International Free Electron Laser Conference, Berlin, Germany, August 27 - September 1, 2006 (THPPH041).

Terahertz SASE-FEL using a Strong Focusing Wiggler, *S. Kashiwagi, Y. Kon, R. Kato, T. Igo, G. Isoyama, Proc. of the SANKEN International Symposium on Nanoscience and Nanotechnology 2006 (SISNN-2006), Osaka, Japan, September 19-20, 2006, p.63.

Stability Evaluation of the L-Band Electron Linear Accelerator at ISIR, OSAKA University, *R. Kato, S. Kashiwagi, T. Igo, Y. Kon, T. Yamamoto, S. Suemine, G. Isoyama, Proc. of the SANKEN International Symposium on Nanoscience and Nanotechnology 2006 (SISNN-2006), Osaka, Japan, September 19-20, 2006, p.64.

Performance of the Renewed L-band Linac and Recent Progress of Development of FEL and SASE at Osaka University, *G. Isoyama, R. Kato, S. Kashiwagi, T. Igo, Y. Kon, T. Yamamoto, S. Suemine, Proc. of 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, December 8-9, 2006, p.90.

Distributed Control System based on PCs and PLCs for the L-band Electron Linac, *R. Kato, S. Kashiwagi, T. Yamamoto, S. Suemine, G. Isoyama, Proc. of 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, December 8-9, 2006, p.91.

New Method of Femtosecond Electron Beam Generation for Reaction Analysis in Nano-space, *S. Kashiwagi, T. Kondo, J. Yang, R. Kato, G. Isoyama, Y. Yoshida, A. Masuda, T. Nomoto, K. Sakaue, M. Washio, Proc. of 5th 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Awaji, Japan, December 8-9, 2006, p.92.

Publications in Domestic Meetings

The 3rd Annual Meeting of Particle Accelerator Society of Japan and the 31st Linear Accelerator Meeting in Japan, August 2-4, 2006, Sendai, Japan	9 papers
The 5th Scientific Meeting of the Japanese Society of Radiation Safety Management, November 29- December 1, 2006, Nagoya University, Nagoya, Japan	3 papers
The 23rd Annual Meeting of the Japan Society of Plasma Science and Nuclear Fusion Research, November 28-December 1, 2006, University ot Tsukuba, Tsukuba, Japan	1 paper

Academic Degrees

Doctor Degree for Science

T. Igo	Study of the Short-Range Longitudinal Wake Field Produced by a High-Intensity Electron Beam in a Linear Accelerator and its Influence on the Energy Spectrum

Master Degree for Science

Y Kon	Fast Control of the Phase and Amplitude of the RF Power Provided to the Electron Linac for Producing the Highly Bright Electron Beam for the Free Electron Laser

Sponsorships

Grant-in-Aid for Scientific Research (C)

R. Kato	Development of the longitudinal phase-space monitor for high-brightness electron beams	¥2,100,000

Grant-in-Aid for Young Scientists (B)

S. Kashiwagi	Basic study of SASE using the edge-focusing wiggler in the far-infrared region.	¥600,000

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.	¥800,000

Other Research Fund

G. Isoyama	KEK Accelerator Supporting Project	Technology Development and Applications of SASE-FEL in the Long Wavelength Region	¥2,000,000

Department of Beam Materials Science

Professor:	Seiichi TAGAWA
Associate Professor:	Shu SEKI
Research Associate:	Kazuo KOBAYASHI, Akinori SAEKI
Appointed Professor:	Kazuyuki HORIE
Appointed Researcher:	Shin-ichi FUJITA
Research Students:	Kikuo FURUKAWA
Graduate Students:	Satoshi TSUKUDA, Hiroki YAMAMOTO, Yoshiko KOIZUMI, Ryuhei YAMAGAMI, Yuko OHNISHI, Kenichiro NATSUDA, Ryo HIROSE
Under Graduate Students:	Takehiro FUKUYAMA, Masafumi TANAKA
Supporting Staff:	Kaoru KOJIMA

Outline

Main subjects of the present department are utilization of quantum beams for molecular science, research on mechanisms of phenomena induced by quantum beams, and analysis of microscopic structure of materials. Quantum beams mean both beams such as photons and beams inducing interactions with materials in the microscopic level of quantum mechanics. The beams cause completely different physico-chemical reactions in condensed matters from conventional chemical reactions. Features of beams are highly developed for electrons, ions, positrons, as well as photons (synchrotron radiation, gamma-rays, and lasers).

Current Research Projects

1. Analysis of Primary Process in Interactions between Beams and Molecular Materials

Physico-chemical reactions, which occur within nano- and pico- second region, are considered to dominate followed reactions and products in molecular materials. High-accuracy spectrum acquisition system was developed using CCD camera, highly-stable femtosecond white light continuum, and double pulse detection technique, resulting in approximately two orders of magnitude higher performance than conventional system. The direct observation of reactive intermediates is carried out to elucidate the mechanisms and to control the reaction. Aromatics have high radiation resistance. The characteristic has been used in electron beam lithography. Especially, the radiation–induced reaction of aromatics is important to improve and understand the resist materials. Primary process of irradiated aromatics from nano- to picosecond time scale is investigated by electron beam pulse radiolysis.

2. Development of Ultrafast Measurement System Using Electron and Photon Pulses

The measurement system was developed to trace ultrafast phenomena by ultra short

pulses of electrons and photons in the current program. Transient spectroscopy is done within 0.8 psec approaching to shorter time region. Dynamics of short-lived intermediates have been observed for several molecular materials.

3. Electronic Structure and Physical Properties of σ-and π-Conjugated Polymers

Polysilanes and polygermanes containing only silicon and germanium in the backbone are attached considerable attention because of their interesting electro-optical properties which are due to conjugated bondings in the main chain. The electronic structure of conjugated skeleton is investigated in the present program, which leads to improve the physical properties of the conjugated polymers.

4. Reaction Mechanisms in Polymeric Materials for Microelectronics

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

Using time-resolved microwave conductivity (TRMC) which enables us to measure nano-scale electric conductivity in organic semiconductors, we investigated electric and optical properties of super-molecular nanotubes, pentacene thin films, and sigma-conjugated polymer: polysilane. Regarding the super-molecular nanotube, anisotropic charge carrier mobility along the long axis of the nanotube was successfully measured. Moreover, the nanotube laminated by electron acceptor layers was found to show extraordinary conductivity, due to its programmed structure on nano-scale. For pentacene thin films, transient conductivity signals were considerably dependent on the grain size and show high intrinsic charge carrier mobility comparable to that in amorphous silicon. Real and imaginary conductivities were separated into independent components, demonstrating the large contribution of real conductivity.

6. Ionizing Radiation Induced Damage in DNA

Deprotonation of the guanine radical cation ($\mathbf{G}^{+\cdot}$) in DNA is an important step in hole hopping and mutagenesis. In experiments using 5-substituted cytosine-modified oligonucleotides, changes of the cytosine C5 hydrogen to methyl or bromine groups resulted in an increase or decrease, respectively, in the rate constants of the slower kinetic component. Kinetic solvent isotope effects on the oxidation kinetics of deoxyguanosine (dG) and oligonucleotide duplexes were examined in H_2O and D_2O. The rate constant of formation of $G(-H)^{\cdot}$ in dG was larger by a factor of 1.7 than was the same rate constant in H_2O . In the oligonucleotide, on the other hand, a remarkable solvent isotope effect of 3.8 was observed in the slower kinetic phase. These results suggest that the slower kinetic phase is due to the deprotonation of oxidized

hydrogen-bridged G-C base pair by a water molecule.

Publications

Original Papers

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Resists for Post-Optical Lithography: Acid Yield and Deprotonation Behavior of Poly(4-hydroxystyrene) and Poly(4-methoxystyrene), A. Nakano, T. Kozawa, K. Okamoto, S. Tagawa, T. Kai and T. Shimokawa, Jpn. J. Appl. Phys., 45 (2006) 6866-6871.

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Electrodeless Measurement of Charge Carrier Mobility Probed by Microwave, A. Saeki, S. Seki, and S. Tagawa, , Jpn. Soc. Radiat. Chem. 81 (2006) 29-39.

Books

Ion Beam and Nano-structure, H. Koizumi, S. Seki, Recommendation of Radiation Chemistry, ed. by Jpn. Soc. Radiat. Chem., Gakkai Shuppan-center (2006) 134-135.

Lithography and Resist, T. Kozawa, Recommendation of Radiation Chemistry, ed. by Jpn. Soc. Radiat. Chem., Gakkai Shuppan-center (2006) 52-54.

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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, 31st Int. Symp. Microlithography 2006, San Jose, California, USA, Feb. 22-25, 2006.

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The Reaction Mechanism of Poly[4-hydroxystyrene-co-4-(1,1,1,3,3,3-hexafluoro-2-hydroxypropyl)-styrene], *H. Yamamoto, T. Kozawa, K. Okamoto, S. Tagawa, T. Ando, M. Sato and H. Komano, 31st Int. Symp. Microlithography 2006, San Jose, California, USA, Feb. 22-25, 2006.

Line Edge Roughness in Chemically Amplified Resist of Electron Beam Lithography, *A. Saeki, T. Kozawa, S. Tagawa, and H. B. Cao, EIPBN, Baltimore, USA, May 31-June 2, 2006.

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Electrodeless Measurement of Charge Carrier Mobility in Pentacene by Microwave and Optical Spectroscopy Techniques, *A. Saeki, S. Seki, S. Tagawa, Gorden Research Conference, Colby College, USA, July 2-8, 2006.

Formation of Aggregated Radical Cations of Benzene and Polystyrene in Condense Phases, *K. Okamoto, S. Seki, T. Kozawa, Y. Yoshida, S. Tagawa, Gorden Research Conference, Colby College, USA, July 2-8, 2006.

The Mobility of Holes through DNA, *R. Yamagami, K. Kobayashi, A. Saeki, S. Seki, and S. Tagawa, Gorden Research Conference, Colby College, USA, July 2-8, 2006.

Self-Assemble Properties of Oligofluorenes with Amphiphilic Side Chains, *Y. Koizumi, S. Tsukuda, S. Seki, S. Tagawa, Gorden Research Conference, Colby College, USA, July 2-8, 2006.

Pico/subpicosecond Pulse Radiolysis and Research on Nanolithography by EB/EUV, *A. Saeki, T. Kozawa, S. Tagawa, Gorden Research Conference, Colby College, USA, July 2-8, 2006.

Synthesis and Self-Assemble Properties of Oligofluorenes With Amphiphilic Side Chains, *Y. Koizumi, S. Tsukuda, S. Seki, S. Tagawa, 11th Tihany Symposium on Radiation Chemistry, Eger, Hungary, Aug. 26-31, 2006.

Femtosecond Pulse Radiolysis Based on Photocathode Electron Accelerator, Y. Yoshida,

J. Yang, T. Kondoh, T. Kozawa, S. Tagawa, Asian and Pacific Symposium on Radiation Chemistry (APSRC) , Shanghai, China, Sep. 17-21, 2006.

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Acid Generation in Chemically Amplified EUV Resists, *T. Kozawa, S. Tagawa, H. Oizumi and I. Nishiyama, EUVL Symposium, Barcelona, Spain, Oct. 16-20, 2006.

Exposure Dose Dependence on LER of Latent Image in EB/EUV Lithographies Studied by Monte Carlo Technique, *A. Saeki, T. Kozawa, S. Tagawa, H. B. Cao, H. Deng, and M. J. Leeson, EUVL Symposium, Barcelona, Spain, Oct. 16-20, 2006.

Polymer Structure Dependence of Acid Generation in Chemically Amplified EUV Resists, *H. Yamamoto, T. Kozawa, S. Tagawa, H. B. Cao, Hai Deng, and M. J. Leeson, EUVL Symposium, Barcelona, Spain, Oct. 16-20, 2006.

Critical Issues of EUV Resists and New Research Approach, *S. Tagawa, T. Kozawa, A. Saeki, EUVL Symposium, Barcelona, Spain, Oct. 16-20, 2006.

Effect of Acid Diffusion and Polymer Structure on Line Edge Roughness, *H. Yamamoto, T. Kozawa, A. Saeki, K. Okamoto, S. Tagawa, K. Ohmori, M. Sato and H. Komano, Int. Microprocesses and Nanotechnology Conf., Kamakura, Japan, Oct. 25-27, 2006.

Proton Dynamics and Amines in Chemically Amplified Resist, *K. Natsuda, T. Kozawa, K. Okamoto and S. Tagawa, Int. Microprocesses and Nanotechnology Conf., Kamakura, Japan, Oct. 25-27, 2006.

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	10 papers
Atomic Energy Society of Japan	2 papers
The Japan Society of Applied Physics:	3 papers

Academic Degrees

Doctor Degree for Engineering

S. Tsukuda	Formation mechanisms of polymer nano-structures by high energy ion beam

Master Degree for Engineering

K. Natsuda	Study on proton dynamics in chemically amplified resists
Y. Ohnishi	Structural dynamics of polysilanes using ultrafast transient absorption spectroscopy

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas

S. Tagawa	Femtosecond Pulse Radiolysis Study on Time Profile of Radiation-Induced Processes in Nanoscopic Region	¥19,700,000

Grant-in-Aid for Young Scientists (A)

S. Seki	Formation and characterization of nano-structures generated via chemical reactions by single ion beam	¥9,700,000

Grant-in-Aid for Special Purposes

S. Seki	Electrode-less evaluation of one-dimensional electric conductivity of single conjugated polymer chain by microwave technique	¥1,300,000

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	¥1,000,000

Grant-in-Aid for JSPS Fellows

S. Tsukuda	Formation mechanisms of polymer nano-structures by high energy ion beam	¥900,000
H. Yamamoto	Creation of novel lithographic process based on nano-beam-induced reaction mechanisms	¥1,000,000
Y. Koizumi	Contact-less evaluation of intrinsic conductive property of single conjugated polymer chain	¥1,000,000

Entrusted Research

S. Tagawa	Basic research of nuclear safety	Development of visible dosimeter for keeping safety based on advanced research of radiation chemistry	¥11,765,000
S. Tagawa	ASET	Research on reaction mechanism of chemically amplified resist	¥1,000,000
S. Seki	INSS	Elucidation of degradation process of polymer upon exposure to radiation studied	¥2,683,000

		by microwave detection technique	

Other Research Fund

S. Tagawa	Mitsubishi gas chemical company	Basic study on ArF photo resist	¥1,000,000
S. Tagawa	SELETE	Research on EUV resists	¥1,680,000

Division of Next Industry Generation

Outline

Three new research departments have been established. The goal of each department is to provide advances in science and technology via close relationships with industry, which will lead to create a novel industry in the 21st century.

The departments are:

-Department of New Industry Projection

Perform research on new projects that can lead to industrial-structure innovations in the next generation.

-Department of New Industry Generation System(s)

Investigate and develop novel business systems that enable transfer of academic research outcomes to a new industry effectively and promptly, and that intend to improve productivity through responding to social demands.

-Department of Intellectual Property Research

Perform the strategic world-leading study of intellectual property linked with potential needs of the society, where the academia is required to create intellectual properties efficiently from the wide-ranging knowledge accumulated from academic research of the new interdisciplinary fields of material, information, and biology.

Achievement

- Comparison analysis between Japanese major manufacturing industries
- Position of the finance industry in the Japanese economy
- Shareholding network of Japanese listed companies
- Development of a new intellectual property map
- Discussion group for the future drug concept
- Discussion group for the new era of life science research, business, and industry
- Science & Business Club (in preparation)
- Launch of study group of management of intellectual property and technology
- Intellectual properties management seminar series

Department of New Industrial Projection

Professor: Hiroshi KATAYAMA-YOSHIDA
Designated Research Assoc.: Makoto NAKAZAWA
Supporting Staff: Mika ASADA, Ryoko ITO

Outline

Now in the 21st century, Japanese industrial structure is being transformed from a traditional industrial society to a knowledge-based society. In the knowledge-based society, instead of process innovation ("how to make"), product innovation ("what to make") is required. Thus new strategy for the change of the industrial structure is needed. We aim for the establishment of a framework to project new industries in future society (including the projection of the basic research required in the society) based on the analysis of the existing industries.

Current Research Projects

Comparison Between Japanese Major Manufacturing Industries

An analysis is made between the automobile and the electric industries which are qualified as the Japanese leading industries. The total market values of Toyota, Honda and Nissan belonging to the automobile industry at the end of March 2006 are all about twice compared to the standard values at the end of January 1985. On the other hand, the total market values of the companies belonging to the electric industry are still substandard. Similarly, although the operating profit on sales of the automobile industries shows an upward trend at recovering from slower a growth during a certain period in the past, that of the electric industry have declined as yet.

Position of The Finance Industry in The Japanese Economy

Since the total assets of the Japanese companies show the power low distribution, the distribution is denoted by a straight line in the log-log plot. However, the straight line changes its slope at one trillion yen. By examining the scatter plot for the sales and the total assets, it is concluded that the bent of the line is due to the finance industry (banks are the main constituent companies) locating over one trillion yen of the total assets. In addition, the total assets of the banks are dozens of times compared to those of the manufacturing industries with almost the same sales as the banks, and the banks make higher profit on sales.

Shareholding Network of Japanese Listed Companies

The characteristics of the shareholding network constructed from Japanese listed companies are studied, by schematically representing a company by a dot and its relationship to shareholders by a line. This analysis shows, while the clustering coefficient and the degree (the number of lines connected to a dot) negatively correlates, the betweenness centrality (the number of shortest paths on a network that run through the dot of interest) and the degree positively correlates. The former shows that the

shareholding network has a tree-like structure, and the latter indicates that the hub (the dot which has high-degree lines) takes an important role for connecting companies.

Development of Intellectual Property Map

The method for visualizing technology and market can be a very powerful tool to project new industries. To this end, we have developed an intellectual property map created by mapping both patent descriptions of interest and the keywords selected from the patent descriptions at the calculated position in the same plane. As an example, the analysis of the patent descriptions relevant to fuel cell applied by Toyota, Honda and Nissan was made. This analysis makes it visually clear that the application relevant to the polyelectrolyte membrane by Honda is unique and the number of applications overwhelms others.

Publications

Patents

“Transparent ferromagnetic alkali/Chalcogenide compound comprising solid solution of transition metal or rare earth metal and method of regulating ferromagnetism thereof”, H. Yoshida, M. Seike, K. Sato, A. Yanase, EU-Patent EP1634979A1

“Magnetic Random Access Memory Device”, H. Yoshida, K. Sato, Korean-Patent 0557387

“Magnetic Random Access Memory Device”, H. Yoshida, K. Sato, H. Yoshida, K. Sato, Taiwan-Patent I-262593

“Ferromagnetic IV Group Based Semiconductor, Ferromagnetic III–V Group Based Compound Semiconductor, or Ferromagnetic II–IV Group Based Compound Semiconductor, and Method for Adjusting Their Ferromagnetic Characteristics”, H. Yoshida, K. Araki, K. Sato, TAIWAN-Patent-I 252521

“Circular Polarization Spin Semiconductor Laser Using Magnetic Semiconductor and Laser Beam Generating Method”, H. Yoshida, K. Araki, K. Sato, JAPAN-3797936

“Circular polarized light-generating spin-based semiconductor laser source using magnetic semiconductor and method of generating laser light”, H. Yoshida, K. Sato, KOREA-Patent-10-0603057

“Method for gettering transition metal impurities in silicon crystal”, H. Yoshida, KOREA-Patent 10-0596701

“II-VI or III-V ferromagnetic single crystal compound and their adjustable method of ferromagnetism”, H. Yoshida, K. Sato, TAIWAN-Patent I254088

“Ferromagnetic p-type single crystal zinc oxide and method for preparation thereof”, H. Yoshida, K. Sato, US-Patent US7022182B1

“Verfahren zur herstellung von diamanten des n-type mit niedrigem widerstand (Method for synthesizing n-type diamond having low resistance)”, H. Yoshida, Germany-Patent DE69926985T2

“Ferromagnetic ZnO-type compound including transition metallic element and method for adjusting ferromagnetic characteristics thereof”, H. Yoshida, K. Sato, US-Patent US7115213B2

Publications in Domestic Meetings

The Physical Society of Japan	1 paper
Japan Society for Intellectual Production	1 paper

Department of Next Industry Generation Systems

Specially Appointed Professor: Mototaka Senda

Outline

This Department was initiated from April, 2006 under the Division of Next Industry Generation including Department of New Industry Projection and Department of Intellectual Property Research, which will lead to create a novel industry in the 21st century. The Department focuses on investigation and development of novel business systems that enable transfer of academic research outcomes to a new industry effectively and promptly, and that intend to improve productivity through responding to social demands.

Current Research Projects

- Functional Think Tank for Ideas, Technologies, Intellectual Properties and Business Opportunities in the University –

1.Discussion Group for the Future Drug Concept (New Drug Generation Business from Academic Seeds)
2.Discussion Group for the New Era of Life Science Research, Business, and Industry (New Interdisciplinary Fields Generation)
3.Research for Management of Intellectual Property and Technology (New Methodology for Intellectual Property Generation)
4.Science & Business Club (in preparation: New Relationship between Academia and Industry)

Department of Intellectual Property Research

Specially Appointed Professor: Hirokazu SHIMIZU

Outline

The object of this department is to perform the strategic world-leading study of intellectual property linked with potential needs of the society, where the academia is required to create intellectual properties efficiently from the wide-ranging knowledge accumulated from academic researches of the new interdisciplinary fields of material, information, and biology.

Current Research Project

Intellectual Property Engineering
Engineering method is studied to put intellectual properties of scientific knowledge to definite expression of patents and also to make detailed analysis and evaluation of published patents. This study has been made in collaboration with Department of Knowledge Systems and Human Interface Research Group.

Intellectual Property Management
Management of intellectual properties has an important role in the evolution of industries. Strategic management approaches of intellectual properties have been discussed and derived in the series of lectures given by the invited speakers from business world. This program was carried out in collaboration with Department of New Industry Generation Systems.

Publications

Patents
Optical semiconductor device and its production method and apparatus, H. Kobayashi and H. Shimizu, Japanese Patent application 2006-239646

Activities of Centers

Nanoscience and Nanotechnology Center

Director Professor: Katsuaki SUGANUMA
Support Staff: Aya KOMOTO

Outline

Nanoscience and Nanotechnology Center was founded in April 2002 for developing Bottom-up Nanotechnology, Top-down Nanotechnology, and their Industrial Application. This center consists of four divisions; (1) Nanomaterial and Nanodevices, (2) Beam Science for Nanotechnology, (3) Nanoscience and Nanotechnology for Industrial Applications and (4) Nanocharacterization together with five laboratories (Radiation Laboratory, Electron Microscope Laboratory, Electronic Processing Laboratory, Nanofabrication Shop and Open Laboratory) and Nanotechnology Process Foundry.

Division of Nanomaterials and Nanodevices

Outline

The main purpose of this division is to construct function harmonized nano-materials which can mimic flexible data processing like human body. By using typical "Bottom-up Nanotechnology" of artificial lattice technique, we combine metal, inorganic and (bio)organic materials at an atomic/molecular level to new nano-materials. The object of this division is also to research molecular-scale devices based on the function of single molecule. We are developing new techniques for the measurement of physical and chemical properties of single or several molecules. Furthermore, design and syntheses of supramolecules such as artificial DNA, proteins, photosynthetic molecules, and nanoparticles having more efficient and selective functions than those of single molecules are being investigated towards constructions of organized supramolecular systems such as artificial living cells and nanodevices exhibiting multifunction, complex properties, and conjugated functions. Proteins and their complexes with other biomolecules are regarded as nano bio devices. The research of our group is focused on structural and functional studies on such devices. We are also interested in developing highly sensitive biosensors and nano machines.

Achievement

- Construction of functional nano-materials, which can mimic flexible data processing like human body.
- Investigation of relationship with structure and material properties at nano-scale.
- Control of nano-scale interface among organic, inorganic, and metal materials.
- Development of bottom-up nanotechnology system.
- Creation of super-five senses sensor and brain type memory.
- Programmed self-assembly and self-organization for molecular device.
- Control of electrode-molecule interface for molecular devices.
- Fabrication of top-contact nanoelectrode by nanoscale transfer-printing.
- Development of electrostatic force microscopy for insulating substrates.
- Methodological development of time-resolved electrostatic force detection.
- Electric property measurement of molecular interface and networks by point-contact current-imaging atomic force microscopy.
- Molecular recognition imaging by frequency modulation atomic force microscopy.
- Charge transfer through DNA nanoscaled assembly programmable with DNA building blocks.
- Mechanism of photosensitized one-electron oxidation of DNA.
- Dual activation in the enantioselective coupling of 2-naphthols catalyzed by chiral dinuclear vanadium complexes.
- Development of functionalized nanoparticles by self-assembly.
- Structural analysis of reaction intermediates formed on the catalytic cycle of copper amine oxidase.
- Biochemical and molecular biological studies on the biogenesis mechanism of quinohemoprotein amine dehydrogenase.
- Determination of the crystal structure of bacterial major multidrug exporter AcrB with substrates.

Department of Artificial Nanomaterials for Bio-Information Systems

Professor:	Hitoshi TABATA
Research Associate:	Hiromasa SAEKI
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Outline

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.

The future substance invention in a strong correlation system substance thin film or an artificial lattice is carried out using the laser MBE method in which crystal structure control on an atomic level is possible. For example, device research of basic research, a spin transistor and a photo-excited spin element, a synapse junction type memory, etc. on the dimension nature of an oxide magnetic body, a spin glass, and a relaxor ferroelectric, or fluctuation and physical properties is done. In addition, new type of functional materials so called multi-ferroics have been discovered by our group which are one of the families on garnet type ferrites. Spintronics based on oxide wide gap semiconductors. Spin glass and dipole glass (relaxor) enable us to construct new type devices called “Yuragi” devices. Moreover, aiming at the nano biotechnology device, invention of the bio-memory by the nano structure control using the self-organization of a DNA molecule and cloning and research on the nano domain physical properties using the scanning probe microscope are done.

Current Research Projects

Creation of room temperature multiferroics by garnet type ferrite strained films

Multiferroic materials, which show ferromagnetism and ferroelectricity at the same time, have been expected not only for practical application such as memory devices but also for generating new physical properties in magnetic-electric interaction. So far,

perovskite type materials are well known as multiferroic materials. In essence, this candidate multiferroic materials fall into two categories namely, iron (Fe) oxide system and manganese (Mn) oxide system. As an example of the former, $BiFeO_3$ is given. As the latter, $YMnO_3$, $BiMnO_3$, $TbMnO_3$ is given. The studies of multiferroics have been providing fundamentally important results about the cross correlation between ferromagnetism and ferroelectricity yet it has appeared at too low temperature and its magnitude has remained too small. This factor is considered because, in most cases, their ferromagnetic properties can be observed only at low temperature due to the week magnetic correlation energy comparing with that of dipole interaction. It is necessary for application in devices that the properties show near room temperature. So, to push up the magnetic interaction energy, we select ferrimagnetic materials which have Neel temperature as high as ferroelectric Curie temperature.

