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MEMOIRS OF THE

Institute of Scientific and Industrial Research

OSAKA UNIVERSITY

Contents

Foreword

The Institute of Scientific and Industrial Research was started as a part of Osaka University in 1939. Since then, the Institute had developed into one of the leading research organization for science and engineering in our country. We are hoping that our research on materials/devices, information/intelligence, biology/biotechnology, and their interdisciplinary areas will contribute to the industries, and ultimately to the next generations. "Memoirs of the Institute of Scientific and Industrial Research (ISIR)" has witnessed the sixty-four years' history of the Institute, since it was published in 1940, one year after the foundation of ISIR.

The roles of Memoirs had been changed with time. During the first decade, its main role was to publish original research papers. However, staff of the Institute started to publish their original work in international journals, and Memoirs became a vehicle for reviews of joint researches and abstracts of papers published by the members of the Institute. Since 1997, Memoirs has become our annual publication summarizing the scientific activities of ISIR.

We report here information such as current research programs and recent findings of each laboratory, list of publications, financial supports from granting agencies, and all other scientific activities. We hope that this publication will be useful and stimulating for researchers in universities, research institutes and industries, and young scientists outside as well as inside our Institute.

Tomoji Kawai
Director,
The Institute of Scientific and
Industrial Research

Outline of ISIR

1. Research Activities

1) History and Organization

The Institute of Scientific and Industrial Research (ISIR) was founded in 1939 as a part of Osaka University, in response to the strong requests from the industrial community of the Kansai area in Japan. The original buildings were constructed in Sakai supported financially by an association of leading private enterprises in Osaka. ISIR moved to the present place in Suita Campus in 1968. For more than half a century, ISIR has been very active as a University-associated research Institute, and dedicated to the advance of basic and applied sciences, especially in the fields of electronics, computer science, metallurgy, inorganic chemistry, organic chemistry, biochemistry, and radiation science. The Institute also has been developing industrial applications of the results obtained by staff members. We celebrated the fiftieth anniversary in 1989.

In April 1995, ISIR was reorganized in order to respond effectively to the highly developed science and technology in this country. It has modified its structure to expand basic original research, and to promote interdisciplinary programs based on the three major fields: material sciences, information sciences, and biological sciences. ISIR has at present six research divisions and two institute-associated research centers. The organization of ISIR is shown on the next page. A new building was constructed in 2001 and in 2003 in response to the increased number of scientists and the development of Nanotechnology, respectively. The Nanotechnology and Nanoscience Center has started in April 2002. In April 2005, Materials Science and Technology Research Center for Industrial Creation has started, in order to promote technology tarnsfer from ISIR to the industry.

The number of staff scientists is 105 in total, including full professors, associate professors, and assistant professors. Ages and Alma Maters of professors and research staff are shown below. In almost all the large national universities in this country, most of the faculties are graduates of their own university. However, more than half of the staff scientists in ISIR were graduated from other universities. This is an exceptional case in this country, and contributes to promoting scientific activities of the Institute.

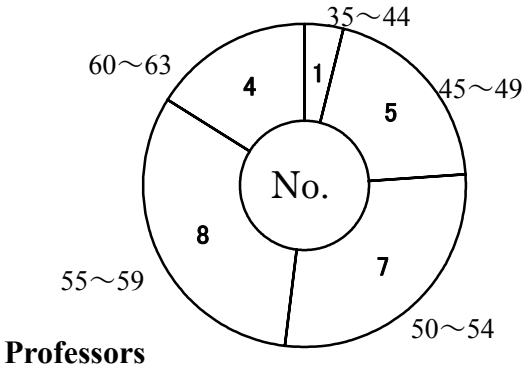
Divisions	Departments
Quantum Engineering	Quantum Molecular Devices Photonic and Electronic Materials Semiconductor Electronics Condensed Matter Physics
Advanced Materials Science & Technology	Structural Characterization and Design Metallic Materials Process Atom Scale Science Functional Ceramic Materials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

Research Centers (Two Centers)