Next, as regard of ferroelectricity, it is necessary for arising the spontaneous polarization that ions breakdown a central symmetry. J. H. Haeni et. al. realized this by a strain effects using positively lattice mismatch for substrates. They reported $SrTiO_3$, well-known as quantum paraelectric materials, showed ferroelectricity at room temperature because of spatial symmetry breakdown using lattice mismatch for substrates. Our material design of room temperature maltiferroic materials is that $SrTiO_3$ is replaced with room temperature ferrimagnets and we make the materials show at the same time ferromagnetism (ferrimagnetism) and ferroelectricity at room temperature.

According to condition of arising the spontaneous polarization, it is necessary that this ferrimagnets have high resistance. Therefore, we focused rare earth garnet ferrites. Rare earth garnet ferrites now have been widely used as optical devices and have a big advantage when it will adopt the devices with multiferroic property. Consequently, scope of this study is to fabricate room temperature multiferroic materials and observe properties in magnetic-electric interaction.

We have shown a new method to make multiferroic materials. That is to add ferrimagnets to ferroelctricity by a strain effects using positively lattice mismatch for substrates. By using this method, I have succeeded to fabricate films which show ferrimagnetism and ferroelectricity at room temperature. For this film, in the cross term measurement, it has been measured the increase of residual polarization caused by existence of residual magnetization. The magnitude of change indicates a possibility of a new phenomenon caused by coexistence of ferromagnetism and ferroelectricity. By further research, it will become clear.

Control of growth mode and magnetic properties of $Zn_{1-x}Co_xO$

Dilute magnetic semiconductors have unique physical properties relation with spin, photon and carrier. Interesting magneto optical properties have been observed in Co modified ZnO films which have good optical property. In this year, we have tried to control 2D growth and emission properties.

1) Growth mode control

The heteroepitaxy of Mg-rich $Mg_{0.37}Zn_{0.63}O$ layers on ZnO (0001) substrates was carried out usinglaser molecular-beam epitaxy. $Mg_{0.37}Zn_{0.63}O$ layers changed from a

two-dimensional (2D) to three-dimensional growth mode at a layer thickness tc between 38 and 100 nm throughlattice-strain relaxation. For tc 100 nm, hexagonal nanodots with a density in the order of 10^9 cm^{-2} formed naturally by the Stranski-Krastanov mode. The individual nanodots possessed pyramidal hillocks with lateral sizes raging from 100 to 200 nm, and phase separation to Mg-rich and Mg-poor regions in the $Mg_{0.37}Zn_{0.63}O$ alloys was found from the results of atomic force microscopy and microphotoluminescence spectroscopy. A suitable layer thickness of $Mg_{0.37}Zn_{0.63}O$ concerning quantum barriers was speculated as being 38 nm from a theoretical calculation based on the Matthew and Blakeslee model, the top surface of the $Mg_{0.37}Zn_{0.63}O$ layer was very flat due to the curtailment of 2D growth. This contributed to the coherent growth of Mg-rich $Mg_{0.37}Zn_{0.63}O$/ZnO multi-quantum-well structure (MQWS) with high crystallinity, as characterized from structural analyses using high-resolution x-ray diffraction. The two-dimensional properties of the MQWS were confirmed from the anisotropic optical property and electrical conductivity with 2D electron transport at low temperatures.

2)Magnetic control

We have demonstrated a new growth technique realizing the simultaneous control of growth mode and ferromagnetic ordering in Co-doped ZnO layers. Remarkable changes in growth occurred as a result of doping with Co ions. Exposure to O_2 plasma to generate an oxygen-rich atmosphere was indispensable for the fabrication of undoped ZnO layers given stabilization of the negatively charged growing surface in a twodimensional (2D) mode. In contrast, the 2D mode of $Zn_{0.94}Co_{0.06}O$ layers was adequately retained in the absence of a plasma source, and was attributable to the covalence provided by the 3d character of Co ions compared with the 4s character of Zn ions. Spontaneous magnetization of $Zn_{0.94}Co_{0.06}O$ layers was closely correlated with the number of free electrons, which was controlled by the activation energy of donor levels. This was also confirmed for O-polar $Zn_{0.94}Co_{0.06}O$ layers. Ferromagnetic (FM) ordering was observed at nevalues close to the Mott transition and led to hopping conduction between shallow donor bands. However, levels of pO_2 below 10^{-6} mbar that yielded FM ordering generated a pitted surface and led to crystalline deterioration. Given our understanding of the formation mechanism of pits, we applied a periodic oxygen pressure-modulated epitaxy that resulted in the coherent growth of Co-doped ZnO layers with a 2D mode. This specific growth was effective in producing pit-free surface uniformities over large areas that maintained FM ordering.

Terahertz spectroscopy and imaging of DNA-related biomaterials

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. Additionally the DNA hybridization was recognized by THz spectrum. This is because the hydrogen-bond vibration mode of $–NH_2$ structure between complementary DNA. However, nobody has clarified the vibration mode of DNA systematically. We succeeded to obtain the vibration mode less than 1.0 THz related to DNA hybridization using simple DNA oligomer (11mer) having G-G mismatch.

The sample was DNA thin-film deposited on a glass substrate. The samples are commercial 11mers of 5'-CTAACGGAATG-3' and 5'-CTAACGGAATG-3' which have G-G mismatch in the center position. The aqueous solutions (2mM) of each 11mer were mixed at room temperature and deposited on glass substrate and dried in the air at room temperature.

A typical THz-TDS system was used in this work. Photoconductive dipole antennas (LT-GaAs) were used as both THz emitter and receiver, but a ZnTe crystal was sometimes used as emitter. The pump laser was 800 nm in wavelength and 100 fs in pulse-width and the repetition frequency was 50 MHz.

A clear peak was found in < 1.0 THz region. This result shows that the vibration mode related to the hybridization appears in low frequency (< 1.0 THz). Although baseline increase due to DNA hybridization have already reported in the previous paper, unfortunately any clear peak structures can not be found because of the long-length DNA strand. We successfully showed a very clear peak structure by using simple DNA of 11mers.

We successfully distinguished the THz spectra of single and double strand DNA and found a clear peak structure. The spectrum detection of thin film biomaterials in this preliminary work should become basic database for the future development of nanobio-devices.

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Book

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International Conferences

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Charge Transport Properties of DNA Molecules Measurements by Nano-gap Electrodes (Invited), *H.Tabata, Charge Migration in DNA, Manitoba, Canada, Jun. 6-9, 2006

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Rump Session B Nanotechnology-Impact on Electronics, Photonics and Biology-(Invited), *H. Tabata, SSDM2006, Yokohama, Japan, Sep. 13-15, 2006

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Advances in Nonpolar ZnO Homoepitaxy: 1D Surface Nanostructure and Electron Transport (Invited), *H. Matsui and H. Tabata, Photonics West-2007, San Jose, USA, Jan. 20-25, 2007

Contributions to International Conferences and Journals

H. Tabata	International Conference on Solid State Devices and Materials 2006 (SSDM2006) (Publishing Committee Committee Chair)
H. Tabata	International Conference on Solid State Devices and Materials 2006 (SSDM2006) (Publishing Committee)
H. Tabata	13th International Workshop on Oxide Electronics (International Committee)
H. Tabata	6th Japan-Korea Conference on Ferroelectricity Publication Committee（Committee Chair）
H. Tabata	Associate Editor of JJAP in special issue
H. Tabata	Chief aid of publication office in Japan Society of Applied Physics
H. Tabata	The 45th a Representative of Japan Society of Applied Physics

Publications in Domestic Meetings

The Japan Society of Applied Physics	9papers
Other	1paper

Academic Degrees

Doctor Degree for Engineering

O. Nakagawara	Epitaxially Grown Aluminum Thin Films on Piezoelectric Single Crystal Substrates and Their Applications.

Master Degree for Engineering Science

K. Tsuruta	Studies on Photo Excited Magnetism and Multiferroic Properties of Ferrite Thin Films

Sponsorships

Grants in aid for scientific research

Fundamental Research (B)

H. Tabata	Symmetry Broken Ferroelectric Relaxors Formed by Artificial Superlattices and Brain Mimetic Memories	¥2,800,000

Exploratory Research

H. Tabata	Non Fluorescent Labeling DNA Transistor Formed by Self Organized Semiconductor	¥800,000

Grantinaid for Young Scientists(B)

H. Saeki	Exploring of Spintronic Materials in Multilayered Homologous Serious	¥2,600,000

Grantinaid for Young Scientists(B)

H. Matusi	Modulation of Hetero-interface in a Surface Nano-structure and their Electric and Magnetic Properties	¥2,100,000

Other Allocation

Scientific Research in Priority Areas

H. Tabata	Development and Application of Computational Nano-Materials Design Engine	¥600,000

Scientific Research in Priority Areas

H. Tabata	Self Organized 3D Structural Multiferroic Devices	¥13,500,000

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	¥600,000

Department of Single-Molecular Integrated Devices

Professor: Tomoji KAWAI
Associate Professor: Takuya MATSUMOTO
Research Associates: Masateru TANIGUCHI
Researcher: Akihiko TAKAGI
Support Staff: Yumiko NOGI

Outline

Notwithstanding the great anticipation of the potential of molecular-scale electronics, it is very difficult to fabricate molecular-devices, owing to the lack of effective technologies for wiring molecules and connecting molecules to electrode. Self-organization is a promising route to fabricating complicated nanostructure by “bottom-up” process with highly selective chemical-reactions.

The object of this department is to research molecular-scale devices based on the function of single molecule. We are developing new techniques for the measurement of electrical properties for molecular nanostructures. We are also developing an interconnect method to program three kinds of component molecules with their own functions, and to create a molecular device between nano-scale electrodes in a self-organized manner.

Current Research Projects

Anchoring Gold Nanoparticles onto a Mica Surface by Oxygen Plasma Ashing for Sequential Nanocomponent Assembly.

Water-soluble gold nanoparticles can be immobilized in both polar (water) and nonpolar liquid (chloroform) on hydrophilic mica surface by oxygen plasma ashing. It was demonstrated that a DNA with a thiol at an extremity is attached to the immobilized nanoparticles due to the gold-thiol coupling, and stretched in the flow direction of the following water rinse. This technique allows a sequential integration of nanoparticles and molecules for various solutions, since the nanoparticles remains on a solid surface rather than dissolve into the solution. The technique is being used for bottom-up construction of molecular nanostructures.

Surface potential and capacitance image of biological molecules on *insulating* substrates

We found that potential and capacitance images of nanoscale adsorbates on *insulating* substrates can be obtained by frequency-mode surface potential microscopy. This finding is beyond the common understanding based on parallel-plate condenser model because the field modulation between tip and insulator surface should be too small to probe the surface potential variation, and the charges of surface adsorbates should be almost negligible in comparison with that of bulk substrate. However, the assumption of these consideration collapsed because the external electric field just below a sharp tip apex was enough strong to modulate tip-adsorbates electrostatic interactions. We are

conducting systematic analysis for electrostatic force imaging on insulating substrate.

Characterization of Nano-Photoswitching Molecular Device Created by Self-Organized Interconnect Method

Recently, we have developed an interconnect method for molecular devices that can control electrode-molecule binding, molecular orientation, and device functions. Our interconnect technique is a self-organized method in which three types of molecules are programmed to have different functions, and are connected sequentially between the nano-scale electrodes. By using this technique we demonstrated a conduction wire and optical switching device. In the measurement of the temperature characteristics of the nano-photoswitching molecular device in the ON state, we found that the molecule has the thermal activation type conduction mechanism, just like the molecular wire with stilbene, and that the activation energy in the high temperature range was 117meV. The long length of the orientational control molecule indicates that the orientational control molecule has a hopping conduction mechanism and the conduction mechanism of the entire molecular wire is dominated by the hopping conduction of the orientational control molecule.

Control of the Electrode-Molecule Interface for Molecular Devices

We systematically investigated the bonding property and the electronic states of the monolayer of benzeneselenol or diphenyl ditelluride for the first time, which was a guide material for benzenethiol used most frequently in molecular devices. To date, Au-S bonds have often been used in molecular devices as an extension of self-assembled films. However we found that the Au-Se bond was more suitable for molecular devices than the other bonds. This result is expected to contribute to improving the electric conduction property of currently developed molecular devices and to enhancing the device properties.

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Patents

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Time-Resolved Scanning Force Microscopy, *T. Matsumoto, T. Kawai, 9th International Conference on Non-contact Atomic Force Microscopy, Kobe, Japan, July 16-20, 2006.

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Contributions to International Conferences and Journals

T. Matsumoto	Program Committee International Symposium on Surface Science and Nanotechnology (ISSS-5)
T. Matsumoto	Editorial Board e-Journal of Surface Science and Nanotechnology

Publications in Domestic Meetings

The Japan Society of Applied Physics	10papers
Discussion meeting for molecular structures	2papers
The Physical Society of Japan	1paper
Others	9papers

Academic Degrees

Master Degree for Science

K. Yokota	Studies on Electric Properties of Molecular Wires and the Molecular-electrode Interface

Sponsorships

Grant-in-Aid for Scientific Research (B)

T. Matsumoto	Stroboscopic Scanning Probe Microscopy and Time-Resolved Molecular-Scale Imaging of Photoexcited Carriers	¥3,800,000

Grant-in-Aid for Young Scientists (B)

M. Taniguchi	Development of Self-Organized Molecular Devices	¥3,000,000

Scientific Research in Priority Areas

M. Taniguchi	Development of Control Technique of Molecule-Electrode Interface	¥2,300,000

Entrusted Research

T. Matsumoto	Japan Science and Technology Corporation	Mesoscopic Devices of Huge Porphyrin Arrays	¥900,000

Cooperative Research

T. Matsumoto	Matsushita Electric Industrial Company	Electric property measurements of Si nano-wire by scanning probe microscopy	¥2,000,000
M. Taniguchi	Matsushita Electric Industrial Company	Development of new functional materials based on pi-conjugated molecules coverd with CD	¥3,250,000

Other Research Fund

T. Matsumoto	Japan Science and Technology Corporation	Mesoscopic Devices of Huge Porphyrin Arrays	¥15,800,000
T. Matsumoto	Ogasawara Science Fundation	Magnetoresistance Device Using Self-organized Nano-scale Molecular Arrays.	¥1,200,000
M. Taniguchi	Shin-Etsu	Development of FET	¥2,000,000

	Chemical Co., Ltd		
M. Taniguchi	Kansai Research Foundation from Technology Promotion	Development of High-mobility FET Based or Polymers Using Inkjet Process	¥900,000

Department of Supramolecular Chemistry

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Specially Appointed-Research Associates:	Kazuhiro TAKENAKA

Outline

Towards the construction of organized supramolecular systems with multifunctionality, the design and syntheses of supramolecules such as spherical nanoparticles, artificial DNA, proteins, photosynthetic molecules, and metal-bridged polymers having more efficient and selective functions than those of single molecules have been investigated.

Current Research Projects

1. Charge transfer through DNA nanoscaled assembly programmable with DNA building blocks

DNA nanostructures based on programmable DNA molecular recognition have been developed, but the nanoelectronics of using DNA is still challenging. A more rapid charge-transfer (CT) process through the DNA nanoassembly is required for further development of programmable DNA nanoelectronics. We succeeded in direct absorption measurements of the long-range CT over a 140-Å DNA assembly based on a GC repetitive sequence constructed by simply mixing DNA building blocks. We show that a CT through DNA nanoscale assembly is possible and programmable with the designed DNA sequence.

2. Mechanism of Photosensitized One-Electron Oxidation of DNA

To investigate the importance of the reaction rate of radical anion of the photosensitizer with O_2 during the photosensitized DNA damage reactions through the one-electron oxidation pathway, photosensitized DNA damage reactions were compared between two well known DNA damaging photosensitizer, naphthalimide (NI) and napthaldiimide (NDI). NI and NDI have similar photophysical properties but differ in their redox properties, that is, the reaction rates of their radical anion with O_2 are supposed to be somewhat different. NI- and NDI-modified DNA were synthesized and a combination of laser flash photolysis kinetic studies and quantitative HPLC analyses of photosensitized DNA damage reactions were investigated. It was clearly demonstrated that the reaction rate of radical anion of the photosensitizer and O_2 is one of the critically important factors determining the efficiency of photosensitized DNA damage. These results may provide us with new strategies for the future design of the Sens for therapeutic and biochemical applications.

3. Metal-bridged Polymers as Enantioselective Catalysts

Immobilization of catalysts facilitates environmentally benign processes by enabling their recovery and reuse. We have developed a novel approach for the effective immobilization of the multicomponent catalysts utilizing metal-bridged polymers which is formed by a metal-mediated self-organization of bis(bidentate) ligand. Treatment of (*R*,*R*)-6,6'-bi(BINOL) with either $LiAlH_4$ or $Ti(O\text{-}i\text{-}Pr)_4$ generates a chiral metal-bridged polymer which catalyzed Michael reaction and carbonyl-ene reaction respectively with high enantioselectivities.

4. 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 $Ti(O\text{-}i\text{-}Pr)_4$ 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.

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Spectroscopic Investigation of Oxidative Hole Transfer in DNA (Invited), *K. Kawai and T. Majima, International Symposium on “Photochemistry of Nanomaerials, SANKEN, Dec 7, 2006.

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Development of New TiO_2 Photocatalysts (Invited), *T. Majima, The 8th International Conference on ECOMATERIALS, Kitakyusyu International Conference Center, Jan 11-14, 2007.

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Annual Meeting of Chemical Society of Japan	13 papers
Congress of Organic Chemistry	2 papers
Symposium on Radiation Chemistry	3 paper
Symposium on Photochemistry	10 papers
FIBER Forum 2006	1 paper
Symposium of SORST Saito Team	1 paper
Annual Meeting of Electron Spin Science Society	1 paper

Sponsorships

Grand-in-Aid for Scientific Research (S)

T. Majima	Nanoscience of Photofuctionalized DNA	¥19,240,000

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

T. Majima	Fundamental Science and Technology of Photofunctional Interfaces	¥10,200,000
H. Sasai	Development of Chiral Organocatalyst with Synergistic Effect	¥2,100,000

Grand-in-Aid for Basic Scientific Research

T. Majima	Formation of Carbon Nanotubes Arrays based on DNA Self-assembly	¥1,000,000

Grand-in-Aid for Encouragement of Young Scientists

K. Kawai	Construction of Nano-DNA Charge-Separation System	¥2,500,000

Grand-in-Aid for Encouragement of Young Scientists

K. Kawai	Photo-Current Conversion by Nano DNA Constructs The Science and Technology Foundation of Japan	¥1,000,000

Grand-in-Aid for Fixed-Term Young Scientists

S. Takizawa	Preparation of Functionalized Nanoparticles by Selfassembly	¥19,430,000

Entrusted Research

T. Majima	IDEC Co.	Selection of plastic by laser	¥4,510,000

	Satake Co.	light	
H. Sasai	Japan Science and Technology Agency	Preparation of Novel Medicinal Intermediates Based on Enantioselective Reactions Using Chiral Spiro Ligands	¥3,250,000

Other Research Fund

T. Majima	Matsushita Electric Industrial Co.	Study of highly reactive TiO_2 nanotuve photocatalysts	¥1,155,000
T. Majima	Mitsubishi Chemical Co.	Basic research on chemical reaction via higher excited states	¥1,000,000
T. Majima	Asahi Glass Co.		¥1,000,000

Department of Nanobiology

Professor: Katsuyuki TANIZAWA
Associate Professor: Toshihide OKAJIMA
Research Associate: Ryousuke NAKASHIMA

Outline

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 Projects

Structural analysis of reaction intermediates formed on catalytic cycle of copper amine oxidase

The catalytic reaction of copper amine oxidase comprises the reductive and oxidative half-r eactions, divided on the basis of the redox state of the covalently-bound organic cofactor, topaquinone (TPQ). A substrate amine reduces TPQ to an aminoresorcinol form in the reductive half-reaction. The reduced TPQ is then re-oxidized by dioxygen in the following oxidative half-reaction. It has been proposed that the TPQ cofactor changes its conformation during the catalytic cycle, serving as a mediator of $2H^+$- and $2e^-$-transfers from substrate to oxygen. To unravel the dynamic movement of TPQ directly associated with these transferring processes, we have determined X-ray crystal structures of catalytic intermediates formed in the recombinant enzyme from *Arthrobacter globiformis* (AGAO) and its variants, including a mutant enzyme lacking the catalytic base and those with the bound Cu^{2+} ion being replaced by other metal ions. The structures of Schiff-base intermediates formed in the base-less mutant have revealed a 'wedge-shaped' movement of TPQ, which appears to be advantageous for abstraction of substrate α-proton and also for the following hydrolysis. Furthermore, the structures of Cu-AGAO (wild type) and Ni-AGAO with TPQ in the substrate-reduced form have revealed that TPQ exists in an 'on-copper' conformation in Cu-AGAO, which is probably a facile conformation for $1e^-$-transfer to Cu^{2+}, but branching off the normal reaction path. On the other hand, the reduced TPQ in Ni-AGAO is in a catalytically active 'off-copper' conformation without forming a semiquinone radical form of TPQ.

Biochemical and molecular biological studies on posttranslational modification of quinohemoprotein amine dehydrogenase

A heterotrimeric quinohemoprotein amine dehydrogenase (QHNDH) from *Paracoccus denitrificans* contains a quinone cofactor, cysteine tryptophylquinone (CTQ), and intra-peptidyl thioether crosslinks within the smallest γ-subunit, all of which are synthesized by post-translational modification. A putative [Fe-S]-cluster-containing protein (ORF2) encoded between the structural genes for α- and γ-subunits in the operon likely belongs to a Radical SAM (S-Ado-Met) superfamily that includes many proteins involved

in vitamin biosynthesis and enzyme activation. Previously, we constructed an ORF2-gene deleted (ΔORF2) strain of *P. denitrificans* and demonstrated the essentiality of ORF2 for QHNDH biosynthesis. In this study, the roles of ORF2 in the biosynthesis of QHNDH were further studied.

When the ΔORF2 strain was transformed with an expression vector for ORF2, significant QHNDH activity was restored by induction with *n*-butylamine. Site-specific mutations in the [Fe-S]- or SAM-binding motifs of ORF2 neither supported bacterial growth nor restored QHNDH activity. The α- and β-subunit proteins were both detected in the periplasm of the ΔORF2 strain, whereas the γ-subunit protein accumulated in the cytoplasm and was stained negatively for redox-cycling quinone staining. Furthermore, MALDI-TOF mass spectrometric analysis revealed that the cytoplasmic γ-subunit protein isolated from the ΔORF2 strain was not posttranslationally modified, and surprisingly that it contained N-terminal presequence unobserved in the mature form. These results show that the Radical SAM ORF2 protein is involved in the formation of unusual intrasubunit thioether crosslinks of γ-subunit, which is essential for QHNDH biosynthesis.

Crystallographic analysis of xenobiotic exporters.

Xenobiotic extruding pumps have recently been known to be widely distributed in living organisms from mammalian to bacteria as a host-defence mechanism in cellular level. These pumps not only confer multidrug resistance of cancer cells and pathogenic bacteria but also cause hereditary diseases through the mutation. We previously reported the high resolution crystalline structure of the xenobiotic exporter AcrB. This is the first case for the crystal structure determination of multidrug transporters as well as proton coupling one and gives a structural basis for understanding the membrane transport mechanism. We also succeeded in determination of crystal structure of AcrB with substrates in 2006. Only one of three protomers that constitute a trimer has a bound substrate in a phenylalanine-rich pocket in the periplasmic region. We propose that the three different conformations of the protomers represent the three states of drug export: access, binding and extrusion. Presumably, the drugs are exported by a three-step binding change mechanism

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Secretory Production System of Bionanocapsules Using a Stably Transfected Insect Cell Line, T. Shishido, M. Muraoka, M. Ueda, M. Seno, K. Tanizawa, S. Kuroda, H. Fukuda, and A. Kondo: Appl. Microbiol. Biotechnol., 73 (2006) 505–511.

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A New Built-in Type Quinone Cofactor, CTQ, and Intramolecular Thioether Crosslink Structure – Toward Elucidation of the Biosynthetic Mechanism of the Unique Structure - , K. Tanizawa: Enzyme Engineering News, 56 (2006) 5–9.

Present and Future of Bionanocapsules that Enable In Vivo Pin-point Delivery of Genes and Drugs, T. Kasuya, J. H. Jung, K. Tanizawa, and S. Kuroda: Kagaku-to-Seibutsu, 44 (2006) 760–766.

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Pinpoint Drug and Gene Delivery System Using ZZ tag-displaying Bio-nanocapsule and Targeting Molecule-fused IgG Fc protein, *H. Tonoi, H. Tada, A. Ueda, A. Kondo, M. Seno, M. Ueda, K. Tanizawa, S. Kuroda, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto, Japan, Jun. 18-23, 2006.

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ENH1 Scaffolds the PKC_-PKD1 Signaling Complex at the Z-discs of Cardiomyocytes, *M. Ishida, A. Matsurara, M. Iwata, J. V. Lint, K. Tanizawa, S. Kuroda, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto, Japan, Jun. 18-23, 2006.

Novel Functions of a Splice Variant of a RING-IBR Protein RBCK1 in Proteasomal Protein Degradation, *N. Yoshimoto, K. Tatematsu, K.Tanizawa, S. Kuroda, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto, Japan, Jun. 18-23, 2006.

Pinpoint Drug and Gene Delivery System Using ZZ-displaying Bio-nanocapsule and Homing Peptide-fused IgG Fc Protein, *H. Tonoi, A. Ueda, T. Kasuya, K. Tatematsu, T. Okajima, K. Tanizawa, S. Kuroda, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Suita, Osaka, Japan, Sep. 19-20, 2006.

Involvement of a Putative Radical SAM Protein in the Posttranslational Formation of Intra-peptidyl Thioether Crosslinks in Quinohemoprotein Amine Dehydrogenase, *K. Ono, T. Okajima, M. Tani, S. Kuroda, D. Sun, V. L. Davidson, K. Tanizawa, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Suita, Osaka, Japan, Sep. 19-20, 2006.

Publications in Domestic Meetings

Japanese Agricultural Biochemical Society, Kansai Branch Meeting	1 paper
Japanese Agricultural Biochemical Society	1 paper
Bimonthly Meeting of Vitamin B Committee	2 papers

Sponsorships

Grant-in-Aid for Scientific Research (B)

K. Tanizawa	Mechanisms of Biosynthesis and Catalysis of Built-in Type Quinone Cofactor	¥9,200,000
T. Okajima	Mechanism of Proton and Electron Transfer in Enzyme Containing Built-in Type Quinone Cofactor	¥10,920,000

Grant-in-Aid for Young Scientists (B)

R. Nakashima	Crystallization of tetracycline efflux protein	¥1,200,000

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	¥3,675,000
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	¥1,300,000
K. Tanizawa	Bio-oriented Technology Research Advancement Institution (BRAIN)	Development of Innovative and Hypersensitive Bio-sensing Technology Using Yeast-derived Bio-nanocapsule	¥20,000,000
T. Okajima	Bio-oriented Technology Research Advancement Institution (BRAIN)	Development of Drugs Inhibiting Bacterial Signal Transduction Based on X-ray Crystal Structures	¥10,000,000

Other Research Fund

K. Tanizawa	Vitamin B Committee	Research on Cofactors		Built-in	¥250,000

Department of Nanosystem Design

Guest Professor: Joji OHSHITA (2006.4.1-2006.6.30)

Outline

Organosilicon compounds exhibit enhanced emission and conductive properties. Application of organosilicon compounds to organic light emitting diodes and conducting devices needs various improvements in synthetic and fabrication methods. On the other hand, the emission and conductive processes are governed by picosecond-order-processes, while their details are not clear. By using femtosecond laser technique, mechanism of the energy migration along the block copolymer of oligothiophene and oligosilylene was investigated.

Achievement

Decay of fluorescence anisotropy of an alternating block copolymer of oligothiophene and oligosilylene was measured. Anisotropy decay on the order of picosecond can be attributed to the energy migration among oligothiophene blocks in the polymer from the comparison with the theory. The length of the oligothiophenes was an important factor in the energy migration. Detailed structure-energy transfer rate relation was obtained from the investigation on the anisotropy decay of well-defined oligomer model compounds.

Publications

Original Papers

Singlet Energy Migration along an Alternating Block Copolymer of Oligothiophene and Oligosilylene in Solution, M. Fujitsuka, D. W. Cho, J. Ohshita, A. Kunai, and T. Majima, The Journal of Physical Chemistry B, 110 [25] (2006) 12446-12450.

Fluorescence Properties of Si-linked Oligothiophenes, M. Fujitsuka, D. W. Cho, J. Ohshita, A. Kunai, and T. Majima, The Journal of Physical Chemistry C, 111 [5] (2007) 1993-1998.

Department of Nanosystem Design

Guest Associate Professor: Kenji TAKAHASHI (2006.4.1-2006.6.30)

Outline

The Room Temperature Ionic Liquids (RTILs) are liquid salts made of only anion and cation at room temperature. And the RTILs attract attention for new reaction solvent. The RTILs are organic molecules. By changing Chemical structure or anion species or cation species, many kind of molecular design and function design are possible. By nanosecond region electron pulse radiolysis, the solvated electrons which induced by electron beam were measured in ionic liquid by transient optical absorption. Reaction of solvated electrons in RTIL were studied by electron scavenging method using the Pyrenees. By changing the cation species of RTIL, the cation effect of solvated electrons was studied by nano-second pulseradiolysis.

Achievement

Reaction properties of solvated electrons in RTIL (DEMMA-TFSI): Reactions of solvated electrons induced by electron beam in RTIL (DEMMA-TFSI) were measured by nano-second pulseradiolysis. As a result of a Pyrene addition, decay rate constant of solvated electrons was increased and initial yield in nanosecond was decreased. The decay rate constant of solvated electrons was increased depend on the concentration of Pyrene. Reaction properties of solvated electrons in DEMMA-TFSI were studied. And reaction between pre-solvated electrons and Pyrene was measured.

Cation effect of solvated electrons: By changing the cation species of RTIL, the cation effect of solvated electrons was studied by nano-second pulseradiolysis. To change structure of solvated electrons, transient optical absorption spectrum was measured for TMPA-TFSI which has same anion but different cation toward DEMMA-TFSI. Transient absorption spectrum did not so big change.

Publications

Kenji Takahashi, Shingo Sakai, Hiroaki Tezuka, and Yusuke Himejima, Yosuke Katsumura, Masayoshi Watanabe, Reaction between Diiodide Anion Radicals in Ionic Liquids, J. Phys. Chem. B, 10.1021/jp0671087, Published on Web 02/01/2007

Ryuzi Katoh, Yoichi Yoshida, Yousuke Katsumura, and Kenji Takahashi, Electron Photo detachment from Iodide in Ionic Liquids through Charge-Transfer-to-Solvent Band Excitation, J. Phys. Chem.B, 10.1021/jp067107e, Published on Web 01/11/2007

Department of Nanosystem Design

Guest Professor: Fumitoshi KAKIUCHI (2006.7.1-2006.9.30)

Outline

Transformation involving cleavage of chemically stable bonds that have large bond energy is very useful for efficient organic synthesis. The goal of this project is to develop new catalytic reactions involving cleavage of chemically stable bonds by use of transition metal complexes.

Achievement

A new catalytic reaction involving C-O bond cleavage has been developed based on our previous finding that coordination of the neighboring functional group enhances activation of C-H bond of aromatic compounds. Treatment of ruthenium complex with (*o*-aryloxy)pivalophenone resulted in the cleavage of C-O bond by oxidative addition to give (*o*-pivaloylphenyl)(aryloxy)ruthenium complex. This ruthenium complex effectively catalyzed the reaction of (*o*-aryloxy)pivalophenone with phenylboronate producing an ortho-phenylation product. Trace experiment by NMR revealed that C-H bond cleavage is the kinetically favored process while aryl C-O bond cleavage is the thermodynamically favorable one. Chemoselective C-C bond formation using vinylsilanes and organoboronates was achieved due to the difference in the reactivity of C-H and C-O bonds toward the ruthenium complex.

Department of Nanosystem Design

Guest Professor: Qiang YU (2006.7.1 - 2006.9.30)

Outline

In order to develop highly reliable micro-systems, establishment of the design concept for micro-joints is one of the most important issues in the electronic packaging technology. This project focused on the design approach based on CAE (Computer Aided Engineering) for Pb-free solder micro-joints.

Achievement

FEM (Finite Element Method) simulation for deformation and fracture behavior of micro-joints using Pb-free solders during thermal cycles was conducted. The simulation results provided useful information for interpreting the experimental results. The CAE is expected to be the effective approach for structural design of micro-joints in various micro-systems.

Department of Nanosystem Design

Guest Professor: Tamio OGUCHI (2006.10.1-2006.12.31)

Outline

Multiferroic systems show multiple ferroic (or anti-ferroic) orders associated with the electronic degrees of freedom in solids such as spin, orbital and charge (electric dipole). In most cases, these electronic degrees are also coupled with the lattice one at the same time. Multiferroic systems have attracted much attention because of not only the multiple orders themselves but also cross-term effects between them, which lead to novel functionalities applied to the next-generation devices. In this project, we study, on the basis of first-principles electronic structure calculations, possible electric polarization induced by lattice distortion in thin films for oxides systems with perovskite and garnet crystal structure.

Achievement

We considered ferroelectric $PbTiO_3$ (PTO) and $Pb(ZrTi)O_3$ (PZT) with perovskite structure and investigated the lattice instability and emerging electric polarization induced by changing the lattice-constant ratio c/a. We performed first-principles calculations for a typical garnet oxide $Y_3Fe_5O_{12}$ and studied the microscopic mechanism of the ferrimagnetic order of Fe spin moments. The lattice instability of YIG induced by tetragonal distortions is currently under investigation.

Department of Nanosystem Design

Guest Associate Professor: Takeshi KAWAGOE (2006.10.1-2006.12.31)

Outline

Semiconductor spintronics are aimed at the manipulation of spin-dependent phenomena in conventional semiconductor heterostructures as well as in the hybrid systems with combination of magnetic and semiconducting materials. Fabricating semiconductor spintronic devices requires the characterization of magnetic structures in semiconductor heterostructures at the nanoscale. Spin polarized scanning tunneling microscopy and spectroscopy (SP-STM/STS), which has visualized magnetic structures of metal (Co, Cr, Gd, and so on) surfaces with atomic scale, is one of promising candidates for this purpose. We have performed researches on nanotechniques visualizing magnetic structures in dilute magnetic semiconductors (DMSs) by using SP-STM/STS.

Achievement

We have discussed and analyzed fundamental issues for visualizing magnetic structures in DMSs such as GaCrN at the nanoscale by SP-STM/STS, in particular, fabrication methods of ferromagnetic tips, surface preparation techniques of DMSs, and acquisition methods of dI/dV images.

A lecture on visualizing nanoscale magnetic structures of thin films was given to researchers and graduate students. The lecture covered (1) overview of techniques for imaging magnetic structures, (2) principle and set-up of SP-STM/STS, and (3) imaging nanoscale magnetic structures of epitaxial Cr films by using SP-STM/STS.

Department of Nanosystem Design

Guest Professor: Makoto SUNAGAWA (2007.1.1-2007.3.31)

Outline

Antibiotics have greatly contributed to human health by interfering microbial infections. However, the emergence of drug-resistant strains became threat and their rapid dissemination is really worrisome. The ultimate goal of the research is to develop drugs that are able to rescue immunocompromised individuals from hospital-acquired infections caused by multidrug-resistant *Pseudomonas aeruginosa*.

Achievement

One of the major mechanisms underlying bacterial resistance to β-lactam-containing antibiotics is the production of β-lactamases, which are enzymes capable of hydrolyzing β-lactam ring. β-Lactamases have been divided into four classes, A–D, where classes A, C, and D contain a serine in the active site, and class B is the so-called metallo-β-lactamase (MBL) that requires metal ions for catalytic activity. As the MBLs hydrolyze a broad spectrum of lactam-antibiotics including carbapenems, the research focused on inhibitors for MBLs and initiated the project to synthesize rationally designed molecules based on new drug-design concept.

Department of Nanosystem Design

Guest Associate Professor: Makio UWAHA (2007.1.1-2007.3.31)

Outline

It is important with the various scenes of nano-technology to understand how disordered states like the liquid and the vapor evolve into ordered states like crystals. In order to fabricate nanoscale devices in self-organized manners by bottom-up processes, it is important to understand the mechanism and dynamics of self-organization phenomena such as grain growth by diffusion. Collaborative research has been done concerning self organized formation of ordered surface structures like regularly stepped ones from disordered surfaces.

Achievement

Thermal relaxation of surface nano-structures has been studied cooperatively. Evolution of a disordered surface, i.e., mechanically polished $SrTiO_3$(100) surface to regularly stepped one by thermal annealing has been studied experimentally and theoretically. It is established how to describe the thermal relaxation process and the behavior is reproduced by simulation. The achievement has been reported in academic workshops.

Division of Beam Science for Nanotechnology

Outline

The division of beam science for nanotechnology is composed of five research departments: beam science for nanofabrication, quantum beams for nanotechnology, beam processing for nanotechnology, advanced nanofabrication, and ultra-fast spectroscopy of nanostructures. Quantum beam science is one of the most important fields for nanoscience and nanotechnology. The researches are performing by using ultra-short electron beam, slow positron beam, ion beam, electron lithography and so on. The studies such as time-space reaction analysis with ultra-short electron beam, nano-structure analysis with slow positron beam and nano-beam process, are expected for ultimate nanofabrication and a new nano-beam science.

Achievements

- 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

Department of Beam Science for Nanofabrication

Professor: Yoichi YOSHIDA
Associate Professor: Jinfeng YANG
Assistant Professor: Takafumi KONDOH
Graduate Students: Kouji TAKEYA, Kouichi KAN, Youichi KURODA, Susumu TAKEMOTO, Masayoshi HIROSE, Akira ASANO
Research Students: Haruki TANAKA, Hiroaki KASHIMA, 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 femtosecond/attosecond pulse radiolysis based on a photocathode electron beam accelerator is being developed for the study of such ultrafast reactions in nano-space. It is also expected for the development of quantum-beam fabrication process for nanotechnology.

In 2006, an equivalent velocity spectroscopy (EVS) based pulse radiolysis system was constructed to avoid degradation of time resolution due to the velocity difference between the analyzing light and the 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. The technique of rotating the electron bunch was developed. The rotation angle of the bunch was successfully measured by using a femtosecond streak camera. Furthermore, the pulse radiolysis system based on the double-decker electron beam accelerator was constructed. The generation of sub-femtosecond and attosecond electron bunches was studied.

Current Research Projects

1. Equivalent velocity spectroscopy based pulse radiolysis

In order to improve the time resolution of pulse radiolysis into femtosecond time region, a new concept of “Equivalent Velocity Spectroscopy (EVS)” was developed. In EVS, the electron beam and the analyzing laser light were injected into sample with an angle (θ), which is determined by the refractive index of the sample. The electron bunch was also rotated with a same angle to make an overlap of the electron bunch with the laser pulse in sample. The degradation of the time resolution caused by the velocity difference between the light and the electron beam was thus avoided. To rotate the electron bunch, a magnetic bunch compressor, which was constructed with two 45°-bending magnets and four quadrupole magnets (two pairs) to provide a necessary path length dependence on energy, was used. The electron beam generated from the rf gun was accelerated by a linear accelerator up to 32 MeV with energy-phase correlation in the bunch. Finally, the necessary rotation angle of the electron bunch was achieved by passing the electron beam through the compressor and optimizing the magnetic fields of the quadrupole magnets. The rotation angle of the bunch was successfully measured by using femtosecond streak camera technique.

2. Double-decker electron beam accelerator and attosecond pulse radiolysis

A concept of double-decker electron beams, which have vertically different positions and a time delay each other, was proposed for study of ultra-fast electron-induced phenomena by pulse radiolysis technique. One of the double-decker electron beams is used as an irradiation source, and another is converted to Cherenkov light or OTR light for probe light source. In case of the pulse radiolysis using double-decker electron beams, the time jitter between the probe light and the electron beam is drastically reduced. The double-decker electron beams were generated successfully by injecting two Nd:YLF picosecond laser pulses into a photocathode RF gun. The beams were accelerated up to 31 MeV by an S-band booster linear accelerator and compressed by a magnetic bunch compressor into femtosecond. The pulse radiolysis based on the double-decker electron beams was developed.

3. Generation of sub-femtosecond and attosecond electron bunch

The growths of the bunch length due to beam emittance, space-charge and higher-order effects in the magnetic bunch compressor were investigated theoretically to generate sub-femtosecond or attosecond electron bunch. A compensation technique of the high-order effect was proposed by optimizing the bunch distribution in longitudinal phase-space obtained with re-phasing the accelerating RF phase in the linac. In the simulation, a 640-attosecond electron bunch was obtained in the photocathode RF linear accelerator by injecting a femtosecond UV laser light on the photocathode.

Publications

Original Papers

Femtosecond Single Electron Bunch Generation by Rotating Longitudinal Bunch Phase Space in Magnetic Field, J. Yang, T. Kondoh, K. Kan, T. Kozawa, Y. Yoshida, S. Tagawa: Nucl. Instrum. Meth., A 556 (2006), 52-56.

Pulse Radiolysis based on a Femtosecond Electron Beam and a Femtosecond Laser Light with Double-pulse Injection Technique, J. Yang, T. Kondoh, T. Kozawa, Y. Yoshida, S. Tagawa: Radiat. Phys. Chem., 75 (2006), 1034-1040.

Double-decker Femtosecond Electron Beam Accelerator for Pulse Radiolysis, J. Yang, T. Kondoh, A. Yoshida, Y. Yoshida: Rev. Sci. Instrum., 77 (2006), 043302.

Femtosecond Single-bunch Electron Linear Accelerator Based on a Photocathode RF Gun, J. Yang, K. Kan, T. Kondoh, A. Yoshida, Y. Yoshida: Proceedings of EPAC 2006, Edinburgh, Scotland, 2514-2516, 2006.

Equivalent Velocity Spectroscopy Based on Femtosecond Electron Beam Accelerator, S. Takemoto, T. Kondoh, J. Yang, Y. Yoshida: Proceedings of EPAC 2006, Edinburgh, Scotland, (2006), 2511-2513.

Higher-order Effect Compensation in Magnetic Compressor for < 50 fs Electron Bunch Generation, K. Kan, T. Kondoh, J. Yang, Y. Yoshida: Proceedings of EPAC 2006, Edinburgh, Scotland, (2006), 2502-2504.

Development of Double-decker Electron Beam Accelerator for Femto/attosecond Pulse Radiolysis, Y. Kuroda, T. Kondoh, J. Yang, Y. Yoshida: Proceedings of EPAC 2006, Edinburgh, Scotland, (2006), 2505-2507.

Electron Beam Pulse Processing toward the Intensity Modified Radiation Therapy (IMRT), T. Kondoh, S. Tagawa, J. Yang, Y. Yoshida: Proceedings of EPAC 2006, Edinburgh, Scotland, (2006), 2334-2336.

International Conferences

Generation of Femtosecond Electron Beam for Ultrafast Reaction Analysis in Nanospace, J. Yang, K. Kan, T. Kondoh, A. Yoshida, T. Kozawa, Y. Yoshida and S. Tagawa, Handai Nanoscience and Nanotechnology International Symposium, Osaka Univ, Jan.30-Feb.1, 2006.

Generation of 98-Femtosecond Single Electron Bunch in Photocathode Linear Accelerator, *Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.8-9, 2006.

Generation of a Gradation Electron Beam Pulse Toward the Intensity Modified Radiation Therapy (IMRT), T. Kondoh, J. Yang, Akira Yoshida, Tamotsu Yamamoto, Y. Yoshida and S. Tagawa, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.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), Osaka, Japan, Feb.8-9, 2006.

100-femtosecond Electron Beam Generation 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), Osaka, Japan, Feb.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), Osaka, Japan, Feb.8-9, 2006.

A Concept of Double-decker Electron Beam Accelerator for Att/femtosecond Reaction Analysis, Y. Kuroda, J. Yang, T. Kondoh, A. Yoshida, Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.8-9, 2006.

3D-Measurement for Short Electron Bunch, A. Yoshida, Yang J., T. Kondoh, Y. Yoshida, Atsushi Ogata, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.8-9, 2006.

Electron Beam Pulse Processing toward the Intensity Modified Radiation Therapy (IMRT), T. Kondoh, J. Yang, Y. Yoshida and S. Tagawa, Proceedings of the 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006.

Higher-order Effect Compensation in Magnetic Compressor for <50fs Electron Bunch, K. Kan, T. Kondoh, J. Yang, Y. Yoshida, Proceedings of the 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006.

Development of Double-decker Electron Beam Accelerator for Femto/attosecond Pulse Radiolysis, Y. Kuroda, T. Kondoh, J. Yang, Y. Yoshida, Proceedings of the 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006.

Equivalent Velocity Spectroscopy Based on Femtosecond Electron Beam Accelerator, S. Takemoto, T. Kondoh, J. Yang, Y. Yoshida, Proceedings of the 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006.

Femtosecond Single-bunch Electron Linear Accelerator Based on a Photocathode RF Gun, J. Yang, T. Kondoh, Y. Yoshida, Proceedings of the 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006.

High-brightness Electron Source based on Photocathode RF Gun in Osaka Univ., *J. Yang, Agenda for 7th Beam Physics Seminar in Pusan (JSPS Core University Program), Pusan National University, Korea, Sep. 13, 2006.

1 mm-mrad Electron Beam at 1 nC, *J. Yang, Agenda for 7th Beam Physics Seminar in Pusan (JSPS Core University Program), Pusan National University, Korea, Sep. 13, 2006.

Spatial Modulation of Electron Beam for IMRT, T. Kondoh, J. Yang, Tamotsu Yamamoto, Y. Yoshida and S. Tagawa, SANKEN International Symposium on Nanoscience and Nanotechnology 2006 (SISNN-2006), Osaka Univ., Sep. 19-20, 2006.

Ultrashort Electron Beam for Reaction Analysis in Nanofabrication, J. Yang, Koichi Kan, Y. Kuroda, T. Kondoh and Y. Yoshida, SANKEN International Symposium on Nanoscience and Nanotechnology 2006 (SISNN-2006), Osaka Univ., Sep. 19-20, 2006.

Femtosecond Pulse Radiolysis based on Photocathode Electron Accelerator, *Y. Yoshida, J. Yang, T. Kondoh, T. Kozawa, S. Tagawa, The 1st ASIAN-PACIFIC SYMPOSIUM ON RADIATION CHEMISTRY, Shanghai, China, Sep. 17-21, 2006.

Pulse Radiolysis Study on Solvated Electrons in Ionic Liquid with Controlling Water Content, J. Yang, R. Nagaishi, T. Kondoh, Y. Yoshida, The 1st ASIAN-PACIFIC SYMPOSIUM ON RADIATION CHEMISTRY, Shanghai, China, Sep. 17-21, 2006.

Processing of Incident Light by the DMD for the Photocathode RF Gun, T. Kondoh, Hiroaki Kashima, J. Yang, Tamotsu Yamamoto, Y. Yoshida, S. Tagawa, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter- Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006.

Collective Ionization by Attosecond Electron Bunches, A. Ogata, T. Kondoh, J. Yang, Y. Yoshida, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter-Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006.

Simulation Study on Sub-femtosecond Electron Bunch Generation, K. Kan, J. Yang, T. Kondoh, Y. Yoshida, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter- Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006.

Femtosecond Electron Beam and Femtosecond Pulse Radiolysis for Reaction Analysis in Nano-space, J. Yang, T. Kondoh, T. Kozawa, Y. Yoshida, S. Tagawa, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter- Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006.

Publications in Domestic Meetings

Symposium on Advanced Radiation Chemistry	2 papers
The Japan Society of Radiation Chemistry	6 papers
The Particle Accelerator Society of Japan	5 papers
Atomic Energy Society of Japan	2 papers
Chemical Society of Japan	1 paper
Symposium on RF Electron Gun	2 papers
Symposium on TIARA	1 paper

Academic Degrees

Master Degree of Engineering

Yoichi Kuroda	Double-decker electron beam accelerator and attosecond pulse radiolysis
Susumu Takemoto	Equivalent velocity spectroscopy based femtosecond pulse radiolysis

Sponsorships

Grant-in-Aid for Basic Research (A)

Y. Yoshida	Basic Research on Subfemtosecond and Attosecond Pulse Radiolysis	¥29,800,000

Grant-in-Aid for Basic Research (C)

J. Yang	Basic Research on Heavy Ion Pulse Radiolysis	¥1,800,000

Collaborative 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
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

Outline

In this department, we conduct research on development of new measurement methods in the nanometer range using quantum beams, which are expected to form bases for nanotechnology, and on their applications as well as on development of quantum beams. To put it concretely, we are developing a highly intense and bright positron beam using an electron linac and its applications to materials science. Positrons have a nature to concentrate in holes and free volumes in materials and consequently measurements using positrons are widely received as an effective method to analyze sizes and distributions of free volumes. The positron beam is highly expected to play an important role in analyzing not only the sizes but also the distributions of nanometer size spaces and free volumes in porous materials such as polymers. We conduct research for better understanding interactions of positrons and positroniums, which are formed by an electron and a positron as a bound state, with materials, and for analyzing free volumes, surfaces and interfaces in thin polymer films, and finally for developing new materials. Since high-quality positron beams are necessary for conducting such researches, we also make studies on production of intense, bright, and short-pulsed slow positron beams using an electron linac, and on development of new measurement methods. We also take part in management and operation of the Radiation Laboratory, which has the experimental apparatuses for these studies.

Current Research Projects

1. Commissioning of the S-band Linac

The S-band linac, which has been used for production of a slow positron beam, has three acceleration tubes and the nominal energy of the accelerated electron beam is 150 MeV. In the last year, we had several troubles, especially the troubles in the DC high voltage power supply were serious. Many of these troubles were removed but stable operation of linac could not be achieved yet. In this year, similar efforts has been made but were in vain. In order to improve present situation, we decided to make a new frame inside which the power supply, modurator and pulse forming network are equipped, and to review the discharge circuit comprehensively. We expect the linac will be operated stably in the next year.

2. Preparation for Positron Diffraction Experiment

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. 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 could not start the experiment relating to positron diffraction because of the unstable operation of the linac. However, we purchased a new goniometry to handle samples. After recovering of the linac, this kind of experiment will be started.

3. Investigation of Degradation Process of Polymer Electrolyte Membrane by Using Positron

In order to investigate the structural change relating to the proton conductivity by small angle X-ray diffraction or neutron diffraction, periodic structure, for example one consisting of inverted micellar structure, is required to some extent. Therefore available materials to be analyzed by using these methods are restricted. The structural change caused by heating is also detectable using DSC, but the evidence is obtained at rather high temperature than working temperature. On the other hand, positron annihilation spectroscopy (PAS) has advantages, since it can evaluate both nanoscale space size and electronic state at room temperature and proton conductivity of polymer electrolyte membrane (PEM) would be influenced by these features. So far, as most of researches for PEM using positron mainly focused on the estimation of the mean diameter of nanoscale open pores named free volume holes and structural change, the substantial correlation of these properties with ion exchange ability and proton conductivity has little been investigated. In this study, thermal degradation process was investigated by age-momentum correlation measurement (AMOC). Nafion®-117 developed by DuPont was used as perfluoro sulfonic acid (PFSA) throughout this study.

We investigated the differences in non-baked and baked PFSAs by using age-momentum correlation measurement in addition to traditional measurements of lifetime and energy spectrum of annihilation γ-ray. The difference in diameter for two samples was estimated at 0.01 nm, which was derived from the lifetimes of *o*-Ps for two samples. However the S-parameter for baked sample increased, which means the increase of low energy electrons by baking. As the results of AMOC measurements, both of time dependent S-parameters showed monotonic decrease. The component of S-parameters affected only by the annihilation of *o*-Ps were similar value, which means environmental condition for pick-off annihilation of *o*-Ps was not affected by baking. On the other hand, the S-parameter corresponding to the free annihilation of positron increased by baking. This means that the low energy electrons, maybe relating to the thermal radicals, were produced by baking. As a result of four-electrode AC impedance measurements, it was found that the proton conductivity was decreased by baking. The chemical bonding was thought being changed by baking, because the proton conductivity for the baked sample could not be recovered completely even after water uptake.

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. Recently positron annihilation spectroscopy has been used to estimate the size of nanoscale open pore, which is often called free volume hole, in polymers. Injection of positron as well as electron induces ionization. Positronium takes place between thermalized positron and electron. This reaction is competitive with recombination of ion and electron, scavenging of electron by halogenated alkyl. Hence, by taking into account of positronium formation taking place within several picoseconds after positron injection, these competitive reactions would be investigated by analyzing positronium formation. This feasibility study is carried out in this study.

Publications

Original Papers

Analysis of Selling Pocess in Bopolymer Gl byUsing Psitron Anihilation Sectroscopy and Termal Aalysis (in Japanese), H. Mimachi, Y. Akiyama, S. Takeda, Y. Izumi, Y. Honda, S. Nishijima: RADIOISOTOPES, **55**(2006)525-531.

Books

Hoshasen Kagaku no Susume (in Japanese), Y. Honda, Gakkai Shuppan Center, (2006) 169-171.

International Conferences

Study on Plymer EectrolyteMembrane for Fuel Cell by Using AMOC Technique, *Y. Honda, Y. Shibahara, Y. Akiyama, N. Kimura, G. Isoyama, S. Tagawa, S. Takeda, Y. Izumi, S. Nishijima, 14th International Conference on Positron Annihilation, Hamilton, Canada, July 23-28, 2006.

The Investigation of Swollen Process in Gelatin Gel by Using Positron Annihilation Spectroscopy, *Y. Akiyama, Y. Shibahara, S. Takeda, Y. Izumi, S. Nishijima, Y. Honda, 14th International Conference on Positron Annihilation, Hamilton, Canada, July 23-28, 2006.