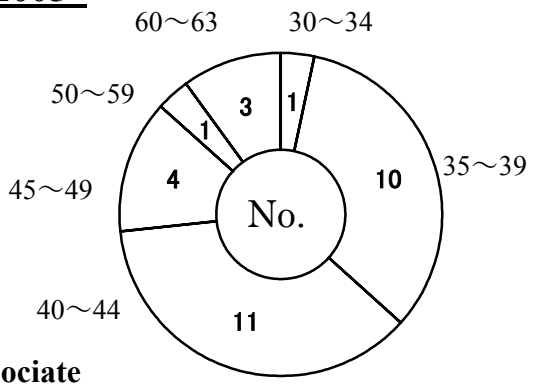
Nanoscience and Nanotechnology Center	**Nanomaterials and Nanodevices** Artificial Nanomaterials for Bio-Information Systems Single-Molecular Integrated Devices Supramolecular Chemistry Nanobiology Nanosystem Design

	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** **Nanotechnology Process Foundry**
Materials Analysis Center	
Service Facilities	Workshop Office of Information Network Laboratory for Radio-Isotope Experiments Library

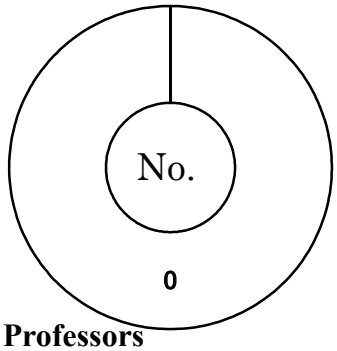
Staffs' Age (years old) –As of 3.30.2005