Study on Polymer Electrolyte Membrane by using Positron Annihilation Spectroscopy, *Y. Honda, Y. Shibahara, Y. Akiyama, N. Kimura, G. Isoyama, S. Tagawa, S. Takeda, Y. Izumi, S. Nishijima, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006.

Tightness of Hydrogen Bonding in Polymers Studied by Positron Annihilation Lifetime Spectroscopy, *N. Kimura, Y. Honda, G. Isoyama, S. Tagawa, SANKEN International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006.

Structure Analysys of Polymer Electrolyte Membrane for Fuel Cell Using Positron Annihilation Spectroscopy, *Y. Akiyama, Y. Shibahara, N. Kimura, S. Tagawa, S. Takeda, Y. Izumi, Y. Honda, S. Nishijima, 5th 21th Century COE “Towards Creating

New Industries Based on Inter-Nanoscience" Internal Symposium, Awaji, Japan, December 8-9, 2006.

Preparation of Polymer Nanogel Using Quantum-ray and Its Swelling-Shrinking Process, *H. Miyauchi, Y. Akiyama, Y. Shibahara, S. Takeda, Y. Izumi, Y. Honda, S. Nishijima, 5th 21th Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Internal Symposium, Awaji, Japan, December 8-9, 2006.

Study of Structural Analysis of Macrocyclic Polyethers Using Positron Annihilation Measurements, *Y. Shibahara, Y. Akiyama, S. Takeda, Y. Izumi, Y. Honda, S. Nishijima, 5th 21th Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Internal Symposium, Awaji, Japan, December 8-9, 2006.

Nano-structural Analysis of Biopolymer Gels Using Positron Annihilation Lifetime Spectroscopy, *Y. Honda, Y. Akiyama, Y. Shibahara, N. Kimura, S. Tagawa, S. Takeda, Y. Izumi, S. Nishijima, 5th 21th Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Internal Symposium, Awaji, Japan, December 8-9, 2006.

Publications in Domestic Meetings

Linear Accelerator Meeting	1 paper
Meeting of Atomic Energy Society of Japan	1 paper

Department of Beam Science for Nanotechnology

Professor: Seiichi TAGAWA
Associate Professor: Takahiro KOZAWA

Outline

The targets of the present department are the establishment of initiatives of quantum beams for nanoscience and nanotechnology. Quantum beams mean both beams such as photons and beams inducing interactions with materials in the nanoscopic level of quantum mechanics. The beams potentially have applicability for imaging with ultra fine patterns, and the present department aims to use the fine patterns as the probes for nano-structured material sciences and devices.

Current Research Projects

Reaction Mechanisms in Polymeric Materials for Micro- and Nano-electronics
Chemically amplified resist system is one of the most practical candidates in the future technology in semiconductor fabrication. Reaction mechanisms in the system are analyzed upon exposure to electron beams, X-rays, and laser beams to design a new lithography technique in the present program.

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.

Nanosize distributions of Polymer Matrices and Acid Generators in Resist Films
The feature sizes in micro-fabrication have shrunken with the progresses in lithography technology. The decrease in deviation of resist pattern has been also needed to molecular size. Thus, distribution of photo-acid generator (PAG) and orientation of polymer matrix have been important issues. X-ray reflectivity measurements were carried out to understand PAG distribution and polymer orientation from the resist film density map in-depth.

Publications

Original Papers
Pulse Radiolysis of Polystyrene in Cyclohexane – Effect of Carbon Tetrachloride on Kinetic Dynamics of Dimer Radical Cation−, K. Okamoto, T. Kozawa, M. Miki, Y. Yoshida and S. Tagawa: Chem. Phys. Lett., 426 (2006) 306-10.

Resolution Blur of Latent Acid Image and Acid Generation Efficiency of Chemically Amplified Resists for Electron Beam Lithography, T. Kozawa and S. Tagawa: J. Appl.

Phys., 99 (2006) 054509-.

Effects of Low Energy Electrons on Pattern Formation in Chemically Amplified Resist, T. Kozawa, H. Yamamoto, A. Saeki and S. Tagawa: J. Photopolym. Sci .Technol., 19 (2006) 361-6.

Reaction Mechanism of Fluorinated Chemichally Amplified Resists, H. Yamamoto, T. Kozawa, K. Okamoto, A. Saeki, S. Tagawa, T. Ando, M. Sato and H. Komano: J. Vac. Sci. Technol. B, 24 (2006) 1833-6.

Acid Generation Efficiency in a Model System of Chemically Amplified Extreme Ultraviolet Resist, T. Kozawa, S. Tagawa, H. Oizumi and I. Nishiyama: J. Vac. Sci. Technol. B, 24 (2006) L27-L30.

Analysis of Acid Yield Generated in Chemically Amplified Electron Beam Resist, T. Kozawa, T. Shigaki, K. Okamoto, A. Saeki, S. Tagawa, T. Kai and T. Shimokawa: J. Vac. Sci. Technol. B, 24 (2006) 3055-60.

Correlation between Proton Dynamics and Line Edge Roughness in Chemically Amplified Resist for Post-optical Lithography, A. Saeki, T. Kozawa, S. Tagawa and H. B. Cao: Vac. Sci. Technol. B, 24 (2006) 3066-72.

Reactivity of Acid Generators for Chemically Amplified Resists with Low-Energy Electrons, A. Nakano, T. Kozawa, S. Tagawa, T. Szreder, J. F. Wishart, T. Kai and T. Shimokawa: Jpn. J. Appl. Phys., 45 (2006) L197-L200.

Acid Generation Mechanism of Poly(4-hydroxystyrene)-Based Chemically Amplified Resists for Post-Optical Lithography: Acid Yield and Deprotonation Behavior of Poly(4-hydroxystyrene) and Poly(4-methoxystyrene), A. Nakano, T. Kozawa, K. Okamoto, S. Tagawa, T. Kai and T. Shimokawa: Jpn. J. Appl. Phys., 45 (2006) 6866-71.

Protonation Sites in chemically Amplified Resists for Electron-Beam Lithography, K. Natsuda, T. Kozawa, K. Okamoto and S. Tagawa: Jpn. J. Appl. Phys., 45 (2006) L1256-L1258.

Relationship between Acid Generator Concentration and Acid Yield in Chemically Amplified Electron Beam Resist, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto, S. Tagawa, T. Kai and T. Shimokawa, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto, S. Tagawa, T. Kai and T. Shimokawa: Jpn. J. Appl. Phys., 45 (2006) 5735-7.

Dependence of Acid Yield on Resist Thickness in Chemically Amplified Electron Beam Resist, T. Shigaki, K. Okamoto, T. Kozama, H. Yamamoto and S. Tagawa: Jpn. J. Appl. Phys., 45 (2006) 5445-9.

Correlation between Width Roughness of Nanowires and Backbone Conformation of Polymer Materials, S. Seki, S. Tsukuda, S. Tagawa, and M. Sugimoto:

Macromolecules7446-7450, 39, 2006.

Line edge roughness of a latent image in post-optical lithography, A. Saeki, T. Kozawa, S. Tagawa and H. B. Cao: Nanotechnology, 17 (2006) 1543-6.

Picosecond Pulse Radiolysis Using Femtosecond White Light with a High S/N Spectrum Acquisition System in One Beam Shot, A. Saeki, T. Kozawa and S. Tagawa: Nucl. Instrum. Meth. A, 556 (2006) 391-6.

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 (2006) 52-6.

Pulse Radiolysis Based on a Femtosecond Electron Beam and a Femtosecond Laser Light with Double-pulse Injection Technique, J. Yang, T. Kondoh, T. Kozawa, Y. Yoshida and S. Tagawa: Radiat. Phys. Chem., 75 (2006) 1034-40.

International Conferences

Analysis of Acid Yield Generated in Chemically Amplified Electron Beam Resist, *T. Kozawa, T. Shigaki, K. Okamoto, A. Saeki, S. Tagawa, T. Kai, T. Shimokawa, Baltimore, 50thEIPBN (Oral), New York, USA, May30-Jun2, 2006.

Line Edge Roughness in Chemically Amplified Resist of Electron Beam Lithography, *A. Saeki, T. Kozawa, S. Tagawa, H. B. Cao, 50thEIPBN, New York, USA, May5-Jun2, 2006.

Formation of Aggregated Radical Cations of Benzene and Polystyrene in Condense Phases, *K. Okamoto, S. Seki, T. Kozawa, Y. Yoshida, S. Tagawa, Gorden Research Conference (Radiation Chemistry), Colby College, ME, USA, Jul2-8, 2006.

Pico/subpicosecond Pulse Radiolysis and Research on Nanolithography by EB/EUV, *A. Saeki, T. Kozawa, S. Tagawa, Gorden Research Conference (Radiation Chemistry), Colby College, ME, USA, Jul2-8, 2006.

Polymer Structure Dependence of Acid Generation in Chemically Amplified EUV Resists, *H. Yamamoto, T. Kozawa, S. Tagawa, H. B. Cao, H. Deng, M. J. Leeson, Barcelona, EUVL Symposium, Barcelona, Spain, Oct 16-20, 2006.

Acid Generation in Chemically Amplified EUV Resists, *T. Kozawa, S. Tagawa, H. Oizumi, I. Nishiyama, EUVL Symposium, Barcelona, Spain, Oct 16-20, 2006.

Exposure Dose Dependence on LER of Latent Image in EB/EUV Lithographies Studied by Monte Carlo Technique, *H. Yamamoto, T. Kozawa, S. Tagawa, H. B. Cao, Hai Deng, M. J. Leeson, EUVL Symposium, Barcelona, Spain, Oct 16-20, 2006.

Critical Issues of EUV Resists and New Research Approach, *S. Tagawa, T. Kozawa, A.

Saeki, EUVL Symposium, Barcelona, Spain, Oct 16-20, 2006.

Effect of Acid Diffusion and Polymer Structure on Line Edge Roughness, *H. Yamamoto, T. Kozawa, A. Saeki, K. Okamoto, S. Tagawa, K. Ohmori, M. Sato, H. Komano, Microprocess and Nanotechnology Conference, Kamakura, Japan, Oct25-27, 2006.

Proton Dynamics and Amines in Chemically Amplified Resist, *K. Natsuda, T. Kozawa, K. Okamoto, S. Tagawa, Microprocess and Nanotechnology Conference, Kamakura, Japan, Oct25-27, 2006.

Single-Component Chemically Amplified Resist Based on Dehalogenation of Polymer, SPIE, *H. Yamamoto, T. Kozawa, S. Tagawa, K. Ohmori, M. Sato, Hiroji Komano, SPIE, San Jose, CA, USA, Feb25-Mar2, 2007.

Contributions to International Conferences and Journals

T. Kozawa	20 th Microprocess and Nanolithograph Conference	(Program Committee)

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	5 papers
Chemical Society of Japan	1 paper
Atomic Energy Society of Japan	2 papers
The Japan Society of Applied Physics:	2 papers

Sponsorships

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

S. Tagawa	Femtosecond Pulse Radiolysis Study on Nano Spatial-temporal Reactions	¥23,900,000

Grant-in-Aid for Scientific Research, Encouragement of Young Scientist (B)(2)

T. Kozawa	Creation of Ultimate Nano Process by Femtosecond Pulse Radiolysis	¥1,100,000

Entrusted Research

S. Tagawa	Japan Nuclear Energy Safety Organization	Development of Color Film Dosimeter Based on Advanced Radiation Chemistry	¥11,765,000
S. Tagawa	Advanced Semiconductor Engineering and Technology	Reaction Mechanism in Chemically Amplified Resist Materials	¥999,000
S. Tagawa	Semiconductor	Study on EUV Resists	¥1,680,000

S. Tagawa	Leading Edge Technology Inc. Intel	Nanoscale Distribution of Acids Generated in Chemically Amplified EUV Resists	¥12,000,000

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: Ulrich HOFER (2006.4.10-2006.5.30)

Outline

Ultrafast non-linear spectroscopy and two-photon photoemission spectroscopy have been applied to elucidate dynamical relaxation processes on surfaces. Laser-induced diffusion, desorption and reactions of atoms and molecules on surfaces have been studied in temporal domains of a few tens of femtosecond.

Achievements

- Ultrafast carrier dynamics in Si(111)-(7x7) dangling bonds probed by time-resolved second-harmonic generation and two-photon photoemission
- Dissociative adsorption of molecular hydrogen on silicon surfaces
- Laser-induced diffusion on oxygen on metal surfaces

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: Xue-Long HOU (2006.7.26-2006.8.25)

Outline

Highly efficient and selective synthesis of desired organic compounds is very important from the viewpoint of decrease in risk on environment and conservation of natural resources. We examined the development of new synthetic reactions utilizing characteristic reactivities of metal catalysts and organic reagents.

Achievement

The addition of benzyltrimethylsilane to imines triggered by fluoride anion gave rise to the corresponding α-benzylated amines in good yields. Moderate to high to diastereoselectivity was obtained in the reactions of *N*-sulfinyl imines. Direct addition of a variety of alkynes to *N*-sulfinyl aldimines in the presence of a suitable base provided the corresponding *N*-sulfinylpropargylamines in high yields with high diastereoselectivity. Combination of cupper salt and chiral P,N-ferrocene ligand effectively catalyzed 1,3-dipolar cycloaddition of nitroalkenes to an imino ester derived from glycine to give *endo*- or *exo*-pyrrolidine derivatives in good yield with high enantioselectivity.

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: James M. HOWE (2006.8.29-2006.9.29)

Outline

Some physical properties of material originated from the atomic bonding nature are closely related to the plasmon-loss spectrum. The aim of this research was to investigate a methodology to relate the mechanical property (like plasticity) of metallic glass and the plasmon-loss spectrum in electron-energy-loss spectroscopy (EELS).

Achievement

The plasticity of material is proportional to the ratio of modulus of rigidity and bulk modulus, and the latter can be obtained from the plasmon-loss. EELS plasmon-loss spectra of several metallic glasses were taken using an energy-filtered transmission electron microscope in ISIR, Osaka University. Detailed discussions were made on the relation between the plasticity of the metallic glasses and their plasmon-loss spectra.

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: Jacqueline BOURDEAU (2007.1.4-2007.3.31)

Outline

Research on organization of instructional design and Instructional theories has been conducted using ontology engineering. Firstly, survey of both theories has been done to build ontological taxonomies of both kinds of theories. Then, each theory has been described in terms of properties extracted for explanation generation about generated scenarios. All the results have been incorporated into a theory-aware authoring tool: SMARTIES under construction.

Achievements

- Release of OMNIBUS: Ontology of learning, instructional and instructional design theories
- Development of instructional design and instructional theories
- Refinement of explanation generation function of SMARTIES

International Conferences

Ontological Support for a Theory-Eclectic Approach to Instructional and Learning Design (Oral)(Plenary), *Y. Hayashi, J. Bourdeau and R. Mizoguchi, First European Conference on Technology Enhanced Learning, EC-TEL2006, Crete, Greece, Oct. 1-4, 2006.

Ontological Modeling Approach to Blending Theories for Instructional and Learning Design (Oral)(Plenary), *Y. Hayashi, J. Bourdeau and R. Mizoguchi. The 14th International Conference on Computers in Education (ICCE2006), Beijing, China, Nov.30-Dec. 4, 2006. (Best Paper Award)

Division of Nanoscience and Nanotechnology for Industrial Applications

Outline

This division involves five laboratories, i.e., Department of Nanomaterials and Environmentally Conscious Technology, Department of Computational Nanomaterials Design, Department of Nano-Bio-Intelligent Systems Science, Department of Propatent Strategy for Nanotechnology (Domestic visiting researcher), Department of Nanotechnology Transfer (Foreign visiting researcher). All of these laboratories have the same direction to make contribution to society and industries through their own nanotechnology. Through the activity of these laboratories in the first year, establishments are listed as follows.

Achievements

Suganuma Lab.

- Basic design and science of high temperature lead-free soldering
- R&D of low temperature lead-free soldering and improvement of oxidation resistance
- Development of Printed Electronics technology with nano particles paste
- Basic design of high reliability conductive adhesives and evaluation methods
- HREM observation and simulation of BCN fullerene materials
- Synthesis and characterization of calcium phosphate-AMP composite material

Mizoguchi Lab.

- Development of a framework for integrated knowledge of functioning-manufacturing process for nano-materials based on ontology engineering
- Development of a design supporting system for nano-materials based on a framework for integrated knowledge of functioning-manufacturing process
- Structuring of knowledge for material design of nanoparticles/films and storing to a computer system
- An evaluation experiment on conceptual design of material using the design support system with the collaboration of domain experts
- Development of contents management system based on nanotechnology ontology

Katayama-Yoshida Lab.

- Development of materials design engine and materials design for semiconductor spintronics
- Development of pseudopotential electronic-structure calculation codes “Osaka2002_nano”
- Material design for superconductivity of icosahedron-based boron
- Mechanism of fast diffusion of Cu impurity in Si
- Material design for Cu gettering in crystal Si
- Microscopic roles of hydrogen in crystal Si

Department of Nanomaterials and Environmentally Conscious Technology

Professor:	Katsuaki SUGANUMA
Associate Professor:	Takeo OKU
Research Associates:	Syunro YAMAGUCHI, Masahiro INOUE
Post Doctoral Fellow:	Junxiang JIANG, Dosop KIM, Yasunori TADA, Sun-sikKIM, Jinting JIU.
Graduate Students:	Jae-Ean LEE , Motoki KANENO, Toshiko NAKAGAWA, Kimihiro YAMANAKA, Seiji KUMAMOTO, Gorou IZUTA, Mitsuru KAWAZOME, Seiji KOMAMOTO, Syun SAITO Naruhiro KOI, Daisuke WAKUDA, Yuhi YORIKADO,
Support Staff:	Mariko HATAMURA, Hiroo HIGUCHI, Noriko KAGAMI, Kozue IDE, Misa MATSUSHITA.

Outline

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 Projects

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 phospate 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

Synthesis of Co Nanocapsules Coated with BN Layers by Annealing of KBH_4 and $[Co(NH_3)_6]Cl_3$,I. Narita, T. Oku, H. Tokoro and K. Suganuma, Solid State Comm., **137**(2006), 44-48.

Simultaneous Measurements of Conductivity and Magnetism by Using Microprobes and Electron holography, Y. Murakami, N. Kawamoto, D. Shindo, I. Ishikawa, S. Deguchi, K. Yamazaki, M. Inoue, Y. Kondo and K. Suganuma, Appl. Phys. Lett. 88, 223103 (2006).

Effect of Curing Conditions on the Electrical Properties of Isotropic Conductive Adhesives Composed of an Epoxy-Based Binder, M. Inoue and K. Suganuma, Soldering & Surface Mount Technology, **18**[2](2006), 40-45.

Synthesis and Structures of Iron Nanoparticles Coated with Boron Nitride Nanomaterials, I. Narita, T. Oku, H. Tokoro and K. Suganuma, J. Electron Microscopy 55[3] (2006), 123–127.

New Glass Sealing Method with Lead-free Solders, K. Sakaguchi, S. Domi, and K. Suganuma Advances in Science and Technology, 45 (2006), 1604-1607.

Synthesis and Characterization of Calcium Phosphate-AMP Layered Materials, M. Kaneno, K. Sakamoto, S. Yamaguchi and K. Suganuma, Key Engineering Materials, 317-318(2006), 769-772.

Formation of Hydroxyapatite from Mechnochemically Treated b-Tricalcium Bis(orthophosphate), M. Kaneno, K. Sakamoto, S. Yamaguchi and K. Suganuma, Key Engineering Materials, 317-318(2006), 781-784.

Development of an Electrophoretic Sol-Gel Coating Process for Porous Metals M. Inoue, S.-K. Hyun, K. Suganuma, H. Nakajima, Mater. Trans., 47 [9], (2006) 2161-2166.

Formation of Ceramic Coatings on Porous Metals by Electrophoretic Sol-Gel Deposition, M. Inoue, S.-K. Hyun, K. Suganuma, H. Nakajima, Porous Metals and Metal Foaming Technology (Proc. of MetFoam 2005, Japan Inst. Metals), ed. by H. Nakajima and N. Kanetake, 655-658 (2006)

Influential Factor in Determining the Thermal Conductivity of Isotropic Conductive Adhesives, M. Inoue, H. Muta, T.Maekawa, S.Yamanaka and K. Suganuma, Proc. EcoDesign 2006 Asia-Pacific Conference, pp.87-92 (2006).

Role of Acidic Amino Acid for Regulating Hydroxyapatite Crystal Growth, T. Matsumoto, M. Okazaki, M. Inoue, J. Sasaki, Y. Hamada and J. Takahashi, Dental Materials Journal, **25** [2] (2006) 360-364.

Synthesis and Structures of Iron Nanoparticles Coated with Boron Nitride Nanomaterials, I. Narita, T. Oku, H. Tokoro and K. Suganuma, J. Electron Microsc. 55 (2006) 123 - 127.

Atomic Structures of Bamboo-Type Boron Nitride Nanotubes with Cup-Stacked Structures, T. Oku, I. Narita and A. Nishiwaki, J. Euro. Ceram. Soc. 26 (2006) 443-448.

Atomic Structures and Formation Mechanism of Boron Nitride Nanotubes and Nanohorns Synthesized by Arc-melting LaB_6 Powders, A. Nishiwaki and T. Oku, J. Euro. Ceram. Soc. 26 (2006) 435-441.

Epitaxial Growth of Cu Nanodot Arrays Using an AAO Template on a Si Substrate, T. Shimizu, M. Nagayanagi, T. Ishida, O. Sakata, T. Oku, H. Sakaue, T. Takahagi and S. Shingubara, Electrochem. Solid-State Lett. 9 (2006) J13-16.

Synthesis and Magnetic Property of Boron Nitride Nanocapsules Encaging Iron and Cobalt Nanoparticles, T. Oku, I. Narita and H. Tokoro, J. Phys. Chem. Solids 67 (2006)

1152-1156.

Fabrication of Hollow and Sandwiched Structure Ag Nanoclusters by High-Dose Iron Implantation, F. Ren, C. Jiang, C. Liu, J. Wang and T. Oku, Phys. Rev. Lett. 97 (2006) 165501-1-4.

Review Papers

Electronic packaging technology using Pb-free solders and electrically conductive adhesives, K. Suganuma, Clean Technology, 16 [3] (2006) 38-4

Current Status and Problems in Joining Technology of Ceramics, K. Suganuma Ceramics, 41 [6] (2006), 416-423

Thermal Stress in Ceramic/Metal Joints, K. Suganuma, Ceramics, 41[6](2006), 434-439.

Development of Super-flexible Tactile Sensor~Development of Soft Skin for Robots~, M.Inoue, K. Suganuma, T. Miyashita, H. Ishiguro, *Kensa-gijutu*,11[10](2006),44-48.

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Contributions to International Conferences and Journals

K.Suganuma	TMS Anunual 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	CIMTEC2006, International Board member
K.Suganuma	Plastic Electronics, Scientific Advisory Board

Publications in Domestic Meetings

Japan Institute of Electronics Packaging	8 papers
Japan Institute of Metals	1 papers
Others	4 papers

Academic Degrees

Doctor Degree for Engineering

J.-E. Lee	Development and reliability analysis of high- and low-temperature lead-free solders
K. Yamanaka	A Study on Solder Electromigration in Cu/Sn-3Ag-0.5Cu/Cu and Cu/In/Cu Flip-chip Joint Systems

Master Degree for Engineering

Y. Yorikado	Study on Generation Mechanism and Suppression Scheme of Sn Whiskers
D. Wakuda	Room Temperature Sintering of Ag Nanoparticle Paste for Fine Electronic Circuit Patterns

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas
Propulsive person in charge of 21th century COE program

K. Suganuma	Development of environmentally conscious fine structural materials using nanostructural control techniques of bi-material interfaces.	¥3,000,000
M.Inoue	Nanostructural control of inter-filler interfaces in super-flexible conductive adhesives	¥900,000

Entrusted Research

K. Suganuma	NEDO	Development of alternative technologyfor high-temperature soldering	¥243,575.000
K. Suganuma	Business innovation Center Osaka	Development of super-flexible tactile sensor systems	¥5,602,000
K. Suganuma	JEITA	Development of prevention techniques for improving the reliability of electronics	¥5,250,000

		packaging systems	
K. Suganuma	i support		¥1,894,000
		Bringing-up program of person of talent for enhancing competitiveness for digital information electronics industry	
K. Suganuma	NEC Co., Ltd.		¥1,050,000
		Interconnection techniques using electrically conductive adhesive	
K.Suganuma	Osaka TLO	Development of electronics information medias using low-temperature sinterable metal nanoparticles	¥25,700,000
K.Suganuma	Research and Development Association for Future Electron Devices	Development of hybrid Ag nano-pastes applicable for SiC device packaging	¥21,000,000

K. Suganuma	BandoChemical Industries, Ltd.	¥500,000
K. Suganuma	Okuno Chemical Industries Co., Ltd.	¥2,000,000
K. Suganuma	Uemura Co., Ltd	￥1,000,000
K. Suganuma	MEC Co., Ltd,	¥500,000
K. Suganuma	Tokuyama Co., Ltd.	¥1,500,000

Department of Computational Nanomaterials Design

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Outline

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 Projects

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 with generalized-gradient approximation and relativistic effects. For molecular dynamic simulation, the force inversion method has been implemented in order to obtain the saddle points of reactions. This method is particularly suitable for simulation of diffusion. Parallel techniques for computation are also implemented partly.

Material Design for Superconductivity of Icosahedron-based Boron

Growing interests are addressed to solid boron and its compounds because of its

superconducting transition at high pressures. Among the variety of polymorphs of boron, α-boron is particularly interesting, because of its high potentiality of superconductivity. A problem of α-boron is difficulty in obtaining good-quality crystals. We have theoretically created the phase diagram for boron, which was previously not available in experiment. Based on this phase diagram, we find a promising path for synthesizing α-boron with good quality.

Simulation of IR excitations for controlling impurities

Recently, in order to achieve selective diffusion of impurity atoms in silicon, use of excitations of the local vibration mode of impurities attracts much attention in the industrial researches. IR laser is such a means to excite local vibration modes. In this study, effectiveness of this method is examined by first-principles MD simulation. This type of MD simulation itself is quite new, and there are various technical problems. On solving such technical problems by some means, we are now applying this simulation technique to real problems of impurity diffusion.

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 variety of impurities and their complexes. Based on these calculations, it is found that a BO complex has an outstanding efficiency for the Cu gettering.

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. However, it is found that the bond Si-H-Si is significantly bending at finite temperatures. We proposed a way of detecting this configuration, based on our first-principles MD simulation.

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. Generally speaking, dilute magnetic semiconductors (DMS) have solubility gap and in thermal equilibrium condition phase separation occurs resulting in spinodal decomposition. We have developed our materials design including

such inhomogeneous impurity distribution. For this purpose, we investigate super-paramagnetic blocking phenomena in DMS systems. The electronic structure of DMS is calculated from first-principles by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. Then, chemical pair interactions between magnetic impurities in the effective CPA medium are estimated by using the generalized perturbation method proposed by Ducastelle et al. Magnetic exchange interactions are calculated by the Liechtenstein's method. The spinodal decomposition of DMS is simulated by the Monte Carlo method. Curie temperatures (T_C) of simulated spinodal decomposition phases are calculated by the random phase approximation. It is shown that for low concentrations, the system is super-paramagnetic (T_C =0) because small isolated clusters are formed in DMS due to the decomposition. However, the Monte Carlo simulation (Dimitorov et al., Phys. Rev. B 54 (1996) 9237) for the magnetization process of the decomposition phases indicates that super-paramagnetic blocking temperature could be higher because the activation energy to flip the magnetization becomes larger for the decomposition phases. We can understand the ferromagnetic behavior of wide gap DMS at high temperature based on this simulation results.

We have already implemented the pseudo-SIC (self-interaction correction) method proposed by Filippetti et al. into the MACHIKANEYAMA2002 KKR-CPA-LDA package in order to treat strongly-correlated materials. We applied the method to the materials design of oxide-based DMS, such as MgO-, CaO-, BaO- and SrO-based DMS. Surprisingly, it is suggested that the ferromagnetism is induced by introducing C impurities at O sites in these oxides. Experimental demonstration is needed to confirm the ferromagnetism without magnetic elements suggested in the present calculations. ZnO-based DMS is also investigated by using the pseudo-SIC method. The experimental photoemission spectra of (Zn, V)O, (Zn, Mn)O and (Zn, Co)O are well reproduced by the present method.

We have also studied $CuAlO_2$-based dilute magnetic semiconductors. In order to calculate Curie temperatures of this system as accurate as possible, firstly, we calculate effective exchange interactions between magnetic impurities in $CuAlO_2$-based DMS from first-principles. 3d transition metal I impurities are considered as possible magnetic elements. The calculations show that TM impurities induce impurity bands in the gap and the ferromagnetic state is stabilized by the double exchange mechanism in Mn-, Fe-, Co- and Ni-doped cases. As a nature of double exchange mechanism, the calculated exchange interaction is short-ranged and the Monte Carlo calculation of T_C reveals that the expected T_C is lower than room-temperature.

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Nano-Scale Spinodal Decomposition Phase in ZnO-based Dilute Magnetic Semiconductors (Oral), *M. Toyoda, K. Sato, H. Katayama-Yoshida, Conference on "Computational Magnetism and Spintronics" CompMag 2006, Forschungszentrum Jülich, Germany, Oct. 2-4, 2006.

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Theory, New Materials Design and Nano-Process Design of Ferromagnetic Semiconductors, *H. Katayama-Yoshida, K. Sato, T. Fukushima, M. Toyoda, H. Kizaki, V. A. Dinh and P. H. Dederichs, Conference on "Computational Magnetism and Spintronics" CompMag 2006, Forschungszentrum Jülich, Germany, Oct. 2-4, 2006.

Pseudo-SIC and Monte Carlo Study of the Frromagnetism in C (N)-doped Alkaline Earth Metal Oxides, *V. A. Dinh, M. Toyoda, K. Sato and H. Katayama-Yoshida, Conference on "Computational Magnetism and Spintronics" CompMag 2006, Forschungszentrum Jülich, Germany, Oct. 2-4, 2006.

Nano-Scale Spinodal Decomposition Phase in ZnO-based Dilute Magnetic Semiconductors (Oral), *M. Toyoda, K. Sato and H. Katayama-Yoshida, The 4th International Workshop on ZnO and Related Materials, Univ. of Giessen, Germany, Oct. 3-6, 2006.

Ab Initio Materials Design for TCO-based New Functional Materials (Invited), H. Katayama-Yoshida, *K. Sato, H. Kizaki, H. Funashima, I. Hamada, T. Fukushima and M. Toyoda, 1st International Symposium on Transparent Conducting Oxides, Crete, Greece, Oct. 23-25, 2006.

Electronic Structures of Dilute Magnetic Semiconductors from LDA+SIC Calculations (Oral), *M. Toyoda, H. Akai, K. Sato, H. Katayama-Yoshida, KKR-Workshop: new developments, applications and collaborations, University of Bristol, Bristol UK, Oct. 20-22, 2006.

Computational Nano-Materials Design for Semiconductor Nano-Spintronics (Invited), *H. Katayama-Yoshida, Handai Nanoscience and Nanotechnology International Symposium 2006 (From Observation of Atoms/Molecules, via Measurement, to Assembly of NanoStructures), Osaka, Japan, Nov. 20-22, 2006.

Materials Design of $CuAlO_2$ based Dilute Magnetic Semiconductors for Semiconductor Spintronics, *H. Kizaki, K. Sato and H. Katayama-Yoshida, Handai Nanoscience and Nanotechnology International Symposium 2006 (From Observation of Atoms/Molecules, via Measurement, to Assembly of NanoStructures), Osaka, Japan, Nov. 20-22, 2006.

LDA+SIC Calculations for ZnO-based Dilute Magnetic Semiconductors, *M. Toyoda, H. Akai, K. Sato, H. Katayama-Yoshida, Handai Nanoscience and Nanotechnology International Symposium 2006 (From Observation of Atoms/Molecules, via Measurement, to Assembly of NanoStructures), Osaka, Japan, Nov. 20-22, 2006.

Ab Initio Design of Fabrication Process and Shape Control of Self-Organized Tera-Bit-Density Nano-Magnets in Dilute Magnetic Semiconductors by Two-Dimensional Spinodal Decomposition, *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, Handai Nanoscience and Nanotechnology International Symposium 2006 (From Observation of Atoms/Molecules, via Measurement, to Assembly of NanoStructures), Osaka, Japan, Nov. 20-22, 2006.

Theoretical Approach to Nanoscale Control of Impurity Diffusion in Silicon: Material Dynamics Design, *K. Shirai, K. Matsukawa and H. Katayama-Yoshida, Handai Nanoscience and Nanotechnology International Symposium 2006 (From Observation of Atoms/Molecules, via Measurement, to Assembly of NanoStructures), Osaka, Japan, Nov. 20-22, 2006.

Ferromagnetism in Oxide-based DMS without Transition Metal Impurities, *V. A. Dinh, K. Sato and H. Katayama-Yoshida, Handai Nanoscience and Nanotechnology International Symposium 2006 (From Observation of Atoms/Molecules, via Measurement, to Assembly of NanoStructures), Osaka, Japan, Nov. 20-22, 2006.

Spinodal Decomposition and Super-Paramagnetism in Dilute Magnetic Nitride Semiconductors (Invited), *K. Sato, T. Fukushima and H. Katayama-Yoshida, 2006 MRS Fall Meeting, Hynes Convention Center & Sheraton Boston Hotel, Boston, USA, Nov. 27-Dec. 1, 2006.

Materials Design of Ferromagnetic Diamond (Oral), *H. Katayama-Yoshida, K. Kenmochi, K. Sato and A. Yanase, 2006 MRS Fall Meeting, Hynes Convention Center & Sheraton Boston Hotel, Boston, USA, Nov. 27-Dec. 1, 2006.

Nano-scale Spinodal Decomposition Phase in ZnO-based Dilute Magnetic Semiconductors (Oral), *M. Toyoda, K. Sato and H. Katayama-Yoshida, 2006 MRS

Fall Meeting, Hynes Convention Center & Sheraton Boston Hotel, Boston, USA, Nov. 27-Dec. 1, 2006.

Ab Initio Design of Fabrication Process and Shape Control of Self-organized Tera-Bit-Density Nano-Magnets in Dilute Magnetic Semiconductors by Two-Dimensional Spinodal Decomposition (Oral), *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, 2006 MRS Fall Meeting, Hynes Convention Center & Sheraton Boston Hotel, Boston, USA, Nov. 27-Dec. 1, 2006.

Spinodal Decomposition and Super-Paramagnetism in Dilute Magnetic Semiconductors (Oral), *K. Sato, T. Fukushima and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Vacancy-Induced Magnetism in HfO_2, *V. A. Dinh, M. Toyoda, K. Sato and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Valence Control of α-Rhombohedral Boron by Electronic Doping, *H. Dekura, K. Shirai and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Local Environment Effects on Exchange Interactions and Curie Temperatures of Dilute Magnetic Semiconductors, *K. Sato, P. H. Dederichs and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

First-Principles Design of Self-Organized Tera-Bit-Density Nano-Magnets in Dilute Magnetic Semiconductors by Spinodal Decomposition, *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Control of Impurity Diffusion on Silicon by IR Laser Excitation, *K. Shirai, H. Yamaguchi and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Materials Design of $CuAlO_2$ Based Dilute Magnetic Semiconductors for Semiconductor Spintronics, *H. Kizaki, K. Sato and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Electronic Structures of Dilute Magnetic Semiconductors from LDA+SIC Calculations, *M. Toyoda, H. Akai, K. Sato and H. Katayama-Yoshida, International Conference on Quantum Simulators and Design (QSD2006), Hiroshima, Japan, Dec. 3-6, 2006.

Local Environment Effects on Exchange Interactions and Curie Temperatures in Dilute Magnetic Semiconductors, *K. Sato, P. H. Dederichs and H. Katayama-Yoshida, 5th 21st

Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Awaji, Japan, Dec. 8-9, 2006.

Computational Nano-Materials Design for Semiconductor Spintronics, *H. Katayama-Yoshida, K. Sato, T. Fukushima, H. Kizaki, M. Toyoda, V. A. Dinh, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Awaji, Japan, Dec. 8-9, 2006.

First-Principles Study of $CuAlO_2$ Based Dilute Magnetic Semiconductors, *H. Kizaki, K. Sato and H. Katayama-Yoshida, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Awaji, Japan, Dec. 8-9, 2006.

First-Principles Design of Self-Organized Tera-Bit-Density Nano-Magnets in Dilute Magnetic Semiconductors by Spinodal Decomposition, *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International symposium, Awaji, Japan, Dec. 8-9, 2007.

Inhomogeneity and its Effects on the Ferromagnetism of Dilute Magnetic Semiconductors (Invited), *K. Sato, The 2nd Indo-Japan Seminar “Novel Magnetic Materials and their Electronic Structures”, Feb. 27 – Mar. 1, 2007, Univ. of Tokyo, Tokyo, Japan

Contributions to International Conferences and Journals

H. Katayama-Yoshida	24rd International Conference on Defects in Semiconductors : ICDS24 (International Steering committee members)
H. Katayama-Yoshida	International conference on Quantum Simulators and Design (Organizing Committee)
H. Katayama-Yoshida	4th 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)
K. Shirai	16th International Symposium on Boron, Borides and Related Compounds (Organizing Committee)

Publications in Domestic Meetings

The Physical Society of Japan	11papers
The Japan Society of Applied Physics	7 papers
The Japan Society of High Pressure Science and Technology	2 papers

Academic Degrees

Doctor Degree for Engineering

K. Matsukawa	Materials design for the gettering of diffusive 3d transition elements in silicon

Doctor Degree for Science

N. Mitsuda	First principles study on the bonding states and diffusion of CN molecule in crystalline silicon

Master Degree for Engineering

K. Takeuchi	First-principles Molecular Dynamics Simulations of Al/Alq_3 Interfaces: Atomic Geometries and Electronic Properties.
A. Nagoya	First-principles Simulation of Self-Assembled Monolayers on Au.
M. Hiramatsu	First-Principle Theoretical Study of Adsorption of Hydrogen on the Rutile TiO_2(110) surface

Master Degree for Science

H. Dekura	Metalization of solid boron by impurity doping and its electronic structure
H. Minai	Ab initio study on the ferromagnetism and magnetic excitations in dilute magnetic semiconductors

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas

K. Sato	Development and application of computational nano-materials design engine	¥10,400,000

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

K. Sato	Ab initio calculation for electric transport properties by non-local CPA method	¥1,200,000

Entrusted Research

H. Katayama-Yoshida	JSPS Core-to-Core Program –Integrated Action Initiative-	Computational Nano-Materials Design	¥16,000,000

Other Research Fund

H. Katayama-Yoshida	Japan Science and Technology Corporation	Case study on advanced measurements and analysis	¥1,960,000
H. Katayama-Yoshida	Japan Atomic Energy Agency	Analysis and Materials design simulation in Grid computing	

H. Katayama-Yoshida	Institute for Materials Research, Tohoku Univ.	Materials design, fabrication and device application for transparent high-T_C ferromagnetic semiconductors spintronics
K. Shirai	SPring8	Novel-material processing by IR excitation
K. Shirai	Renesas Technology Corp.	Materials design for Cu gettering in Si
K. Shirai	U. of Tokyo, Okayama Sci. U, NIMS	Superconductivity research in icosahedron-based semiconductor boron

Department of Nano-Bio Intelligent Systems Science

Professor: Riichiro MIZOHUCHI
Research Associate: Kouji KOZAKI

Outline

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

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. In 2006, we extended the system as a web service which the users access it through the internet.

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. In 2006, we did an evaluation experiment on conceptual design of material using our system with the collaboration of domain experts.

An Environment for Ontology Development and its Use

We developed ***Hozo,*** an ontology engineering environment, which enables a user to build and use an ontology and instance models. It consists of Ontology editor, Concept factory and ontology server.

Ontology editor

It provides a friendly user interface as well as powerful functions necessary for ontology building and editing.

Concept factory

A guidance system based on AFM (Activity-First Method) has been implemented to guide ontology developers who build an ontology from technical documents.

Ontology server

A server for ontologies and models has been developed. It is based on the client-server architecture and enables human/computer agents to access them through internet.

We published the Ontology editor at the web site (http://www.hozo.jp), and we improved the Graphical User Interface of the system based on feedbacks from its users. And we developed API for ontology-based system and applied it to our content management system and creative design support system. In 2006, we developed a prototype of Model Editor which is a tool to construct instance models based on ontologies. Furthermore, in order to maintain consistency of ontologies built in a distributed manner, we have developed two functionalities to manage the dependencies between component ontologies and to help users keep and restore consistencies among them when they are changed.

Publications

Books

A Primer of Ontology Development, K. Kozaki, Y. Kitamura, M. Sasajima and R. Mizoguchi, Ohmsya, (2006)

International Conferences

Fundamental Consideration of Role Concepts for Ontology Evaluation (Oral), *K. Kozaki, E. Sunagawa, Y. Kitamura and R. Mizoguchi, Evaluation of Ontologies for the

Web (EON2006) 4th EON Workshop, Edinburgh, United Kingdom, May 22, 2006

Role Organization Model in Hozo (Oral), E. Sunagawa, K. Kozaki, Y. Kitamura, *R. Mizoguchi, EKAW 2006 - 15th International Conference on Knowledge Engineering and Knowledge Management Managing Knowledge in a World of Networks, Podebrady, Czech Republic, Oct. 2-6, 2006

Development of Contents Management System Based on Light-Weight Ontology (Oral), *K. Kozaki, Y. Kitamura and R. Mizoguchi, The 2007 IAENG International Conference on Internet Computing and Web Services, Hong Kong, March 21-23, 2007

Contributions to International Conferences and Journals

R.Mizoguchi	European Project on SEKT (Steering committee member)
R.Mizoguchi	Semantic Web Science Association (Vice-president)
R.Mizoguchi	International Artificial Intelligence in Education Society (Executive Committee member)
R.Mizoguchi	Asia-Pacific Society for Computers in Education(APSCE) (Board member)
R.Mizoguchi	The 1st Asian Semantic Web Conference (ASWC2006) (PC Chair)
R.Mizoguchi	The 14th International Conference on Computers in Education (ICCE2006) (PC Chair)
R.Mizoguchi	The 3rd European Semantic Web Conference (ESWC2006) (PC member)
R.Mizoguchi	Fifth international semantic web conference (ISWC2006) (PC member)
R.Mizoguchi	The 15th International Conference on Knowledge Engineering and Knowledge Management (EKAW2006) (PC member)
R.Mizoguchi	The 15th International World Wide Web Conference Semantic Web Track (PC member)
R.Mizoguchi	The 8th International Conference on Intelligent Tutoring Systems (ITS2006) (PC member)
R.Mizoguchi	The First European Conference on Technology Enhanced Learning (EC-TEL 2006) (PC member)
R.Mizoguchi	The 12th International Conference on Artificial Intelligence: Methodology, Systems, Applications (AIMSA 2006) (PC member)
R.Mizoguchi	2006 IEEE International Conference on Information Reuse and Integration (IEEE-IRI 06) (PC member)
R.Mizoguchi	The First International Conference on Knowledge, Information and Creativity Support Systems (KICSS 2006) (Technical Committee and International Advisory Committee)
R.Mizoguchi	IFIP AI 2006: Artificial Intelligence in Theory And Practice (PC member)

R.Mizoguchi	The Ninth Pacific Rim International Conference on Artificial Intelligence (PRICAI2006) (Workshop Chair)
R.Mizoguchi	the Sixth International Symposium on Tools and Methods of Competitive Engineering (TMCE 2006)(PC member)
R.Mizoguchi	International Workshop on Applications of Semantic Web Technologies for E-Learning (SW-EL) (PC member)
R.Mizoguchi	LORNET Conference I2LOR 2006 (PC member)
R.Mizoguchi	International Journal of Applied Ontology(Editorial board)
R.Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
R.Mizoguchi	International Journal of Artificial Intelligence in Education (Editorial board)
R.Mizoguchi	International Journal of Web Semantics (Editorial board)
R.Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	1 paper
Japan Reserch Group for Medical Ontology	2 papers
Nippon Association for Librarianship	1 paper
The Association for Natural Language Processing	1 paper

Sponsorships

Grant-in-Aid for Scientific Research on Priority Areas

R. Mizoguchi	Technical documents integration based on an artifact ontology	¥5,400,000

Grant-in-Aid for Encouragement of Young Scientists (B)

K. Kozaki	A Development of Knowledge Management System Based on Ontology and its Application for Nanotech Knowledge	¥1,500,000

Grant-in-Aid for JSPS Fellow

R. Mizoguchi	Ontological Modeling of Second Language Learning Interferences and an Experimental Computer Application	¥700,000

Entrusted Research

R. Mizoguchi	The Society of Chemical Engineers, Japan	Surveillance Study for Development of Structued Knowledge Platform for Nano-Materials and Products of Nano-particle and Nano-carbon (1) Brush up of	¥3,150,000

Basic Systems and Information Gathering about Nano-particle and Nano-carbon to expand the Contents

Department of Nanotechnology Transfer

Guest Associate Professor: Supab CHOOPUN (2006.4.–5.)

Outline

We have tried to developed new type nano-fabrication technique, so called, bottom-up nanotechnology. Which is opposite approach to 3D nano-structural fabrication comparing with conventional EB lithography and Focused Ion Beam (FIB) techniques. By controlling a position of metallic nano-particles, metal-oxide nano-rods have been formed. We have also controlled a size and density of the nano-rods and tried to create new phenomena such as localized DOS and quantum properties.

In addition, nano-scale controlled spintronics devices have been constructed by introducing magnetic ions and constructing low dimensional structures.

Achievement

We have succeeded to fabricate new type of nano-rods formation process. It is so called laser induced VLS technique with is different form conventional VLS method. It is opposite approach to 3D nano-structural fabrication comparing with top-down techniques. By controlling a position of metallic nano-particles, metal-oxide nano-rods have been formed. We have also controlled a size and density of the nano-rods and tried to create new phenomena such as localized DOS and quantum properties.

In addition, nano-scale controlled spintronics devices have been constructed by introducing magnetic ions and constructing low dimensional structures.

Department of Nanotechnology Transfer

Guest Professor: Tulsi Mukherjee (2006.5-6.)

Outline

Quantum beam can deposit its energy on nanoscale region in materials and is expected to play an important role in the future nanotechnology fields. Elucidation of quantum-beam-induced reaction in materials is important for the application of excellent properties of quantum beams to nanotechnology fields.

Achievement

Chemical reactions induced by ionizing radiation and photon, in particular, radiation chemistry of free radicals and excited molecules, were investigated. These intermediates are highly reactive and play a key role in chemical reactions. In this study, radiation-induced reactions of amines in alkanes were made clear using pulse radiolysis methods and ^{60}Co radiolysis.

Department of Nanotechnology Transfer

Guest Associate Professor: Lifeng Yan (2006.6-7.)

Outline

1) The STM-induced luminescence of a conjugated polymer poly[2-methoxy-5-(20-ethyl-hexyloxy)-p-phenylene vinylene] (MEHPPV) on metallic substrates of Ag(111), Ag, Au and Cu and ITO have been investigated in air at room temperature by using Ag or Pt–Ir tip. Molecular fluorescence of MEHPPV was observed from the polymer film on Ag(111), Ag and Au substrates, and all of them show an intensity enhancement compared to the pristine substrates. A mutual enhancement between surface plasmon and molecular fluorescence is suggested for the STM-induced luminescence of MEHPPV on these substrates.
2) The STM-induced luminescence (STML) of a conjugated polymer poly[2-methoxy-5-(20-ethyl-hexyloxy)-p-phenylene vinylene] (MEHPPV) with or without annealing on substrate of Ag(111) were investigated in air at room temperature. The surface morphologies of pure Ag(111), MEHPPV thin film on Ag(111) with or without annealing were modified by STM scans under higher positive or negative sample biases. The experimental results show that for MEHPPV film without annealing, the STML intensity increases after aggregates formation induced by STM scans. However, for annealed MEHPPV film, the negative bias scans decrease the STML intensity. The chain aggregations among MEHPPV molecules are believed to be the key factor for the behavior.

Achievements

Based on the research results, two papers had been published:

1) Mutual Enhancement between Plasmon and Molecular Fluorescence of Conjugated Polymer on Metal Substrates Induced by STM, Lifeng Yan, Hongwen Liu, Hiroshi Iwasaki: Chem. Phys. Lett., 433 **(**2007) 312-316.
2) STM-induced Light Emission of Conjugated Polymer Thin .lm in Different Chain Aggregations, Lifeng Yan, Hongwen Liu, Hiroshi Iwasaki: Physica B393 (2007) 6-10.

Department of Nanotechnology Transfer

Guest Professor: Emil Pínčik (2006.7-8.)

Outline

Semiconductor elements form the backbone of electronic devices which are indispensable for the modern society. Properties of both ultra-thin dielectric films/semiconductor interfaces and dielectric films greatly affect device characteristics and thus, studies on these physical properties are important in both basic and applied researches. For this aim, we have been developing the advanced transient charge processor. The findings obtained by the transient measurements have been analyzed in conjunction with the optical and the crystal structural information to investigate the interface properties both experimentally and theoretically.

Achievement

We have concentrated on the interface properties for ultra-thin SiO_2/Si interfaces for metal-oxide-semiconductor (MOS) structure and the hydrogenated amorphous Si (a-Si:H) thin films used for active layers in a-Si solar cells. The electrical measurements using charge deep level transient spectroscopy (Q-DLTS) method, UV-visible and infrared spectroscopy, and grazing incidence X-ray diffraction (GIXRD) measurements were executed for the observation of metastable defect states and the characterization of interfaces properties. Several ultra-thin SiO_2/c-Si and SiO_2/a-Si:H samples have been used for the measurements. Chemical oxidation by use of nitric acid aqueous solutions, followed by passivation in HCN solutions was found to be the best technique for formation of high quality interfaces of ultra-thin SiO_2/a-Si:H structures. In the case of SiO_2/c-Si structures formed by the plasma enhanced chemical vapor deposition (PECVD) using tetraethyl orthosilicate (TEOS) (or thermally formed-SiO_2/c-Si structures), followed by the low temperature annealing, interface state densities were not suppressed below 10^{12} (or 10^{11}) $eV^{-1}cm^{-2}$. We suppose that positively charged states formed in a-Si:H layers were absolutely passivated by cyanide ions.

The following international conference has been organized by us;
Fifth International Workshop in the series of the Solid State Surfaces and Interfaces (SSSI 2006) (Conference chairman).

Publications

Original Papers

Passivation of Si and a-Si:H surfaces by thin oxide and oxy-nitride layers, E. Pinčík, H. Kobayashi, J. Rusnák, M. Takahashi, R. Brunner, M. Jergel, A. Morales-Acevedo, L. Ortega and J. Kákoš: Appl. Surf. Sci., 252 (2006) 7713-7721.

On a presence of Si_mH_n clusters in a-Si:H/c-Si structures, M. Kopani, E. Pinčík, H. Kobayashi, M. Takahashi, N. Fujiwara, R. Brunner, M. Jergel and L. Ortega: Appl. Surf.

Sci., 252 (2006) 7722-7725.

International Conferences

Photoluminescence of Very Thin Oxide/a-Si:H Structures Passivated in HCN Solutions (Invited), *E. Pinčík, H. Kobayashi, M. Takahashi, M. Kučera, R. Brunner, 5th International Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

Solution of the Optical Parameters of the Thin Film Systems and Interfaces, *S. Jurečka, E. Pinčík, R. Brunner, 5th International Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

Infrared Spectroscopy of Si_mH_n Clusters in a-Si:H/c-Si Structures, *M. Kopáni, E. Pinčík, H. Kobayashi, M. Takahashi, N. Fujiwara, R. Brunner, M. Jergel, L. Ortega, M. Mikula, 5th International Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

Structural Properties of SiO_x Layer Deposited on Flexible PET Foil, *M. Mikula, E. Pinčík, 5th International Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

On Formation of Ultra-thin and Very Thin Oxide Films When Treated Semiconductor Surfaces Interact with Plasmas or Low-Energy Particle Beams or Liquid Solutions, *E. Pinčík, H. Kobayashi, M. Takahashi, J. Rusnák, R. Brunner, 5th International Workshop in the series of the Solid State Surfaces and Interfaces, Smolenice, Slovak Republic, Nov. 19-24, 2006.

Very Thin and Ultrathin Oxide/a-Si:H Structures and Polycrystalline-Si MOS type of Solar Cells, *E. Pinčík, H. Kobayashi, R. Brunner, R. Hajossy, H. Glesková, M. Takahashi, M. Mikula, International Conference SILICON 2006, Rožnov pod Radhoštěm, Czech Republic, Nov. 7-10, 2006.

On Solar Energy Demand and Si-based Solar Cell Technology, *E. Pinčík, R. Brunner, and M. Mikula, International Conference SILICON 2006, Rožnov pod Radhoštěm, Czech Republic, Nov. 7-10, 2006.

Brief Solar Photovoltaic Industry Overview with Focus to Japan Production, *E. Pinčík, R. Brunner, H. Kobayashi, M. Takahashi, M. Mikula, and J. Rusnák, International Conference Rural Development in the Knowledge Based Society, Bratislava, Slovak Republic, Oct. 16-17, 2006

Solar Photovoltaic Industry Overview and Remarks to Other Renewable Sources of Energy, *E. Pinčík, R. Brunner, J. Rusnák, International Conference Rural Development in the Knowledge Based Society, Bratislava, Slovak Republic, Oct. 16-17, 2006.

MOS Solar Cells. *E. Pinčík, R. Brunner, H. Kobayashi, M. Takahashi, International Conference Rural Development in the Knowledge Based Society, Bratislava, Slovak Republic, Oct. 16-17, 2006.

Reflectance Properties of a-Si:H Based Solar Cell Structures, *R. Brunner, E. Pinčík, H. Kobayashi, M. Takahashi, International Conference Rural Development in the Knowledge Based Society, Bratislava, Slovak Republic, Oct. 16-17, 2006.