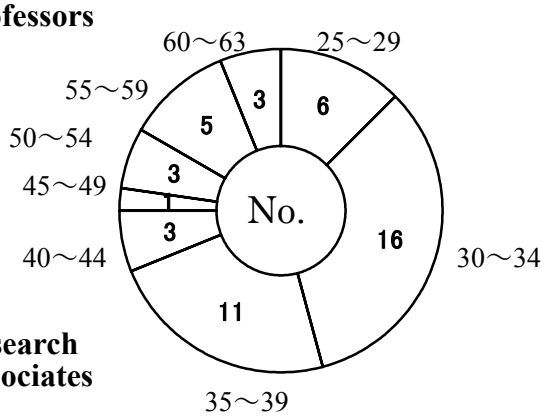
Professors



Associate Professors

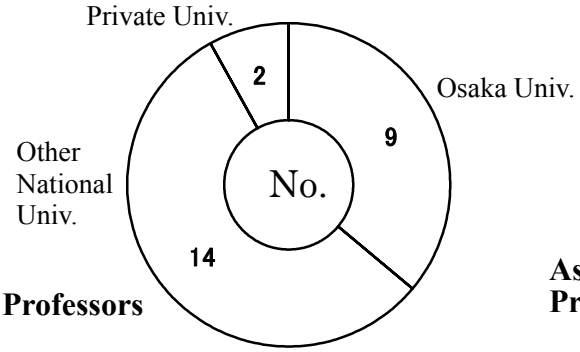


Assistant Professors

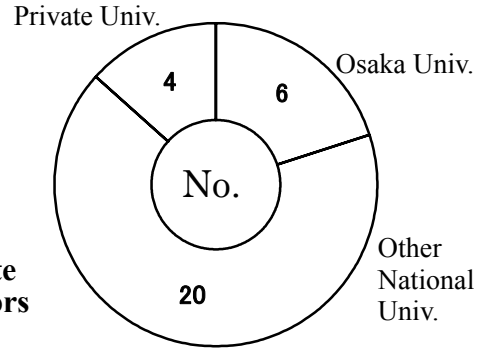


Research Associates

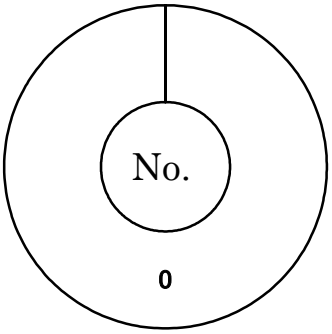
Staffs' Alma Mater –As of 3.30.2005



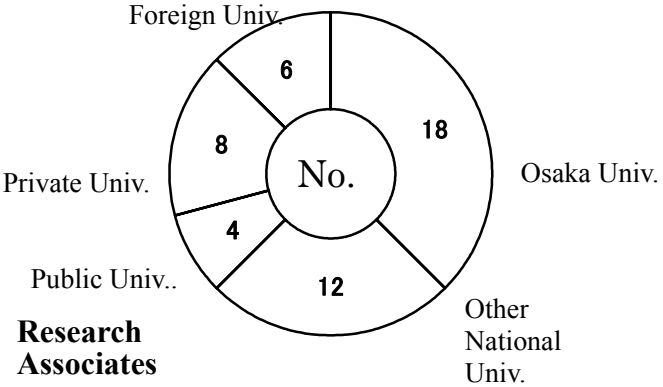
Professors



Associate Professors



Assistant Professors



Research Associates

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, 2005 is Professor Tomoji Kawai.

Important matters of ISIR are discussed and determined by the Faculty Council, which consists of the Director and all the full 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 Institute budget, 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. Institute budget is composed of various items including Project Research. Project Research was planned in the Research Plan Committee of ISIR and the plan was proposed to Ministry. After the judgment of Ministry, the budget was granted to the Institute.

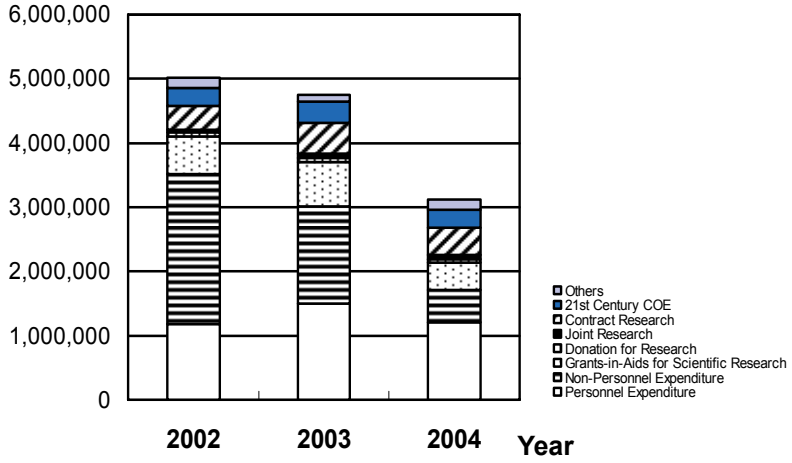
In 2002, the following project has been selected as a 21st Century Center of Excellence (COE) program from the Ministry of Education, Culture, Sports, Science and Technology.

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 2004 is 423,960,000 yen.

Donation for Research

Donation for Research is accepted after the Judgement of Committee and the amount in these two years are as follows.

(Unit : kilo yen , ( ) Number)

Division / Year	Quantum Engineering	Advanced Materials Science and Technology	Organic Molecular Science	Intelligent System Science
2003	1,500 (2)	24,300 (20)	10,250 (13)	6,480 (5)
2004	1,111 (2)	30,811 (23)	3,950 (7)	4,352 (8)

Division / Year	Biological Science	Quantum Beam Science and Technology	Nanoscience and nanotechnology center	Others	Total
2003	8,350 (9)	2,000 (3)	11,050 (14)	1,000 (1)	64,930 (67)
2004	3,833 (5)	1,111 (2)	9,010 (12)	1,480 (18)	55,658 (77)

4) Cooperative Research

Cooperative Researches and Contract Researches in the fiscal year 2003-2004 are as follows: Cooperative Researches are carried out with 22 organizations. The budget for the fiscal year 2003-2004 is 61,989,000 yen. Contract Researches are 44. The budget for the fiscal year 2003-2004 is 429,474,000 yen.