Department of Nanotechnology Transfer

Guest Professor　　ANISHCHIK Sergey Vladimirivich（2006.8～ ）

Outline

On the next generation nano-fabrication, for further refining, Extreme Ultra Violet (EUV) light will be used. Wavelength of the EUV is 13.5nm. Because the photon energy exceeds the ionization potential of materials, many problems remain. Solving these problems, because it actualizes the next generation extremity nano- fabrication, elucidation of ultra fast phenomena in reaction process is necessary. Therefore geminate pair recombination process in the none-polar solvent is researched. Microwave field effects on the time dependence of recombination fluorescence from non-polar solution are studied.

Achievement

Study of the geminate pair creation and recombination in hydro-carbon: As a standard non-polar organic molecule sample, n-Dodecane was used. Transient optical absorption spectrum was measured by nano-second pulse radiolysis. Time profile of excited states of n-Dodecane and cation radical of n-Dodecane was measured. Time profile of optical absorption of cation radical was measured in nano-second region. As a result of these measurements, geminate recombination in n-Dodecane was very fast, in pico-second region. For measurement of geminate recombination in n-Dodecane, pico-second pulseradiolysis experiments were carried out. In pico-second pulseradiolysis, pico-second pulse laser which generated electron beam was used for analyzing light. Pulseradiolysis system which has extremely low timing jitter between analyzing light and electron beam was achieved. Geminate recombination in n-Dodecane was measured in pico-second time region.

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 nanoprocesses, 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

- Development of comprehensive analysis of amorphous structures using high-resolution electron microscopy and electron diffraction.
- A study on soft phonon mode in phase-change optical recording materials.
- Structural characterization of phase-change optical recording material using TEM with the field emission gun.
- Elucidation of fundamental processes of structural instability on semiconductor surfaces induced by low-energy electron-beam irradiation.
- Findings of surface phase transition and removal of plane fragments on graphite surface induced by femtosecond laser excitation.
- Developments of energy-resolved differential STM-Image analysis method and quantitative evaluation of charge transfer around point defects on semiconductor surfaces.
- Nano-Characterization of Surface and Interface in Spintronics Devices.
- XAFS Characterization of Atomic Arrangement of Low Temperature Grown GaN-Based Ferromagnetic Semiconductors.
- STM Characterization of 100nm MOSFET.

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 Project

Local structure and recrystallization process in amorphous Fe-Si layers

Microstructural changes of ion-beam-synthesized amorphous Fe-Si layers on thermal annealing were investigated using transmission electron microscopy. Single crystal Si(111) substrates were irradiated with 120keV Fe^{+} ions at cryogenic temperature to a fluence of $4.0\times10^{17}cm^{-2}$, followed by thermal annealing at 200–700°C. The amorphous Fe-Si layer separated into epsilon-FeSi and amorphous Fe-Si layers at 300 °C for 2 h. The remaining amorphous Fe-Si layer crystallized to polycrystalline beta-$FeSi_2$ layers at 500 °C for 2 h and the phase transformation from epsilon-FeSi to beta-$FeSi_2$ was observed with increasing annealing temperature.

Damage recovery process in Fe implanted Si

The effect of ion fluence on microstructure of recrystallized layers in Fe ion implanted Si was investigated. In the case of the high-fluence sample, the continuous polycrystalline beta-$FeSi_2$ layer was obtained on the Si substrate with a smooth interface after annealing at 800 °C for 2 h. In the low-fluence sample, a continuous amorphous layer in the as-implanted sample recrystallized into beta-$FeSi_2$ fine particles incorporated into polycrystalline Si layer by post-implantation thermal annealing. Also, a defective layer with a thickness of ~70 nm was formed between polycrystalline Si layer and Si substrate. In the high-fluence sample, such defective region was observed in the 600 °C-annealed sample but not in the 800 °C-annealed one. Bright-field images and elemental maps reveled that excess Fe atoms generated by epsilon-to-beta phase transformation migrate toward the defective region along grain boundaries within the buried beta-$FeSi_2$ layer in the high-fluence sample. By reacting with Si atoms, these Fe atoms contributed to the elimination of the defects within the recrystallized Si layer.

Publications

Original Papers

Local Atomic Ordering and Nanoscale Phase Separation in a Pd-Ni-P Bulk Metallic Glass, Y. Hirotsu, T. G. Nieh, A. Hirata, T. Ohkubo and N. Tanaka, Phys. Rev. B 73 (2006) 012205(1)-012205(4).

Local Structure Studies of Fe-Nb-B Metallic Glasses using Electron Diffraction, A. Hirata, Y. Hirotsu, T. Ohkubo, E. Matsubara and A. Makino, J. Microsc. 223 (2006) 191-194.

Structural Investigation of Ge-Sb-Sn Thin Film using Transmission Electron Microscopy, M. Naito, M. Ishimaru, Y. Hirotsu, M. Takashima and H. Matsumoto, J. Mater. Sci. 41 (2006) 2615-2616.

Formation Process of beta-$FeSi_2$/Si Heterostructure in High-Dose Fe Ion Implanted Si, M. Ishimaru, K. Omae, I.-T. Bae, M. Naito, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, J. Appl. Phys. 99 (2006) 113527(1)-113527(7).

Solid Phase Crystallization of Amorphous Fe-Si Layer Synthesized by Ion Implantation, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, Appl. Phys. Lett. 88 (2006) 251904(1)-251904(3).

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, Nucl. Instrum. Meth. B 250 (2006) 283-286.

Structural Evolution in Fe Ion Implanted Si upon Thermal Annealing, K. Omae, I.-T. Bae, M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, Nucl. Instrum. Meth. B 250 (2006) 300-302.

Low-Temperature Crystallization Caused by Ultrasound in $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ and $Pd_{40}Ni_{40}P_{20}$ Bulk Metallic Glasses, T. Ichitsubo, E. Matsubara, K. Anazawa, N. Nishiyama, M. Naito and Y. Hirotsu, Mater. Sci. Eng. A 442 (2006) 273-277.

Amorphous Structure of Ion-Beam-Synthesized Fe-Si Thin Layer, M. Naito, M. Ishimaru and Y. Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1771.

High-Dose Fe Ion Implanted Si: Ion-Beam-Induced and Annealing-Induced Microstructures, M. Ishimaru, K. Omae, I.-T. Bae, M. Naito and Y. Hirotsu, Proc. the 16th Int'l Microscopy Cong. (2006) 1856.

Books

Nanostructure Analysis of Metallic Materials (in Japanese), K. Hono and Y. Hirotsu, AGNE Gijutsu Center (2006)

Patents

Ferromagnetic Particles and Their Production Methods, Y. Hirotsu, A. Kovács and K. Sato: Tokugan 2006-220037.

International Conferences

Change of Nanostructure in $(Fe_{0.5}Co_{0.5})_{72}B_{20}Si_4Nb_4$ Metallic Glass on Annealing

(Invited), *Y. Hirotsu, A. Hirata, K. Amiya, N. Nishiyama and A. Inoue, International Conference on Processing & Manufacturing of Advanced Materials (THERMEC' 2006), Vancouver, Canada (July 4-8, 2006).

Effects of Additive Elements on Atomic Ordering and Hard Magnetic Properties of $L1_0$-Type FePt and FePd Alloy Nanoparticles (Invited), *Y. Hirotsu, K. Sato, H. W. Ryu and A. Kovács, 48th IUVSTA Workshop, Innovatial Training Course on "Influence of Trace Elements on the Nucleation and Growth of Thin Films", Budapest, Hungary (August 26-31, 2006).

Amorphous structure of ion-beam-synthesized Fe-Si thin layer (Oral), *M. Naito, M. Ishimaru, and Y. Hirotsu, The 16th International Microscopy Congress, Hokkaido (September 3-8, 2006).

Atomic Ordering and Hard Magnetic Properties of $L1_0$-Type FePtCu Nanoparticles Studied by Transmission Electron Microscopy and Electron Diffraction (Invited), *Y. Hirotsu, H. W. Ryu and K. Sato, 6th Japanese-Polish Joint Seminar on Materials Analysis -New Developments and Analysis for Fabrication of Functional Nanostructures-, Toyama (September 10-13, 2006).

Formation process of beta-$FeSi_2$ from amorphous Fe-Si, *M. Naito, A. Hirata, M. Ishimaru, Y. Hirotsu, J. A. Valdez and K. E. Sickafus, 15th International Conference on Ion Beam Modification of Materials, Taormina, Italy (September 18-22, 2006).

Local Structure Studies of Metallic Glasses using HREM and Electron Diffraction (Invited), *Y. Hirotsu, A. Hirata and T. Ohkubo, International Workshop on Bulk Metallic Glasses: Sicence & Technology, Bangalore, India (January 12-17, 2007).

Contributions to International Conferences and Journals

Y. Hirotsu	5th International Bulk Metallic Galsses Conference (Co-Chair)
Y. Hirotsu	16th International Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	The IUMRS International Conference in Asia 2006 (Session Organizer)
Y. Hirotsu	International Conference on Magnetism 2006 (Organizing Committee)
Y. Hirotsu	6th Japan-Polish Joint Seminar on Materials Analysis (Organizing Committee)

Publications in Domestic Meetings

The Japan Society of Applied Physics 1 paper

Sponsorship

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

Y. Hirotsu	In situ observation of atomistic structures in metallic liquid and metallic glass	¥8,400,000

Grant-in-Aid for Scientific Research (S)

Y. Hirotsu	Fabrication and characterization of hard magnetic alloy nanoparticles produced by vapor quenching	¥11,100,000

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

Department of Advanced Characterization for Nano-Processing

Professor: Katsumi TANIMURA
Associate Professor: Jun'ichi KANASAKI

Outlines

For fabricating highly functional nano-structured devices in future technology, it is important to establish the ways to control structures and compositions of materials in atomic levels. Electronic excitations, which induce and promote atomic processes with strongly site-sensitive rates, can be a promising method for creating nano-scaled structures possessing new properties and functions that are not achieved by conventional thermal process. Our targets are to understand completely the fundamentals of underlying physics concerning the excitation-induced atomic processes, and finally to establish advanced surface nano-processing technologies fully exploiting unique features of electronic-excitation effects. For this purpose, we have studied laser- or low-energy electron induced structural changes of semiconductor and graphite surfaces by means of the direct imaging of the surface structures using scanning tunneling microscopy (STM). Also, we have studied carrier dynamics on graphite surface by means of femtosecond reflection spectroscopy.

Current Research Project

Hydrogen Removal on Si(001)2x1:H Surface Excited by Ordinary Low-Energy Electron Beams

The inelastic interaction of low-energy electrons with surface atoms (and molecules), leading to their electronic and vibrational excitation, induces variety of atomic motions, like diffusion, bond breaking, desorption, chemical reactions etc, but its mechanism is still controversial. We have studied structural changes of Si(001)-(2x1):H surface irradiated with ordinary electron beams of energies ranging from 2.6 to 12.6 eV. Direct atomic-scale imaging by means of STM has revealed that the excitation removes hydrogen atoms at individual atomic sites, resulting in the formation of un-terminated single dangling bond (DB) on the surface. The concentration of DB sites increases initially with excitation dose, followed by saturation at the levels that depend on the beam-current density. Quantitative analyses of the results determine the Si-H bond rupture cross section to be $1.3 \times 10^{-20} cm^2$, which is constant for the energy regime studied. Also, we have demonstrated that re-termination process of DBs with hydrogen is accelerated under electron irradiation. Based on the results, we suggest that the Si-H $\sigma \rightarrow \sigma^*$ electronic transition is responsible for the bond rupture on this surface.

Bond Breaking on InP(110)1x1 Surface Induced by Hole-Injection from a STM Tip

In contrast to the case of laser excitation, the STM tip can inject either electrons or holes selectively onto the surface. This selectivity provides a strong benefit to elucidate

the relative roles of carriers in the electronic bond breaking processes. We have studied structural changes of InP(110)-(1x1) surfaces induced by carrier injection from the STM-tip. Direct imaging of hole-injected areas has shown the prominent formation of P-atomic vacancies, while no structural change is induced by electron-injection. Important finding is that monovacancies are mainly formed on p-type InP, while vacancy clusters are efficiently formed on n-type InP, similar to the case of laser excitation. The striking difference in surface-defect morphologies is successfully explained by electrostatic interaction among injected holes and monovacancies charged positively (negatively) on p-type (n-type) surfaces. The bond-breaking rate increases quadratically as tunneling current increases. These features suggest that localization of two-holes injected from the STM tip plays an important role in the tip-induced bond breaking process.

Structural Instability of Graphite Surface by Femtosecond-Laser Excitation

We have studied the structural changes of graphite surfaces excited with femtosecond laser pulses. Direct imaging by using STM has revealed that the excitation with p-polarized laser lights forms nano-scaled vacancy clusters double-layer deep, indicating the fragmentary removal of two-neighboring surface atomic layers. The femtosecond time-resolved reflection spectroscopy can detect the transient reflection peak at 2 eV, which is short-lived and formed only under p-polarized pump pulse. The peak has been theoretically predicted for the transient excitonic state generated by interlayer charge transfer excitation. The observed features can be explained reasonably by the model which assumes local vertical lattice relaxation of surface carbon atoms by Coulomb attraction between localized electron-hole pairs generated in adjacent two layers.

Publications

Original Papers

Fomation and Clustering of Surface Vacancies under Electronic Excitation on Semiconductor Surfaces, J. Kanasaki: Physica, B376-377 (2006) 834-840.

Two-Hole Localization Mechanism for Electronic Bond Rupture of Surface Atoms by Laser-Induced Valence Excitation of Semiconductors, K. Tanimura, E. Inami, J. Kanasaki, and W. Hess: Physical Review, B74[3] (2006) 035337-1-8.

Excitation-Induced Structural Instability of Semiconductor Surfaces, K. Tanimura and J. Kanasaki: J. Physics: Condensed Matter, 18[30] (2006) 1479-1516.

Review Papers

Laser-induced desorption from semiconductor surfaces and its electronic mechanism (in Japanese), J. Kanasaki, K. Tanimura: Journal of the Vacuum Society of Japan 49[10] (2006) 581-587.

International Conferences

Graphite-to-Diamond Phase Transformation Induced by Femtosecond-Laser Excitation

(Oral), K. Tanimura, *****J. Kanasaki, K. Nasu**,** The 5th International Symposium on Ultrafast Surface Dynamics, Abashiri, Japan, May 21-26, 2006.

Femtosecond Laser-Induced Phase Transformation on Graphite Surface –Creation of a Novel Crystalline Phase of sp^3-Bonded Carbon－, *K. Kimura, J. Kanasaki, K. Tanimura, K. Nasu, 24th European Conference on Surface Science, Paris, France, September 4-8, 2006.

Structural Instabilities Induced by Injected Tunneling Carriers on Cleaved InP(110)-(1x1) Surfaces, *J. Kanasaki, K. Ichihashi, J. Tsuruta, E. Inami, K. Tanimura, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006.

Photo-Induced Phase Transformation on Graphite Surface, *K. Kimura, J. Kanasaki, K. Tanimura, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, Japan, September 19-20, 2006.

Femtosecond Laser-Induced Phase Transformation on Graphite Surfaces, *K. Kimura, J. Kanasaki, K. Tanimura, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9, 2006

Structural Instabilities Induced by Carrier Injection from Scanning Tunneling Microscope Tips on Cleaved InP(110)-(1x1) Surfaces, *E. Inami, J. Kanasaki, K. Tanimura, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9, 2006.

Excitation-Induced Processing for Highly Functional Nano-Structured Materials, E. Inami, *J. Kanasaki, S. Tanaka, and K. Tanimura, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Japan, December 8-9, 2006.

Structural Iinstabilities on InP(110)-(1x1) Surfaces Induced by Hole-Injection from the STM Tip, E. Inami, J. Tsuruta, and *J. Kanasaki, 11th International Workshop on Desorption Induced by Electronic Transitions (DIET-VI), Berlin, Germany, March 11-15, 2007.

Excitation-Induced Atomic Desorption and Structural Instability of Semiconductor Surfaces (Invited), K. Tanimura, 11th International Workshop on Desorption Induced by Electronic Transitions DIET-VI, Berlin, Germany, March11-15, 2007.

Contributions to International Conferences and Journals

K.Tanimura International Workshop on Desorption Induced by Electronic Transitions (International Steering Committee)

Publications in Domestic Meetings

The Physical Society of Japan 4 papers

The Japan Society of Applied Physics	1 paper
The Surface Science Society of Japan	1 paper

Sponsorship

Grant-in-Aid for Scientific Research (A)

K. Tanimura	Study of Excited-State Properties of Quasi-Two Dimensional Semiconductor Surfaces	¥13,700,000

Grant-in-Aid for Scientific Research (C)

J. Kanasaki	Structural Instability of Semiconductor Surfaces Induced by Low-Energy Electron Beam Excitation	¥500,000

Department of Quantum Materials and DevicesCharacterization

Professor: Hajime ASAHI
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 Project

1. Nano-Characterization of Surface and Interface in Spintronics Devices

Ferromagnet/Nonmagnet/Ferromagnet trilayer structure is a basic structure for the spintronics devices. We have studied the the relationship between the growth condition of GaCrN/AlN/GaCrN trilayer structure and the surface and interface smoothness with atomic force microscopy (AFM). We found that the surface morphology of GaCrN layer is degraded during the increase of substrate temperature from 700°C to 800°C at the interface of AlN/GaCrN. By optimizing the AlN growth condition for the 700°C growth, we have obtained the smooth surface AlN layer with only one atomic layer step. Under this condition, we have grown GaCrN/AlN/GaCrN trilayer structure and obtained good current-voltage characteristics.

2. XAFS Characterization of Atomic Arrangement in the Low Temperature Grown GaCrN and GaGdN

To improve the magnetization characteristics for the diluted magnetic semiconductors, it is useful to grow at lower temperatures through the high concentration of magnetic ions. We have grown GaCrN and GaGdN layers at the substrate temperature of below 400°C and observed ferromagnetism with much increased concentration of magnetic ions. With XAFS measurements we confirmed the substitution of Cr and Gd atoms at Ga sites even for these samples and no observation of secondary phases, such as precipitation of Cr (Gd) and formation of CrN.

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. In 2006, we have studied the effect of cutting the MOSFET out. We observed the asymmetric current image corresponding to the potential profile, while observed the symmetric topographic image corresponding to the device structure. This difference was understood with the simulation on the 2-dimensional p-n junction.

Publications

Original Papers

Emission spectra from AlN and GaN doped with rare earth elements, S.W. Choi, S. Emura, S. Kimura, M.S. Kim, Y.K. Zhou, N. Teraguchi, A. Suzuki, A. Yanase, and H. Asahi, J. Alloys and Compounds 408-412 (2006) 717-720.

Ferromagnetic cubic GaCrN epitaxial growth over MgO substarte – effect of growth condition, S. Kimura, S. Shanthi, Y.K. Zhou, M.S. Kim, S. Kobayashi, S. Emura, S. Hasegawa and H. Asahi, Jpn. J. Appl. Phys. 45 (1A) (2006) 76-78.

Evaluation of Device Configurations through Cross-Sectional Planes along Gates of 0.1um Metal-Oxide-Semiconductor Field-Effect Transistors by Scanning Tunneling Microscopy/Scanning Tunneling Spectroscopy, S. Hasegawa, W. Doi, A. Yabuuchi and H. Asahi, Jpn. J. Appl. Phys. 45 (3B) (2006) 2033-2036.

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, Phys. Stat. Sol. (c) 3(6) (2006) 2250-2253.

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, Jpn. J. Appl. Phys. 45 (4B) (2006) 3522-3525.

Ferromagnetism in short-period GaGdN/GaN superlattices grown by RF-MBE, S.W. Choi, Y. K. Zhou, M. S. Kim, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, Phys. Stat. Sol. (a) 203 (11) (2006) 2774-2777.

Local crystal structure and local electronic structure around Cr in low-temperature-grown GaCrN layers, M. Hashimoto, S. Emura, H. Tanaka, T. Honma, N. Umesaki, S. Hasegawa and H. Asahi, J. Appl. Phys. 100 (2006) 103907-1 - 103907-6.

Tunnel magnetoresistance in GaCrN/AlN/GaCrN ferromagnetic semiconductor tunnel junctions, M.S. Kim, Y.K. Zhou, M. Funakoshi, S. Emura, S. Hasegawa and H. Asahi, Appl. Phys. Lett. 89 (2006) 232511-1 – 232511-3

Review Papers

Semiconductor Nanospintronics and Devices, Y.K. Zhou and H. Asahi, Vacuum 49(12)

(2006) 722-727 (in Japanese).

Patents
Ferromagnetic Materials: Y.K. Zhou and H. Asahi, JP2006-294577.

Magnetism Control Method: S. Emura, H. Asahi and Y.K. Zhou, JP2006-319153.

International Conferences
Growth of GaCrN/AlGaN/GaCrN Trilayer Structures and Observation of Tunnel Magneto-Resistance Effect (Invited), H. Asahi, M.S. Kim, S. Matsuno, Y.K. Zhou, S. Emura and S. Hasegawa, International Symposium on Hybrid Nano Materials Toward Future Industries, Nagaoka, Japan, February 3-5, 2006.

Ferromagnetism in short-period GaGdN/GaN superlattices grown by RF-MBE, Y.K. Zhou, S.W. Choi, M. S. Kim, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, 15th International Conference on Ternary and Multinary Compounds, Kyoto, Japan, March 6-10, 2006.

Cr atom alignment in Cr-delta-doped GaN, S. Kimura, S. Emura, H. Ofuchi, Y. Nakata, Y.K. Zhou, C.W. Choi, Y. Yamauchi, S. Hasegawa and H. Asahi, The XIII International Conference on XAFS, Stanford, USA, July 9-15, 2006.

New Cr-cluster formation in diluted magnetic semiconductor GaCrN, S. Kimura, S. Emura, S. Kobayashi, S.W. Choi, M.S. Kim, Y.K. Zhou, H. Asahi and H. Ofuchi, The XIII International Conference on XAFS, Stanford, USA, July 9-15, 2006.

Magnetic properties of GaGdN/GaN superlattices grown by RF-MBE, S. W. Choi, Y. K. Zhou, S. Kimura, S. Emura, S. Hasegawa, and H. Asahi, International Conference on Physics and Applications of Spin Related Phenomena in Semiconductors, Sendai, Japan, August 15-18, 2006.

Electronic State and Local Structure Analysis of GaGdN by HX-PES and XAFS, S. Emura, S.W. Choi, J.J. Kim, S. Kimura, S. Kobayashi, Y.K. Zhou, K. Kobayashi, H. Asahi, N. Teraguchi and A. Suzuki, International Conference on Physics and Applications of Spin Related Phenomena in Semiconductors, Sendai, Japan, August 15-18, 2006.

Growth and Characterization of Ferromagnetic Cubic GaCrN, S. Kimura, S. Kabayashi, Y. Zhou, S. Choi, S. Subashcandran, H. Ofuchi, M. Ishimaru, Y. Hirotsu, S. Emura, S. Hasegawa and H. Asahi, 14th International Conference on Molecular Beam Epitaxy, Tokyo, Japan, September 3-8, 2006.

Evolution of Cr-doped and Gd-doped GaN layers grown at low temperatures (Best Paper Awards), Y.K. Zhou, S.W. Choi, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, IUMRS International Conference in Asia 2006, Jeju, Korea, September 10-14, 2006.

Magnetic properties of Gd-doped GaN single layer and GaGdN short period superlattices grown by RF-MBE, S.W. Choi, Y.K. Zhou, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, IUMRS International Conference in Asia 2006, Jeju, Korea, September 10-14, 2006.

Electronic structure of ferromagnetic element Cr in DMS GaCrN observed in X-ray absorption spectra, S. Emura, S. Kimura, M. Hashimoto, S. Kobayashi, S.W. Choi, M.S. Kim, Y.K. Zhou and H. Asahi, IUMRS International Conference in Asia 2006, Jeju, Korea, September 10-14, 2006.

Unique Lattice Alignment around Cr Atoms Doped in GaN under Some Growth Condition, S. Emura, S. Kobayashi, S. Kimura, Y. Yamauchi, S.W. Choi, Y.K. Zhou, H. Ofuchi, S. Hasegawa, H. Asahi, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, September 19-20, 2006.

Growth and characterization of ferromagnetic cubic GaCrN, S. Kimura, S. Emura, H. Ofuchi, S. Shanthi, M. Ishimaru, Y. Hirotsu, Y. K. Zhou, S. Hasegawa and H. Asahi, Sanken International Symposium on Nanoscience and Nanotechnology 2006, Osaka, September 19-20, 2006.

Growth and characterization of GaN-based diluted magnetic semiconductors for semiconductor spintronics (Invited), S. Hasegawa, M. Funakoshi, Y. Yamauchi, Y.K. Zhou, S. Emura and H. Asahi, Handai Nanoscience and Nanotechnology International Symposium 2006, Osaka, November 20-22, 2006.

GaN-based diluted magnetic semiconductors for nano-spintronics, H. Asahi, S. Hasegawa, S. Emura and Y.K. Zhou, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Growth and characterization of cubic GaCrN, S. Kimura, S. Emura, Y.K. Zhou, S. Shanthi, Y. Yamauchi, Y. Hiromura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Defect analysis on MBE grown ferromagnetic GaCrN epitaxial layers, S. Shanthi, S. Kimura, Y.K. Zhou, S. Emura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Epitaxial growth and magnetic properties of GaGdN/GaN superlattice structures, S.W. Choi, Y.K. Zhou, S. Kimura, M. Funakoshi, S. Emura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Low temperature growth of GaCrN and GaGdN layers and their properties, Y.K. Zhou,

S.W. Choi, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, International Symposium of Fifth 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience, Awaji, Hyogo, December 8-9, 2006.

Contributions to International Conferences and Journals

H. Asahi	14th International Conference on Molecular Beam Epitaxy (Organizing Committee Vice-Chair, Program Committee Chair)
H. Asahi	15th International Conference on Ternary and Multinary Compounds (Program Committee member)
H. Asahi	The Third International School and Conference on Spintronics and Quantum Information Technology (Spintech III) (Organizing Committee member)
H. Asahi	2006 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	14th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (Publication Committee member)
H. Asahi	18th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	2007 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	19th International Conference on Indium Phosphide and Related Materials (Organizing Committee member, International Steering Committee member)
H. Asahi	International Symposium on Compound Semiconductors 2007 (Organizing Committee member, Program Committee member)
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 (B) (2)

H. Asahi	Study on Room Temperature Ferromagnetic Nitride Semiconductor Nanostructures and Application to Nanospintronics Devices	¥7,500,000

Nanotechnology Process Foundry

Professor:	Tomoji KAWAI
Visiting Associate Professor:	Masakazu MURASUGI
Visiting Associate Professor:	Toshio KAWAHARA (to Nov.15)
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 final year of this project in 2006, and most of our efforts resulted in supporting 36 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.

Current Research Project

Bring-up Nanotechnology Process Foundry

The 180 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.

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.

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.

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

Dependence of Acid Yield on Chemically Amplified Electron Beam Resist Thickness, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto, and S. Tagawa, Jpn. J. Appl. Phys., Part 1 45 (2006) 5445-5449.

Relationship between Acid Concentration and Acid Yield in Chemically Amplified Electron-Beam Resist, T. Shigaki, K. Okamoto, T. Kozawa, H. Yamamoto, and S. Tagawa, Jpn. J. Appl. Phys., Part 1 45 (2006) 5735-5737.

Reaction Mechanism of Fluorinated Chemically Amplified Resists, H. Yamamoto, T. Kozawa, K.Okamoto, and S. Tagawa, J. Vac. Sci. Technol. B 24 (2006) 1833-1836.

Acid Generation Mechanism of Poly(4-hydroxystyrene)-based Chemically Amplified Resists for Post-optical Lithography －Acid Yield and Deprotonation Behavior of Poly(4-hydroxystyrene) and Poly(4-methoxystyrene) －, A. Nakano, T. Kozawa, K.a Okamoto, S. Tagawa, T. Kai, and T. Shimokawa, Jpn. J. Appl. Phys. Part 1 45 (2006) 6866-6871.

Protonation Sites in Chemically Amplified Resists for Electron-Beam Lithography, K. Natsuda, T. Kozawa, K. Okamoto, and S. Tagawa, Jpn. J. Appl. Phys. Part 2 45 (2006) L1256-L1258.

Pulse Radiolysis of Polystyrene in Cyclohexane -Effect of Carbon Tetrachloride on Kinetic Dynamics of Dimer Radical Cation-, K. Okamoto, T. Kozawa, M. Miki, Y. Yoshida, and S. Tagawa, Chem. Phys. Lett. 426 (2006) 306-310.

Formation of Trimer and Dimer Radical Cations of Methyl Substituted Benzenes in γ-Irradiated Low Temperature Matrices, K. Okamoto, S. Seki, and S. Tagawa, J. Phys. Chem. A 110 (2006) 8073-8080.

Analysis of Acid Yield Generated in Chemically Amplified Electron Beam Resist, T. Kozawa, T. Shigaki, K. Okamoto, A. Saeki, S. Tagawa, T. Kai, and T. Shimokawa, J. Vac. Sci. Technol. B 24 (2006) 3055-3060.

Review Papers

Control of temperature dependence of the ferroelectric $BaZr_xTi_{1-x}O_3$ superlattice films, T Kawahara, T Ohno, H Tabata, T Kawai, T Hino, Ultra Sonic Techno, 9-10 (2006)

31-34.

Patents
Cleaning method for metal nano cluster surfaces. Y. Agawa, M. Matsuura, T. Kawahara, T. Kawai, Tokugan2006-343794.

International Conferences
Formation of aggregated radical cations of benzene and polystyrene in condensed phases. (poster), *K. Okamoto, S. Seki, T. Kozawa, Y. Yoshida and S. Tagawa Gordon Research Conference (2006 GRC on Radiation Chemistry), ME, USA, Jun. 2-7, 2006

Magnetic and Electric Properties of Fe-Doped ITO Thin Films.(poster), *S. Kohiki, T. Ohno, T. Kawahara, M. Murasugi, H.Tanaka and T. Kawai International Conference on Magnetism (ICM-2006), Kyoto, Japan. Aug. 22-30, 2006

Nanotechnology Process Foundry in ISIR for the Supporting of the Nanotechnology in Japan (poster), *M. Murasugi, T. Kawahara, T. Ohno, Y. Matsui, K. Okamoto, and T. Kawai SISNN-2006, Suita, Japan, Sep. 19-20, 2006

Sponsorship

Entrusted Research

T. Kawai	MEXT(RR2002) Nanotechnology Support Project	¥90,000,000

Open Laboratory

Professor (concurrent, manager):	Yoichi YOSHIDA
Professor (concurrent):	Kazuhiko MATSUMOTO
Professor (concurrent):	Hikaru KOBAYASHI
Professor (concurrent):	Hiroaki SASAI
Technical Staff:	Akira YOSHIDA, Kimihiro NORIZAWA
Supporting Staff:	Kayoko OHASHI

Outlines

Open Laboratory supports the comprehensive research for creative and advanced academic research on materials and devices, which should become the foundation of scientific and technological development on nanotechnology.

Current Research Project

On 2006, the following 27 researchers used Open Laboratory for 32 projects.

Prof. Mitsuru AKASHI	Graduate School of Engineering
Prof. Kazuyoshi IKUTA	Research Institute for Microbial Diseases
Prof. Yukichi UMAKOSHI	Nanoscience and Nanotechnology Research Center
Prof. Hisao OHTAKE	Graduate School of Engineering
Prof. Masanori OZAKI	Graduate School of Engineering
Prof. Tomoyuki KAKESHITA	Graduate School of Engineering
Prof. Tomoji KAWAI	Institute of Scientific and Industrial Research
Assoc. Prof. Shun'ichi KURODA	Institute of Scientific and Industrial Research
Prof. Susumu KUWABATA	Graduate School of Engineering
Prof. Hikaru KOBAYASHI	Institute of Scientific and Industrial Research
Prof. Takatomo SASAKI	Graduate School of Engineering
Prof. Katsuaki SUGANUMA	Institute of Scientific and Industrial Research
Prof. Seiichi TAGAWA	Institute of Scientific and Industrial Research
Prof. Naoyuki TANIGUCHI	Research Institute for Microbial Diseases
Prof. Hideo NAKAJIMA	Institute of Scientific and Industrial Research
Prof. Yasufumi FUJIWARA	Graduate School of Engineering
Prof. Kiichi FUKUI	Graduate School of Engineering
Prof. Hiroshi MASUHARA	Graduate School of Engineering
Prof. Riichiro MIZOGUCHI	Institute of Scientific and Industrial Research
Assoc. Prof. Seiichi MURASUGI	Institute of Scientific and Industrial Research
Prof. Hirotaro MORI	Research Center for Ultra-High Voltage Electron Microscopy
Assoc. Prof. Yusuke MORI	Graduate School of Engineering
Assoc. Prof. Yoshimitsu YAMASAKI	Graduate School of Medicine
Prof. Masahiko YAMAMOTO	Graduate School of Engineering
Prof. Hiroshi YOSHIDA	Institute of Scientific and Industrial Research
Prof. Yoichi YOSHIDA	Institute of Scientific and Industrial Research
Assoc. Prof. Takehiko WADA	Graduate School of Engineering

Radiation Laboratory

Professor, Director:	Tetsuro MAJIMA
Professors	Seiichi TAGAWA, Goro ISOYAMA, Yoichi YOSHIDA
Associate Professors:	Ryuko KATO, Yoshihide HONDA, Shu SEKI, Mamoru FUJITSUKA, Takahiro KOZAWA, Kiyohiko KAWAI, Jinfeng YANG
Specially Appointed Associate Professors:	Masayuki ENDO
Research Associates:	Toshiji IKEDA, Norio KIMURA, Kazuo KOBAYASHI, Sachiko TOJO, Shigeru KASHIWAGI, Akinori SAEKI
Specially Appointed Research Associates:	Tachikawa Takashi, Masanori Kondo Takafumi Kondo
Technical Staff:	Tamotsu YAMAMOTO, Kumiko BABA
Support Staff:	Naoko KAWAGUCHI (-1.19.2007)

Outline

The Radiation Laboratory was newly established in the fiscal year 2002 in the Nanoscience and Nanotechnology Center as a successor of the *Radiation Laboratory*, which was a facility directly attached to the Institute but had been reorganized to be part of the center, for operating experimental equipment previously owned by the *Radiation Laboratory*. The main pieces of the equipment are the 40 MeV L-band electron linear accelerator (linac), the 150 MeV S-band electron linac, the 40 MeV RF-gun electron linac, and the ^{60}Co γ-ray irradiation facility. Among them, the L-band linac and the γ -ray irradiation facility are open to users in Osaka University. The staff of the Radiation Laboratory is composed of the full-time members, who are 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.

Achievement

L-band linac

The L-band electron linac has four operation modes, which are transient, steady, single-bunch, and multi-bunch modes, in combination with either the short or long pulse duration of injected electrons and operation of the sub-harmonic buncher or not, and has ability to accelerate an electron beam up to the maximum energy 40 MeV and the highest charge per bunch 91 nC in the single bunch operation mode or the maximum current injected from the electron gun 30.6 A in the transient mode at the repetition rate 60 pulses per second at maximum. The machine time of the L-band linac in the fiscal year 2006 is as follows; 108 days including 13 days for maintenance are allocated in the first term and 118 days including 18 days for maintenance in the latter term. The operation days in the year are 195 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.

S-band linac

The S-band linac can accelerate an electron beam of the nominal energy 100 MeV and a peak current 0.2 A at the repetition rate 30 Hz, and it has been used for production of the slow positron beam.

RF-gun linac

The 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 operated the linac for 950 hours in eight months. The operation of the linac was satisfactory for the most part.

^{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 and the total utilization time is about 2520 hours, which is longer than a value in last year.

Join-use

The number of joint-uses this fiscal year is 26 subjects from our institute, 12 subjects from other departments in the university, and 4 subjects from groups including members outside the university, and these are adding up to 42 subjects in total.
We held two workshops; “Development and Utilization of Quantum Beams” held on November 10, 2006, and “Mechanism and Application of Quantum Beam Induced Reactions” held on January 19, 2007. In addition, we held the annual meeting for presenting results obtained in the fiscal year 2006 on March 14, 2007 at the auditorium of the institute. We received more than 240 visitors to the Radiation Laboratory.

Radiation safety management

The number of radiation users in ISIR is 151 persons in the fiscal year 2006. An education and training course for users was held on April 13, 14, 2006 at the MO-hall in the Convention Center of Osaka University. An education and training course for new users was held on May 14, 2006 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 2006, the 300kV TEM served as an important equipment for the nano-structure characterization researches of 8 laboratories in ISIR with operation times as many as 319.

Electronic Processing Laboratory

Professor: Hajime ASAHI
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 nanotechnology-related research by use of equipments and special skills for nanotechnology researchers and students belonging to ISIR. In addition, this shop fabricates nano-devices for the ISIR researchers and develops devices for researchers who want to apply those devices for their own experiments.

Activities

On demand fabrication requests

We have received requests from 6 laboratories in ISIR. Total number of their requests reached 45 and 153 samples were provided.

Practice seminar of fabrication and application of micro-devices

We have held a practice seminar under the support of the 21COE project. This program contained not only fabrication of micro-devices but also application of them. It took 2 days and was held 3 times. Total participants were 8 people.

Participation in “nanotech 2007”

We have made a poster exhibition and micro-devices demonstration in the booth of Nanotechnology Center in the international nanotechnology exhibition and conference “nanotech 2007” which was held on 21st to 23rd of February in 2007.

Materials Analysis Center

Professor Director:	Hiroaki SASAI
Associate Professor:	Takeyuki SUZUKI
Research Associate:	Yoshio TAKAI
Technical Staff:	Hitoshi YAMDA
	Takanori TANAKA
	Tuyoshi MATSUZAKI
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 oxidation: development and applications

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. Tishchenko reaction of the corresponding aldehydes were developed using the same catalyst. Furthermore, we have developed two intramolecular cyclization of ketoaldehydes.

The pheromone of the Biprorulus bibax, was synthesized by the iridium catalyzed oxidative lactonization

Publications

Original Papers

Enantiocontrolled Synthesis of the Epoxycyclohexenone Moieties of Scyphostatin, a Potent and Specific Inhibitor of Neutral Sphingomyelinase, T. Katoh, T. Izuhara, W. Yokota, M. Inoue, K. Watanabe, A. Nobeyama, T. Suzuki, Tetrahedron, 62 (2006) 1590-1608.

Convergent and Enantioselective Total Synthesis of (−)-Nalanthalide, a Potential Kv1.3 Blocking Immunosuppressant**,** T. Abe, K. Iwasaki, M. Inoue, T. Suzuki, K. Watanabe, T. Katoh, Tetrahedron Lett., 47 (2006) 3251-3255.

Synthesis of the Hemiacetal Pheromone of the Spined Citrus Bug Biprorulus Bibax Utilizing a Iridium Catalyzed Oxidative Lactonization, T. Suzuki, K. Morita, H. Ikemiyagi, K. Watanabe, K. Hiroi, T. Katoh, Heterocycles, 69 (2006) 457-461.

International Conferences

Iridium-catalyzed oxidative dimerization and Tishchenko reaction, T. Suzuki, T.

Yamada, T. Matsuo, K. Watanabe, T. Katoh, 7th Tetrahedron Symposium, Kyoto, Japan, May.24, 2006.

Development of Oxidative Reactions Catalyzed by Ir Complex, N. K. Mangu, T.Suzuki, T. Yamada, T. Matsuo, K. Watanabe, T. Katoh, H. Sasai, the 10th International KYOTO Conference on New Aspects of Organic Chemistry, Kyoto, Japan, Nov.13-17, 2006.

Iridium-catalyzed oxidative dimerization and Tishchenko reaction, T. Suzuki, T. Yamada, T. Matsuo, K. Watanabe, T. Katoh, XXII International Conference on Organometallic Chemsitry, Zaragoza, Spain, July 23-28, 2006.

Publications in Domestic Meetings

Symposium on Organometallic Chemistry	1 paper
Symposium on Organic Synthesis	1 paper
The Chemical 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	¥700,000

Entrusted Research

T. Suzuki	KRI	Research of Materials Analysis	¥300,000

Other Research Fund

T. Suzuki	Tokuyama Science Foundation	Iridium-catalyzed oxidative dimerization and Tishchenko reaction	¥240,000
T. Suzuki	The Uehara Memorial Foundation	The development of environmentally benign oxidation using iridium catalyst and application for the synthesis of bioactive compounds	¥5,000,000

Materials Science & Technology Research Center for Industrial Creation (MSTeC)

Outline

Materials Science & Technology Research Center for Industrial Creation (MSTeC) was founded in April 2005 for contributing to the creation of new industry through the complementary cooperation with Institute of Multidisciplinary Research for Advanced Materials, Tohoku University. This center consists of two projects: P1 Materials Research Project and P2 Human Interface Research for Safety and Security Project which are divided to four groups: G1 Hard Materials Research Group, G2 Soft Materials Research Group, G3 Medical Sciences Research Group, and G4 Human Interface Research Group.

Director: Prof. T. Majima

P1 Materials Research Project

G1 Hard Materials Research Group: Group leader: Prof. H. Nakajima

G2 Soft Materials Research Group: Group leader: Prof. T. Majima

P2 Human Interface Research for Safety and Security Project

G3 Medical Sciences Research Group: Group leader: Prof. A. Yamaguchi

G4 Human Interface Research Group: Group leader: Prof. H. Tabata (until Nov. 30, 2006) and Prof. H. Yoshida (from Dec. 1, 2006)

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 invironmentally 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 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
- Fabrication of lotus-type porous ultra-high purity ion
- Functionalization of lotus-type porous materials by modification of surface
- 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
- Development of spiro chiral ligands for novel Pd catalyzed enantioselective reactions

Hard Materials Research Group

Professor: Hideo NAKAJIMA, Katsuaki SUGANUMA
Designated Associate Professor: Soong-Keun HYUN
Designated Research Associate: Keun-Soo KIM, Shunkichi UENO

Outline

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 magnesium, 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. Fabrication of Lotus-type Porous Ultra-high Purity ion

We successfully prepared a lotus type porous ultra-high purity ion by a continuous zone melting method in pressurized hydrogen atmosphere. We made clear the role of impurity on the formation of pores during the unidirectional solidification. Since the number of nuclei decreases with increasing the purity, the number of pores, pore size and pore length along the solidification direction increased with increasing the purity. This study was performed by a collaboration work with Prof. Isshiki Tohoku University.

3. Functionalization of Lotus-type Porous Materials by Surface Modification

A technology of a modification for lotus-type porous copper by Ar ion irradiation was developed. Micro whiskers grow on the surface of inner pore. The whisker consisted with Cu_2O. And the aspect ratio of the whisker can be controlled by heat treatment and power of Ar beam. This technology promised a development of gas filter and catalyst support using lotus-type porous metals. This study was performed by a collaboration work with Prof. Tanaka Tohoku University.

4. 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.

Room temperature fabrication enables to use the wide variety of functional materials

into one circuit board without thermal stress or damage as well as environmental consciousness. Metallic nanoparticles can be sintered to form dense microstructure if both the surface of nanoparticles and the environment are clean without any oxidation or contamination. Ag nanoparticles are, however, usually protected by an organic layer. Recently, we developed a new process, by which the paste of Ag nanoparticles protected with them can be successfully sintered at room temperature in air atmosphere. In order to remove the dodecylamine layer, Ag nanoparticles printed as lines on a glass substrate was dipped into methanol for 10 s to 7,200 s. As a result, the sintered Ag wires possess excellent low resistivity, 7.3×10-5 Ωcm after 7,200 s dipping. Thus, a novel room temperature wiring method for Ag nanoparticles has successfully developed in air atmosphere.

5. Development of low temperature interconnection technology

Establishment of lead-free plating technology and whisker countermeasures is one of the critical problems remaining to be solved for lead-free electronics packaging. A new approach to prevent the Sn whisker, by surface treatment on Sn plating, was proposed. Two Ni layers of different thickness were plated on the surface of the Sn plating. Sn whiskers were observed on pure Sn plating samples after 168 hours, however, no Sn whisker was observed on thick Ni/Sn plating samples after 10080 hours. Ni over plating on Sn plating has a great effect in suppressing Sn whisker formation.

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.

Publications

Size Effects on Tensile Strength of Lotus-type Porous Copper, H. Sueno, M. Tane, J.S. Park, S.K. Hyun and H. Nakajima, Mater. Trans., 47[9] (2006) 2203-2207.

Fabrication of Lotus-type Porous Ni_3Al with and without Boron, T. Ide, M. Tane, S.K. Hyun and H. Nakajima, Mater. Trans., 47[9] (2006) 2116-2119.

Effect of pore morphology on compressive yield strength of lotus-type porous copper with various specimen sizes, J.S. Park, S.K. Hyun, H. Sueno, M. Tane, H. Nakajima, Y.S. Um, B.Y. Hur and F. Ono, Mater. Trans., 47[9] (2006) 2208-2212.

Effect of Silica Additive on the Formation of Lotus-type Porous Alumina under Unidirectional Solidification, S. Ueno, L.M. Lin, S.K. Hyun and H. Nakajima, Mater. Trans., 47[9] (2006) 2167-2171.

Effect of Hydrogen Pressure on Moisture-Based Fabrication of Lotus-type Porous Nickel, H. Onishi, S.K. Hyun and H. Nakajima, Mater. Trans., 47[9] (2006) 2120-2124.

Development of an Electrophoretic Sol-gel Coating Process for Porous Metals, M. Inoue, S.K. Hyun, K. Suganuma, H. Nakajima, Mater. Trans., 47[9] (2006) 2161-2166.

Laser Welding of Lotus-Type Porous Iron, H. Yanagino, T. Tsumura, H. Nakajima, S.K. Hyun and K. Nakata, Mater. Trans., 47[9] (2006) 2254-2258.

Electrochemical Behaviour of Lotus-type Porous SUS304L and SUS316L Stainless Steels, M. Fuseya, T. Nakahata, S.K. Hyun, S. Fujimoto, H. Nakajima, Mater. Trans., 47[9] (2006) 2229-2232.

Development of Lotus-type Porous Copper Heat Sink, T. Ogushi, H. Chiba and H. Nakajima, Mater. Trans., 47[9] (2006) 2240-2247.

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Contributions to International Conferences and Journals

H. Nakajima	Materials Letters (Principal Editor)
H. Nakajima	Scripta Materialia (Guest Editor)
H. Nakajima	Fifth International Conference on Porous Metals and Metal Foaming Technology (MetFoam2007) (Organizing Committee Chairman)
H. Nakajima	High Temperature Materials and Process (Editorial Board)
H. Nakajima	High Temperature Materials and Progress (Guest Editor)

H. Nakajima	Advanced Engineering Materials (Guest Editor)
H. Nakajima	Materials Transactions (Guest Editor)
H. Nakajima	Diffusion and Defect Data (Editorial Advisory Board)
H. Nakajima	Materials Science Foundations (Editorial Advisory Board)
H. Nakajima	Fifth Pacific Rim International Conference on Materials (PRICM-5) (Organizing Committee Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	International Conference on Processing & Manufacturing of Advanced Materials (THERMEC'2006) (Organizing Committee Member)
H. Nakajima	2nd International Conference on Diffusion in Solids and Liquids (Editorial Advisory Board)
H. Nakajima	International Conference on Eco-Materials Processing and Design VIII (Editorial Advisory Board)
H. Nakajima	International Symposium on Synergistic Effects of Materials and Processing (ISSEMP2006) (Editorial Advisory Board)
H. Nakajima	International Conference on Diffusion in Materials (Editorial Advisory Board)
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	12Papers
Japan Institute of Electronics Packaging	5 Papers
Others	1 Paper

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

Grant-in-Aid for Scientific Research (C)

S. Ueno	Formation mechanism of high ordered porous ceramics and its application for catalyst support	¥2,500,000

JEITA Project

K. Suganuma	Prevention of tin whiskers	¥5,250,000

JST Project

S.K. Hyun	Development of human body friendly sweet new porous metals	¥1,000

Soft Materials Research Group

Professor: Tetsuro MAJIMA
Specially Appointed Associate Professor: Masayuki ENDO
Specially Appointed Research Associate: Katsuya MATSUI, Masanori SAKAMOTO

Outline

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 Projects

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 protein supramolecular and nanostructures by designing the building blocks. 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. Also we employed porphyrin derivatives for creation of the light-harvesting system in the TMV supramolecular structure. We observed the energy transfer from Zn-porphyrin to free-base porphyrin and enhancement of emission intensity of free base porphyrin. The TMV supramolecular system described in this report allows the integration of aromatic molecules into the TMV scaffold and serves for creating well-ordered self-assembled materials.

Development of 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.

New Asymmetric Spiro-type Ligands

So far we have developed a new type of chiral bis(isoxazoline) ligands with spiro[4.4]nonane skeleton (SPRIXs). Pd(II)-SPRIX catalysts are 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 isoxazoline and isoxazole ring with spiro[4.5]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.

Excited Radicals for Preparation of Nanomaterials

We propose the fabrication method of metal nanoparticles using excited radicals. Radicals in the excited state have a stronger reducing ability than those in the ground state and are favorable reducing agents for metal ion. A variety of excited radicals can be conveniently generated by using two-color two-laser flash photolysis. The specific three-dimensional resolution of two-color two-laser makes the construction of three-dimensional arrays of metal nanoparticles possible. In this year, we tried to fabricate AuNps using the excited benzophenone ketyl radical as a reducing agent. The formation of AuNp was significantly enhanced by the two-color two-laser irradiation. The efficient electron transfer from the excited radical enhanced the formation of AuNps.

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Development of New TiO_2 Photocatalysts (Invited), *T. Majima, The 8th International Conference on ECOMATERIALS, Kitakyusyu International Conference Center, Jan 11-14, 2007.

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Contributions to International Conferences and Journals

T. Majima	2006 International Symposium on Frontier Photoscience (Conference Chair)
T. Majima	Langmuir (Editor)
H. Sasai	ICOB-5 & ISCNP-25 IUPAC International Conference on Biodiversity and Natural Product (Organizing Committee)

Publications in Domestic Meetings

Photochemistry Meeting	12 papers
Radiation Chemistry Meeting	3 papers
85th Japan Chemical Society Meeting	10 papers

Sponsorships

Grand-in-Aid for Scientific Research (S)

T. Majima	Nanoscience of Photofuctionalized DNA	¥19,240,000

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

T. Majima	Fundamental Science and Technology of Photofunctional Interfaces	¥10,200,000
H. Sasai	Development of Chiral Organocatalyst with Synergistic Effect	¥2,100,000

Grand-in-Aid for Basic Scientific Research

T. Majima	Formation of Carbon Nanotubes Arrays based on DNA Self-assembly	¥1,000,000

Entrusted Research

T. Majima	IDEC Co. Satake Co.	Selection of plastic by laser light	¥4,510,000

H. Sasai	Japan Science and Technology Agency	Preparation of Novel Medicinal Intermediates Based on Enantioselective Reactions Using Chiral Spiro Ligands	¥3,250,000
K. Matsui	Japan Science and Technology Agency	Development of a Novel Bifunctional Asymmetric Organocatalysts	¥2,000,000

Other Research Fund

T. Majima	Matsushita Electric Industrial Co.	Study of highly reactive TiO_2 nanotuve photocatalysts	¥1,155,000
T. Majima	Mitsubishi Chemical Co.	Basic research on chemical reaction via higher excited states	¥1,000,000
T. Majima	Asahi Glass Co.		¥1,000,000

Human Interface Research for Safety and Security Project

Outline

Human Interface Research for Safety and Security Project is one of two main projects of Materials Science & Technology Research Center for Industrial Creation, MSTeC, which is the newly established cooperative organization with ISIR and the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University from 2005. This project aimed for developing the sustainable technology of human interface for safety and security. This project contains two groups: 1) medical sciences research group and 2) human interface research group. Main research subjects are xenobiotic exporters as novel drug targets, next generation intensity modulated radiation therapy, novel sensors and software systems. In addition, we also investigate new industrial prediction tools.

Achievements

- Identification of the exporters that mediates secretion of lipophilic signal transducing molecules.
- Roles of xenobiotic transporters in cellular physiology.
- Dynamic optical modulation of electron beam for high performance intensity modulated radiation therapy (IMRT).
- Research on bio-applications of novel nano structures and on integrated operation of the interfaces.
- Research on the modeling framework of functional knowledge externalization, and text mining technique for functional concepts and way knowledge.
- Research on the strategic new industry prediction accompanying change of industrial structure and success factors for high tech. venture companies.
- 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, Kunihiko NISHINO, Takafumi KONDOH

Outline

The main research objective of our group is understood 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 accelerator beam control technology to realize the high performance and high function for the intensity modulated radiation therapy (IMRT).

Current Research Projects

Identification of the exporters that mediates secretion of lipophilic signal transducing molecules.

We are trying to identify the function of orphan ABC transporters as a new target for drug development. We have been analyzing one of the ABC transporters, ABCA5 which is expressing predominantly in brain, lung and testis. Previously we showed that the expression of ABCA5 in lung and testis is lamella body of alveolar type II cells and intracellular vesicles of spermatocyte, respectively. This year we tried to determine what kind of cells are expressing the ABCA5 proteins in brain to elucidate the ABCA5 function in brain cells. Using the co-immuno-staining method with ABCA5 antibodies and each neuron type specific antibody, we found that ABCA5 is mainly expressed in adrenergic neurons that are secreting the epinephrine. Adrenal medulla cells that are secreting the epinephrine are, also expressing ABCA5. These results suggested that the possible role of ABCA5 in epinephrine secreting cells.

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) from the platelet. Using the each transporter specific inhibitors, we proposed that ABC A-type transporters might participate the export of sphingosine-1-phosphate. Among the ABCA type transporters, we showed that ABCA7 is predominantly expressed in platelet. These results suggested that ABCA7 should be a candidate of sphingosine-1-phosphate transporter.