5) International Research Projects

Koichi Niihara	Core University Program (CUP) between Japan and Korea (Joint Research Projects under the Bilateral Programs between JSPS and KOSEF). "New Processing and Nanostructure/Property Relationship for Multi-functional Ceramic Materials" (in the field of Ceramic Materials Technology)

6) Symposia, Seminars, Workshops and Lectures

International Seminar on Core University Program between Japan and Korea (CUP Seminar 2004) was held on October 31 –November 3 in conjunction with the 3rd International Symposium on Science of Engineering Ceramics. In this seminar 60 papers were presented for this project. More than 400 participants from over 20 countries joined in this joint seminar.

The first research conference on membrane export proteins (21 Nov 2004)

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 2004, the symposium was held on November 26. The topics were "Development of New Industries from Interdisciplinary Research".

The eighth SANKEN International Symposium / The third International Symposium on Scientific and Industrial Nanotechnology (SISSIN-2004) on "Advanced Characterization for Nano-materials, Nano-devices and Nano-processing" was held on 6-7 December, 2004 at the Osaka University Convention Hall, Osaka University. In this symposium, invited lectures by 18 outstanding researchers from the world and invited talks by 6 researchers from the ISIR as well as 130 poster papers were presented. The number of participants was over 260.

Japan Bioenergetics Group (16-18 Dec 2004)

The second research conference on membrane export proteins (21 Jan 2005)

The third 21st Century COE Program "Toward Creating New Industries Based on Inter-Nanoscience" International Symposium was held on 9-10 March, 2005 at the Oku-Biwako Makino Prince Hotel (Makino-Cho, Takashima-Gun, Shiga). Invited lectures by 9 outstanding researchers from the world and invited talks by 5 researchers from the 21-COE groups as well as 101 poster papers were presented. The number of participants was over 160.

The third research conference on membrane export proteins (18 Mar 2005)

Other Lectures and Seminars

15 Apr 2004	Duk Yong Yoon (Korea Advanced Institute of Science and Technology, Professor)	Interface Roughening Transition and Grain Growth in Ceramics and Metals
16 Apr 2004	Sylwester POROWSKI (Polish Academy of Sciences, Professor)	High Pressure Research and Blue Lasers
16 Apr 2004	Stanislaw FILIPEK (Institute of Physical Chemistry of the Polish Academy of Sciences, Professor)	New Metal Hydrides Obtained UnderVery High Pressure of Gaseous Hydrogen
14 May 2004	Erja Turunen (VTT Technical Research Centre of Finland, Professor)	Sealing of thermally sprayed coatings for boiler applications
14 May 2004	Tommi Varis (VTT Technical Research Centre of Finland, Professor)	Sealing of thermally sprayed coatings for boiler applications
15 May 2004	Masahiko Koizumi (Kyoto Prefectural University of Medicine, Professor)	Radiation therapy and active oxygen
19 May 2004	Ramasamy RAMARAJ (Madurai Kamaraj University, India, Professor)	Photoelectrocatalytic reactions at chemically modified electrodes and membranes
28 May 2004	Hiroshi Omote (Okayama University, Associate Professor)	Drug transport mechanism of multidrug resistance protein, P-glycoprotein
4 Jun 2004	Kamanio Chattopadhyay	Understanding and designing the

	(Indian Institute of Science, Tata Chem Chair Professor)	microstructure through laser surface alloying
26 Jun 2004	Ryo Shimizu (Tanabe Seiyaku Co., Ltd., Research and Development Dept. Senior Scientist)	Development of New Drugs using Structure-Based Drug Design Technique, Part Ⅰ
26 Jul 2004	Joao Gama (University of Porto, Portugal, Associate Professor)	Learning Decision Trees from Data Streams
11 Aug 2004	Ryo Shimizu (Tanabe Seiyaku Co., Ltd., Research and Development Dept. Senior Scientist)	Development of New Drugs using Structure-Based Drug Design Technique, Part Ⅱ
10 Sep 2004	Ryo Shimizu (Tanabe Seiyaku Co., Ltd., Research and Development Dept. Senior Scientist)	Development of New Drugs using Structure-Based Drug Design Technique, Part Ⅲ
21 Oct 2004	Takahiro Hanyu (Tohoku University, Professor)	Circuit of non-volative Logic-in-memories and their application
21 Oct 2004	Byeong Kang (University of Tasmania, Australia, Senior Lecturer)	Ripple Down Rules and Web Monitoring System
2 Nov 2004	Minoru Kawahara (Graduate School of Engineering, Osaka University, Researcher)	Growth of GaN single crystals with low dislocation-density by the Na flux method
4 Nov 2004	Takeshi Nishimatsu (Institute for Materials Research, Tohoku University, Research Associate)	Automatic calculations of energy surfaces of Perovskite Ferroelectric crystals by first-principles calculations
5 Nov 2004	Roman Nowak (Helsinki University of Tech, Professor)	THICKNES OF THE COMPONENTS OF MULTILAYER-STRUCTURE DETERMINED BY NON-CONTACT INDENTATION
12 Nov 2004	Chrys Chatgilialoglu (Institute for the Organic Synthesis and Photoreactivity, Bologna, Italy, Dr.)	Free radical chemistry in the carbohydrate moiety of nucleosides. Model studies of DNA damage
16 Nov 2004	Koichi Furukawa (National Institute of Advanced Industrial Science and Technology, AIST, Senior Scientist)	Dynamics in formation of B cell repertoire and affinity maturation of antibody
2 Dec 2004	Pang Kwok Pan (Monash University, Australia)	Improving the Centered CUSUMS Statistic for Structural Break Detection in Time Series
7 Dec 2004	Masasuke Yoshida	Structural biology of chaperonin

	(Tokyo Institute of Technology, Professor)	protein
7 Dec 2004	So Iwata (Imperial College London, Professor)	Structural biology of membrane protein: focusing on crystallization and crystallographic analysis of membrane transporter
9 Dec 2004	Dae Won Cho (Seonam University, Namwon, Korea, Professor)	Photophysics of Expanded Porphyrins
17 Dec 2004	Shinya Yoshikawa (University of Hyogo, Professor)	Reaction mechanism of cytochrome *c* oxidase
17 Dec 2004	Genji Kurisu (The University of Tokyo, Associate Professor)	Structure and function of the cytochrome b_6f complex: differences among the complexes from cyanobacteria, green alga and higher plant
17 Dec 2004	Taiji Nakae (Tokai University, Professor)	Problems in the energy transduction in the MexAB-OprM xenobiotic transporter in *Pseudomonas aeruginosa*
17 Dec 2004	Yoshikatsu Kanai (Kyorin University, Professor)	Protein-protein interactions involving organic solute transporters: toward the identification of the transporter complexes that enable functional coupling of multiple transporters
17 Dec 2004	Masasuke Yoshida (Tokyo Institute of Technology, Professor)	Engine and brakes of ATP synthase
17 Dec 2004	Hideo Akutsu (Institute for Protein Research, Osaka University, Professor)	Structural change of H^+-ATPase monomeric β subunit for driving force of the rotation of the F_1 motor
17 Dec 2004	Hiroyuki Noji (The University of Tokyo, Associate Professor)	Ultra-sensitive detection of ATP synthesis by F_1-ATPase with microfabrication and a single-molecule manipulation techniques
17 Dec 2004	Toshio Yanagida (Graduate school of Frontier Biosciences, Osaka University, Professor)	Flexibility of bio-systems revealed by a single-molecule nano-measurement
17 Dec 2004	Keiichi Namba (Graduate school of Frontier Biosciences, Osaka University, Professor)	Self-Assembly and switching of the bacterial flagellum
24 Dec 2004	Hiroaki Koga (National Institute for Materials Science)	A study of crystal growth of cubic boron nitrides by first-principles calculations