Roles of xenobiotic transporters in cellular physiology

Xenobiotic transporters play a major role in the multidrug resistance by extruding antibiotics or biocides out of the cell. Recent discoveries support the notion that at least some xenobiotic transporters have specific physiological substrates because these

transporters have been shown to have roles in bacterial virulence. In this study, we will identify "natural substrates" of xenobiotic transporters in order to understand physiological functions of transporters. This knowledge should promote the development of novel inhibitors or strategies that could counteract the contribution of transporters to drug resistance and virulence.

Dynamic optical modulation of electron beam for high performance intensity modulated radiation therapy (IMRT).
The IMRT is remarkable as the effective therapy of cancer. In this research, the beam control technology of intensity modulated electron beam was developed by the laser photo cathode RF gun LINAC at ISIR. Especially for the Breath synchronization in the therapy, dynamic optical modulation of the electron beam was studied using a photocathode RF gun LINAC.

Publications

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Synthesis of Autoinducer-2 Antagonists in Bacterial Quorum-sensing, *M. Hiraoka, Y. Yano, T. Kawano, H. Hirakawa, A. Kobayashi, T. Hirata, A. Yamaguchi, J. Ohkanda and N. Kato, 5th 21COE International Symposium, “Towards Creating New Industries Based on Inter-Nanoscience”, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006

Bacterial Multidrug Exporters -From the Molecular Structure to the Biological Funciton (invited), *A. Yamaguchi, The 6th Awaji International Forum on Infection and Immunity, The Hyogo Prefectual Awaji Yumebutai International Conference Center, Japan, Sep. 4-8, 2006

Membrane Topology of EmrB, an Outer Membrane Channel-Coupled Multidrug Efflux Transporter, in *Escherichia coli*, *Y. Hisano, N. Tamura, S. Murakami and A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology, Kyoto, Japan, Jun. 18-23, 2006

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Virulence and Drug Resistance Roles of Multidrug Efflux Pumps, *K. Nishino, Sanken Workshop on Nano-Bioscience at Berkeley, University of California, Berkeley, CA, USA, Mar.21, 2007.

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A Biological Function of Multidrug Transporters in Iron Homeostasis, *K. Nishino, T. Hirata, A. Yamaguchi, 5th 21st Century COE “Towards Creating New Industies Based on Inter-Nanoscience” International Symposium, Awaji Island, Dec.8-9, 2006.

Single Cell Measurement of Drug Efflux by RND Family Transporter in Femtoliter Chamber Array, *R. Iino, M. Nakata, K. Nishino, S. Sakakihara, S. Takeuchi, A. Yamaguchi, H. Noji, 5th 21st Century COE “Towards Creating New Industies Based on Inter-Nanoscience” International Symposium, Awaji Island, Dec.8-9, 2006.

Lipopolysaccharide Modifications Mediating Bacterial Resistance to Fe(III) and Al(III), *K. Nishino, E. A. Groisman, A. Yamaguchi, International Union of Biochemistry and Molecular Biology 20th Congress, Kyoto, Jun.21, 2006.

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How Bacteria Resist Killing by Fe(III) and Al(III), *K. Nishino, The 8th Japan-Korea International Symposium on Microbiology, Kanazawa, Japan, Mar.29, 2006.

Plasma Membrane Transporters Participate the Sphingosine 1-phosphate Secretion from the Rat Platelet, *T. Nishi, N. Kobayashi, T. Hirata, A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto, June 22, 2006

Cellular Localization of Mouse ABCA5 Proteins in Mouse Tissues, *M. Ohigashi, T. Nishi, A. Yamaguchi, 20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Kyoto, June 22, 2006

Tissue Specific Expression of the Splicing Variants of the Mouse Vacuolar Proton Translocating ATPase a4 Subunit, *S. Kawasaki-Nishi, A. Yamaguchi, M. Forgac, T. Nishi, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, December 8, 2006

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Electron Beam Pulse Processing toward the Intensity Modified Radiation Therapy (IMRT), *T. Kondoh, J. Yang, Y. Yoshida and S. Tagawa, 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006

Higher-order Effect Compensation in Magnetic Compressor for <50fs Electron Bunch, *K. Kan, T. Kondoh, J. Yang, Y. Yoshida, 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006

Development of Double-decker Electron Beam Accelerator for Femto/attosecond Pulse

Radiolysis, *Y. Kuroda, T. Kondoh, J. Yang, Y. Yoshida, 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006

Equivalent Velocity Spectroscopy Based on Femtosecond Electron Beam Accelerator, *S. Takemoto, T. Kondoh, J. Yang, Y. Yoshida, 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006,

Femtosecond Single-bunch Electron Linear Accelerator Based on a Photocathode RF Gun, *J. Yang, T. Kondoh, Y. Yoshida, 2006 European Particle Accelerator Conference, Edinburgh, Scotland, 26-30 June, 2006

Generation of 98-Femtosecond Single Electron Bunch in Photocathode Linear Accelerator, *Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.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), Osaka, Japan, Feb.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), Osaka, Japan, Feb.8-9, 2006

100-Femtosecond Electron Beam Generation 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), Osaka, Japan, Feb.8-9, 2006

Generation of Femtosecond Electron Beam for Ultrafast Reaction Analysis in Nanospace, *J. Yang, K. Kan, T. Kondoh, A. Yoshida, T. Kozawa, Y. Yoshida and S. Tagawa, Handai Nanoscience and Nanotechnology International Symposium, Osaka Univ, Jan.30-Feb.1, 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), Osaka, Japan, Feb.8-9, 2006

A Concept of Double-decker Electron Beam Accelerator for Att/femtosecond Reaction Analysis, *Y. Kuroda, J. Yang, T. Kondoh, A. Yoshida, Y. Yoshida, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.8-9, 2006

3D-Measurement for Short Electron Bunch, *A. Yoshida, Y. Jinfeng, T. Kondoh, Y. Yoshida, A. Ogata, SANKEN International Symposium 2006 (SIS-2006), Osaka, Japan, Feb.8-9, 2006

Spatial Modulation of Electron Beam for the IMRT, *T. Kondoh, J. Yang, T. Yamamoto, Y. Yoshida, S. Tagawa, SANKEN International Symposium on Nanoscience and Nanotechnology 2006 (SISNN-2006), Osaka, Sep. 19-20, 2006

Ultrashort Electron Beam for Reaction Analysis in Nanofabrication, J. Yang, K. Kan, Y. Kuroda, *T. Kondoh and Y. Yoshida, SANKEN International Symposium on Nanoscience and Nanotechnology 2006 (SISNN-2006), Osaka, Sep. 19-20, 2006

Femtosecond Pulse Radiolysis Based on Photocathode Electron Accelerator,*Y. Yoshida, J. Yang, T. Kondoh, T. Kozawa, S. Tagawa, The 1st Asian-Pacific Symposium on Radiation Chemistry, Shanghai, China, Sep. 17-21, 2006

Pulse Radiolysis Study on Solvated Electrons in Ionic Liquid with Controlling Water Content, *J. Yang, R. Nagaishi, T. Kondoh, Y. Yoshida, The 1st Asian-Pacific Symposium on Radiation Chemistry, Shanghai, China, Sep. 17-21, 2006

Processing of Incident Light by the DMD for the Photocathode RF gun, *T. Kondoh, H. Kashima, J. Yang, T. Yamamoto, Y. Yoshida, S. Tagawa, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter- Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006

Collective Ionization by Attosecond Electron Bunches, *Ogata, T. Kondoh, J. Yang, Y. Yoshida, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter-Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006

Simulation Study on Sub-femtosecond Electron Bunch Generation, *K. Kan, J. Yang, T. Kondoh, Y. Yoshida, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter- Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006

Femtosecond Electron Beam and Femtosecond Pulse Radiolysis for Reaction Analysis in Nano-space, *J. Yang, T. Kondoh, T. Kozawa, Y. Yoshida, S. Tagawa, 5th 21st Century COE ‘’Towards Creating New Industries Based on Inter- Nanoscience’’ International symposium, Awaji Yumebutai International Conference Center, Japan, Dec. 8-9, 2006

Contributions to International Conferences and Journals

A. Yamaguchi Journal of Bacteriology (Editorial Board Member)

Publications in Domestic Meetings

Japanese Society for Bacteriology	6 paper
The Pharmaceutical Society of Japan	3 papers
The Molecular Biology Society of Japan	2 papers
Japanese Society of Chemotherapy	1 paper
Symposium on Microbiology	2 papers
Symposium on Biomembrane-Drug Interaction	1 paper
Workshop on *E. coli*	2 papers
Workshop on Bioenergetics	1 paper
Workshop on Infectious Diseases	2 papers
Workshop on efflux system	1 paper
The Institute of Electrical Engineers of Japan	2 papers
Atomic Energy Society of Japan:	2 papers
Japanese Society of Radiation Chemistry:	5 papers
Particle Accelerator Society of Japan:	5 papers
RF gun meeting:	2 papers

Sponsorships

Grant-in-Aid for Scientific Research (A)

Y. Yoshida	Research on Equivalent velocity spectroscopy for Sub-femtosecond and Attosecond Pulse Radiolysis	¥14,400,000

Grant-in-Aid for Scientific Research (C)

T. Nishi	Elucidation of the secretion mechanism of the lipid mediators.	¥1,800,000

Grant-in-Aid for Young Scientists (Start-up)

K. Nishino	Regulatory Networks of Bacterial Multidrug Resistance and Virulence	¥1,420,000

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	¥6,240,000
A. Yamaguchi	The Program of Founding Research Centers for Emerging and Reemerging Infectious	Exhaustive, systematic analysis of bacterial pathogenicity and transcriptional regulation of multidrug transporters, and new strategy for drug design	¥1,000,000

	Diseases		
K. Nishino	National Agriculture and Bio-oriented Research Organization, entrusted	Regulation of Acquisition of Drug Resistance in *Escherichia coli*	¥3,000,000
K. Nishino	Japan Science and Technology Agency (PRESTO), entrusted	Roles of Xenobiotic Transporters in Cellular Physiology	¥650,000

Cooperative Research

Y. Yoshida	National Institute of Radiological Sciences	The research about the beam control for the particle beam cancer therapy.
Y. Yoshida	Sumitomo Heavy Industries, LTD	Research on photocathode RF gun and high brightness electron beam.
Y. Yoshida	Japan Atomic Energy Agency Takasaki	The research about the ion beam induced chemical reaction process by the ion pulse radiolysis.
Y. Yoshida	Japan Atomic Energy Agency Kansai	Basic research for application of femtosecond electron beam driven by high intensity laser.

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	¥43,400,000
T. Nishi	Takeda Science Foundation	Identificcation of the physiological substrates of the orphan transportes for developing the new drugs.	¥2,000,000
K. Nishino	Japan Science and Technology Agency (PRESTO)	Roles of Xenobiotic Transporters in Cellular Physiology	¥6,000,000
K. Nishino	Inoue Foundation for Science	Analysis of Drug Exporter Gene Libraries Based on Genome Information and Study of Their Regulatory Networks	¥500,000
K. Nishino	Okawa	Studies on the Regulatory	¥1,000,000

	Foundation for Information and Telecommunications	Network of Multidrug Resistance in Pathogenic Bacteria and Complex Functional Systems	
K. Nishino	Japan Research Foundation for Clinical Pharmacology	Development of Inhibitors for Bacterial Regulatory System of Multidrug Resistance	¥2,000,000
K. Nishino	Kato Memorial Bioscience Foundation	Development of Screening Devices for Antimicrobial Reagents	¥1,000,000
K. Nishino	Ohyama Health Foundation Inc.	Virulence and Drug Resistance Roles of Multidrug Efflux System	¥1,000,000
K. Nishino	Novartis Foundation (Japan) for the Promotion of Science	Analysis of Drug Resistance Determinants in Bacterial Genome	¥1,000,000

Human Interface Research Group

Professor:	Hitoshi TABATA(-2006.11.30), Hiroshi KATAYAMA-YOSHIDA Masayuki NUMAO, Riichiro MIZOGUCHI

Specially Appointment Staff

Professor:	Sunao TAKAFUJI
Associate Professor:	Takashi Kei SAITO
Research Associate:	Makoto NAKAZAWA, Ken-ichi FUKUI, Munetoshi SEKI(-2007.3.31)

Outline

Our research interests are building novel sensor and software systems, which enable analyzing human bio-signals, behaviors, 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.

Current Research Projects

Research on bio-applications of novel nano structures and on integrated operation of the interfaces (Tabata, Saito, Seki)

1) We developed the laser induced VLS method and it succeeded in producing the ZnO nano rods as bio-affinity material by bottom-up nano structure control.
2) Using the nano rods, we developed a cell membrane perforating method and established a basic technology of high throughput cell processing.
3) We strengthened the durability of the platform robot for the interface integration and invented a novel manipulator mechanism which drastically extended applicative fields of the robot.

Research on the modeling framework of functional knowledge externalization, and text mining technique for functional concepts and way knowledge (Mizoguchi, Takafuji)

1) The functional knowledge externalization model based on ontology engineering has enhanced several capabilities such as refinement of functional concepts and introducing control structure. We embodied such newest research result of ontology engineering to the modeling tool for functional knowledge externalization for any persons to evaluate.
2) Since we completed the research which purpose is to extract and arrange specific vocabularies, which are the verbs that imply functional concept, from a lot of technical documents, we made a dictionary based on them, and append it to the modeling tool for functional knowledge externalization with improving its usability by suggesting the appropriate usage of a term.
3) In order to build typical way knowledge beforehand, we started the research on

analyzing patent documents and extracting way knowledge, and implemented the basic program which has the functionality of analyzing a patent document in this fiscal year.

Research on the strategic new industry prediction accompanying change of industrial structure and success factors for high tech. venture companies (Katayama-Yoshida, Nakazawa)

1) From a correlation with the achievements of a company and a stockholder network structure, we analyzed a growth strategy. We are preparing a patent map system based on the analysis as a new industry prediction tool.

2) From case analysis of the material companies for semiconductor manufacture, we proposed a new company model which made from the following six success factors - (1) market, (2) technology, (3) cost, (4) future prediction, (5) people and an organization, and (6) finance.

The adaptive interface by the sensor network and machine learning (Numao, Fukui)

1) We proposed a human tracking method which has enough robustness in a multiperson environment and partial lost of the sensing signals, and the method could extract person's habitual paths quite correctly by the data accumulation.

2) We empirically validated the self-organization map for diagnostic support of a novel fuel cell, which performs simultaneously clustering and visualization of large-scale of acoustic emission data.

Publications

Original Papers

Basic Study on the Relationship between the Stimulation Signal to Slowly Adapting Type I Unit and thet Intensities of the Evoked Sensation, T. Suzuki, T. Saito, M. Kunimoto, K. Mabuchi, Transactions of the Virtual Reality Society of Japan, 11[1](2006),95-100.

A Multi-purpose Eight-legged Robot Developed for an Evaluation of a Neural Interface, T. K. Saito, I. Saito, N. Nemoto, K. Takiura, T. Ozeki, N. Kakuta, T. Tohyama, T. Isoyama, T. Chinzei, Springer Tracts in Advanced Robotics, 24 (2006) 385-394.

Influence of Microstructure on the Complex Permeability of Spinel Type Ni-Zn Ferrite, S.T. Mahmuda, A.K.M. Akther Hossain, A.K.M. Abdul Hakim, M. Seki, T. Kawai, H. Tabata, J. Magnetism & Magnetic Materials, 305 (2006) 269-274.

Visualization Architecture Based on SOM for Two-Class Sequential Data, K. Fukui, K. Saito, M. Kimura, M. Numao, Lecture Notes in Artificial Intelligence, 4252 (2006) 929-936.

Patent

Manipulator Mechanism, T. Saito, patent application number: 2006-226099

International Conferences

Getting Daily Human Habitual Behaviours from Infrared Sensor Network, *S. Kurihara, S. Honda, K. Fukui, K. Moriyama, M. Numao, K. Fukuda, T. Hirotsu, T. Takada, T. Sugawara, Proc. 3rd International Conference on Networked Sensing Systems (INSS2006). Chicago, Illinois, U.S.A.. May 31-Jun. 2, 2006.

Towards a Reference Ontology of Functionality for Interoperable Annotation for Engineering Documents, *Y Kitamura, N. Washio, M. Ookubo, Y. Koji, M. Sasajima, S. Takafuji, R. Mizoguchi, Proc. of the European Semantic Web Conference, ESWC2006, Budva, Montenegro, Jun. 11-14, 2006.

Room Temperature Weak Ferromagnetism in Ferroelectric $Pb(Fe,Ta)_{0.5}O_3$ & $Ba(Fe,Ta)_{0.5}O_3$ Thin Films, A. K. M. Akther Hossain, *M. Seki, T. Kawai, H. Tabata, The 17th International Conference on Magnetism, Kyoto, Japan, Aug. 20-25, 2006.

High-efficiency Cell Membrane Perforation Technique Based on Self-organized ZnO Nanorods, *M. Seki, T. Saito, H. Tabata, SSDM2006, Yokohama, Japan, Sep. 13-15, 2006.

Animal Mimic Robot as a Prototype Artificial Body for Nano Integrated Neuro-machine Interface Devices, *T. K. Saito, H. Tabata, Sanken International Symposium on Nanoscience and Nanotechnology 2006,Osaka, Japan, Sept. 19-20, 2006.

Synthesis of Oxide Nanorods by Laser-induced VLS Technique, *M. Seki, T. Fujimura, T. K. Saito, H. Tabata, The 13th International Workshop on Oxide Electronics, Ischia, Italy, Oct, 8-11, 2006.

Evaluation of Sequential AE Signals in SOFC Utilizing SOM, *N. Imanaka, K. Fukui, K. Sato, K. Moriyama, S. Kurihara, M. Numao, Proccedings of the 5th 21st Century COE "Towards Creating New Industry Based on Inter-Nanosicence" International Symposium. Awaji, Japan, Dec, 8-9, 2006.

Self-assembled Oxide Nanorods and Their Applications to Bio Systems, *M. Seki, T. Saito, H. Tabata, 5th 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Awaji, Hyogo, Japan, Dec. 8-9, 2006.

An Ontology-based Annotation Framework for Representating the Functionality of Engineering Devices, *Y. Kitamura, N. Washio, Y. Koji, M. Sasajima, S. Takafuji, R. Mizoguchi, Proc. of IDETC/CIE 2006 ASME 2006 Design Engineering Technical Conferences & Computers and Information in Engineering Conference, Philadelphia, Pennsylvania, USA, Sept. 10-13, 2006.

Photodynamic Perforation of Cell Membrane on Micro Channel Array Toward Intra Cellular Technology, *K. Iso, T. K. Saito, H. Muguruma, H. Tabata, S. Konishi, Proc. of 20th IEEE International Conference on Micro Electro Mechanical Systems (MEMS2007), Kobe, Japan, Jan.21-25, 2007.

Publications in Domestic Meetings

The Japan Society of Applied Physics	4 papers
The Society of Instrument and Control Engineers	1 paper
Japan Society for Intellectual Production	1 paper
The Japanese Society for Artificial Intelligence	2 papers
The Electrochemical Society of Japan	1 paper
The Institute of Electronics, Information and Communication Engineers	1 paper
The Physical Society of Japan	1 paper

Sponsorships

Other Research Fund

T.K. Saito	Toyama Prefectural government	Snow Robot (collaborative project)	¥2,000,000
T.K. Saito	Leadership supporting fund, ISIR,Osaka Univ.	Special facilities Support	¥1,500,000

Activities of Facilities

Workshop

Director Professor: Goro ISOYAMA
Technical Staff
Machine Shop: Michiaki KAKUICHI, Masayoshi OHNISHI
Glassworks: Hiroaki MATSUKAWA, Noriyuki OGAWA

Outline

A machine and carpentry shop and a glass factory, which are predecessors of the Workshop, were set up at the same time when the Institute of Scientific and Industrial Research was founded. The machine and carpentry shop and the glass factory were unified to be the Workshop when the Technical Division was established in 1982. Since research fields studied in the institute covers a wide range, many of experimental apparatuses requested to the Workshop are various and novel. The Workshop, which consists of the Machine Shop and the Glassworks, plays an important role in activities of the institute and contributes to them by making and providing such experimental apparatuses.

The Machine Shop performs design and trial manufacture of experimental apparatuses for science and engineering as well as production of experimental tools made of various metals. Requests of experimental apparatuses for ultra high vacuum or ultra low temperature are increasing recently and accordingly we work in closer cooperation with researchers asking such apparatuses from the design phase to respond to the requests and make apparatuses best fit to experimental purposes. A gate-type machining center was introduced in 2002, 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 Icho-Sai. The machine shop showed machine tools, displayed experimental apparatuses being made, and held a practice course of carved seals and wire handiwork. 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. At the manufacturing school from August 2 to 4, 2006 organized by the Technical Division, the workshop held two teaching courses at the Machine Shop and at Glassworks, titled respectively as "Let's make plates!" and as "Let's make Galileo thermometers!", for elementary school and junior high school students and we taught them fun of manufacturing and interest of science.

We renewed a cutting machine of the Machine Shop and a strain tester of the Glassworks and three work tables of the Glassworks. We also equipped the Machine

Shop with peripheral devices and tools for the machining center for precise machining.

The members of the Workshop organized and participated in the national technical meeting and the symposium on glass works for all the engineers and technicians of universities and national laboratories in Japan.

The Glassworks receives staff members of universities in the Kansai area for technical training in glass work and in 2006 it received persons from Kobe University, Kyoto University, Osaka Prefecture University and coached them for handing skills and technique down to the next generation. In addition, we coach technique individually for the members of the Institute.

1. Number of jobs

Machine Shop: 228 jobs (148 jobs in the previous year).
Glassworks: 240 jobs (216 jobs).

2. Number of users in the open shop

Machine Shop: 55 users (50 users in the previous year).
Glassworks: 25 users (50 users).

3. Number of visitors during Icho-Sai

Machine Shop: 70 persons (60 persons in the practice course).
Glassworks: 110 persons (100 persons).

4. Number of persons being trained

Machine Shop: 8 persons.
Glassworks: 8 persons for 25 subjects, including 10 subjects from the outside.

Office of Information Network

Professor,Director:	Katsumi TANIMURA
Professor:	Katsuaki SUGANUMA
Associate Professor:	Satoshi MURAKAMI
Research Associate:	Kouzou OHARA
Technical Staffs:	Takanori TANAKA, Senjin AIHARA, Yuka OKUMURA
Supporting Staff:	Chiaki DAVIS

Outline

Office of Information Network was inaugurated in March, 1999, to organize the operation of the information network in ISIR, which had been started with support by volunteers, because of the rapid spread of the information network and the growth of its importance in the research environment. The information was constructed as a prototype by the departments in the division of Intelligent System Science in the late 1980's and has been expanded to the whole of ISIR with the development of ODINS (Osaka University Information Network System). Recently it has played an important role in ISIR to release/access the information available in the Internet. Office of Information Network is now supporting researchers and students on the variety areas.

Laboratory for Radio-isotope Experiments

Professor: Akihito YAMAGUCHI

Outline

This laboratory is specially designed for biochemical and molecular biological experiments using radioactive compounds labeled with ^{3}H, ^{14}C, ^{32}P, ^{33}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: Yoichi YOSHIDA
Staff: Yasuko FURUTA

Outline

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, 2007)

	Number of books	Journals	Newspapers
Japanese	12588	292titles	4 titles
Foreign	44587	966titles	1 title

Academia Industry Relations Office

Director, Specially Appointed Professor: Mototaka Senda, Ph.D.
Co-Director, Specially Appointed Professor: Hirokazu Shimizu, Ph.D.

Outline

The Academia Industry Relations Office (AIR Office) of the Institute of Scientific and Industrial Research (ISIR), is dedicated to reinforcing collaboration between ISIR and the industrial community, thereby combining and developing research potential of the two sectors and promoting activities for new industrial creation and innovation. The AIR Office organizes a variety of activities to inform the industrial community of the ISIR's research efficiently through the interaction with the industrial community such as SANKEN Techno Salon (four times a year) and various Lectures events, and studied on prediction of new industry, novel system of new Industry generation, and intellectual property.

The major activities of AIR Office are: 1) A network development between ISIR and Industry, 2) Responding to inquiries from industry, 3) A liaison between academia and industrial research activities, 4) Creation of complementary opportunities for science and technology progress. AIR Office will make proposals for new business opportunity between academia and industry. New venture business activities and novel industrial products are the vision of AIR Office.

Achievements

1. Academia and Industry Renkei (communication and cooperation) Activities

The AIR Office organized to introduce the research activities and intellectual property from ISIR to the industrial community. The activities of the fiscal year 2006 are the following.

(1) A network development between ISIR and Industry: Visiting industrial entities, Exhibition of ISIR activities at various meeting, and participating to the various academic meetings and symposiums.

(2) Liaison between academia and industrial research activities and Responding to inquiries from industry
1) SANKEN Techno Salon:
2) Study groups for the new industry generation
3) Lectures and Seminars with invited speakers
4) WEB site setting
5) WEB promotion through outsourcing
6) Promotion of ISIR research activities at Exhibitions such as Technology information Exchange Exhibition and International Nanotechnology Exhibition.
7) Promotion of ISIR research activities at ISIR US Branch Opening Event

(3) Coordination of collaboration, contract research and projects with a company.
Preparation of Independent Collaboration Research Laboratories.

(4) Supporting Technology Transfer
1) Study groups for the new industry generation
2) New Venture Business Opportunity
3) Investigation of interest group on ISIR's Patents

(5) Promotion of patenting from ISIR's research activity
1) Patenting from technology seeds
2) Consulting for patent application
3) Hearing on invention with Department of Intellectual Property of Osaka University.

(6) Others
Participation as a member to the strategic meeting of Research Association of Industry and Science.
Participation as a part of Industry-Academia RENKEI Organization Meetings.

2. Promotion Activity for the new industry generation

Three seminars with invited speakers were held as a series of lectures titled "Intellectual property management for new industry generation".

Three speakers were invited at our intensive strategic intellectual property lecture series. Dr. Tohru Degawa, business consultant from Tokyo, lectured "Collaboration between Academia and Industry & Intellectual Management". Ms. Suzue Fujimori, esq., a lawyer who came from San Francisco, California, gave a talk titled "Intellectual Property Market in the US". Mr. Giichi Marushima from Tokyo, spoke out the strategic IP management to strengthen an entity on the current trend of our economy.

Public Relations Office

Director Professor: Akihito YAMAGUCHI
Support Staff: Noriko MATSUMOTO

Outline

Public Relations Office was opened on February 1, 2006. We provide the right information of our Research Institute for the public effectively. The major activities of Public Relations Office are: 1) To collect any required file to generate the basic plan of the publicity, 2)To support editing and issue the Memoirs of ISIR (annual report) and publications, 3)To collect any requires document for creating and editing of official WEB of ISIR, 4)To perform Press Release except the subjects related to the section of general affairs, 5)To collect and preserve of any press release related to ISIR.

Technical Division

Head: 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.