29 Dec 2004	Katsuhiko Takagi (Nagoya University, Professor)	Nanocomposites having photoresponsible activity
5 Jan 2005	Todd B. Marder (University of Durham, UK, Professor)	Synthesis and Properties of Conjugated Organoelement Compounds
12 Jan 2005	Kyuho Lee (Seoul University)	Pentacene on Au(001):first-principles calculations using localized basis
18 Jan 2005	Jun-Hyung Cho (Dept. of Physics, Hanyang University)	Adsorption and reaction of unsaturated hydrocarbons on Si(001) and Ge(001)
19 Jan 2005	Yong Hee Kim (Hannam University, Korea, Dr.)	Sensitized Emission of Luminescent Lanthanide Complexes Based on Naphthalene Derivatives through Charge Transfer Process
5 Feb 2005	Minoru Yamaji (Gunma University, Professor)	Dissociation of higher triple excited states
14 Feb 2005	Tomoyuki Higuchi (The Institute of Statisitical Mathematics, Professor)	Data Fusion, Prediction and Discovery based on Bayse Model
15 Feb 2005	Werner Schlegel (University of Geneva Medical School, Foundation for Medical Research, Switzerland, Professor, Director)	Intracellular Signaling and Gene Expression: Immediate early response gene transcription is dynamically controlled at the level of elongation
18 Feb 2005	Masahiro Koiwa (Kyoto University, Emeritus Professor)	Serendipity and Materials Developments
28 Feb 2005	Ryusuke Nakamura (Tohoku University, Lecturer)	Supersaturated vacancy in B2-type intermetallic compounds and self-developments
28 Feb 2005	Yasuhiro Ikeda (Yamaguchi University School of Medicine, Department of Molecular Cardiovascular Biology)	Calcium lon-Regulating Protein as a New Drug Target for Heart Failure
8 Mar 2005	Andreas Ochsner (University of Aveiro, Portugal, Associate Professor)	Elastic and plastic behavior of porous metals under uniaxial stress

7) Public Information Activity

Public information activity of ISIR in 2004 is as follows:

- Bulletin of ISIR (2004) (in both Japanese and English)
- Memoirs of the Institute of Scientific and Industrial Research, Osaka University (Vol.61, 2004) (in English)

- Annual Report of ISIR (2004) (in Japanese)
- SANKEN News Letters, 22-24(in Japanese)
- Report on SANKEN TECHNO SALON (2004) (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 2004 is 481. The details are described in the part of activity of divisions and facilities.

9) Scientific Awards

R.Mizoguchi	JSAI Incentive Award (The Japanese Society for Artificial Intelligence)
H.Nakajima	Tanigawa-Harris Award (The Japan Institute of Metals)
H.Nakajima	Tawara-Best Paper Prize (Iron Steel Institute of Japan)
T.Ikeda	Tawara-Best Paper Prize (Iron Steel Institute of Japan)
T.Aoki	Tawara-Best Paper Prize (Iron Steel Institute of Japan)
T.Kujime	Encouragement Award (High Temperature Society of Japan)
H.Nakajima	Best Poster Prize (International Conference on New Frontier of Process Science and Engineering in Advanced Materials)
T.Ikeda	Best Poster Prize (International Conference on New Frontier of Process Science and Engineering in Advanced Materials)
T.Ide	Best Poster Prize (International Conference on New Frontier of Process Science and Engineering in Advanced Materials)
K.Sato	Young Scientist Award (Japan Institute of Metals)
K.Sato	Excellent Poster Award (High Temperature Society of Japan)
M.Ishimaru	Excellent Poster Award (High Temperature Society of Japan)
Y.Hirotsu	Excellent Poster Award (High Temperature Society of Japan)
T.Sekino	Scientific Encouragement Award (The Japan Society of Pow. and Pow. Metal)
T.Kusunose	Scientific Encouragement Award

	(The Japan Society of Pow. and Pow. Metal)
T.Nakayama	Scientific Encouragement Award
	(The Japan Society of Pow. and Pow. Metal)
T.Kusunose	Ceramographic Award
	(The Ceramic Society of Japan)
T.Sekino	Ceramographic Award
	(The Ceramic Society of Japan)
K.Niihara	Ceramographic Award
	(The Ceramic Society of Japan)
K.Niihara	ECD Bridge Building Award
	(The American Ceramics Society)

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 1, 2005 is as follows.

G.S. / Course	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Course	33	50	16	9	9	3	120
Doctor Course	25	36	6	3	5	0	75
Total	58	86	22	12	14	3	195

Number of students who had obtained Master's or Doctor's Degree in 2004 is as follows.

Field / Degree	Science	Engineering	Engineering Science	Pharmaceutical Science	Information Science and Technology	Frontier Biosciences	Total
Master Degree	15	36	2	4	1	0	58
Doctor Degree	6	8	0	1	1	0	16
Total	21	44	2	5	2	0	74

3. International Exchange

1) Exchange Agreement

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

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

2) Foreign Researchers and Students

Number of foreign researchers and students staying in ISIR as of March 31, 2005 is 30 in total. Details are: Research Associates (6),Visiting Researchers (1), Research Students (4), Graduate Students (Doctor Course) (17), (Master Course) (2). Their nationalities are : Korea (12), China (7), India (4), Thailand (2), Egypt (1), Bangladesh (1), Taiwan (1), Philippines (1), Finland (1) Foreign visitors in 2004 are as follows: U.S.A. (19), Korea (6), Canada (1), India (1), Ukraine (1), Portugal (1), Netherlands (2), Australia (1), Norway (1), Austria (1), U.K. (6), Italy (1), Sweden (3), Switzerland (1), Brazil (1), France(2), Germany (6), Poland (3) Total (57).

3) International Conferences and Symposiums

Number of presentations (plenary, invited, oral and poster in various international conferences and symposia) by staff of ISIR is 816 in total.

Number of ISIR staffs who have been working as committee members of International Conferences or Editorial Board of international academic journals are 189 in total. For more details, see the part of activity of divisions and facilities.

4. Concluding Remarks

(1) Organization and Management System

By the reorganization of the Institute in 1995, previous small research divisions were grouped into larger ones including several professors, associate professors and research associates in order to increase joint research and scientific communication among scientists. 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.

(2) Budget and Facilities

Sufficient research budget has been obtained for the Institute compared with other research institutes. Necessary facilities and equipments for researches have been installed to a considerable level. A new building was constructed in 2001 and in 2003 to the increased number of scientists and the development of Nanotechnology, respectively. Nanosocience and Nanotechnology Center started in April 2002, and in 2005, Materials Science & Technology Research Center for Industrial Creatiuon has launched as a joint center between ISIR and Institute of Multidisciplinary Research for Advanced Materials, Tohoku University. Reconstruction of an old first research building is necessary for the next advance and development of the Institute.

In 1997, Harmonized Materials Research Group was designated as one of the Centers of Excellence (COE) of Ministry of Education, indicating the high research activity of the Institute. The COE budget has been one of the important resources for the Institute for exploiting new and interdisciplinary research through basic science and technology.

(3) Graduate and Undergraduate Education

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

The Sanken Techno-Salon is a forum 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.

(4) Contribution to Societies

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

In 2005, the office for cooperation of university/industry will be settled in order to strengthen cooperation between the Institute and industries.

(5) International Exchange

More foreign researchers and students could be able to join the Institute. We are trying to invite more researchers and students from other countries. International Conferences sponsored by our Institute have been held twice a year since 1998. It's so important to release our results towards all over the world and have a chance to exchange opinions with foreign scientists.

(6) Future Plan and Prospect

In 1998, Future Planning Committee was established in the Institute. Future plan of the Institute has been discussed in this Committee and summarized in annual report which can be seen in the Home Page of ISIR (http://www.sanken.osaka-u.ac.jp/). From 2004, all the committee systems have been reconstructed to promote research and education activities based on the policy of National University Agencies.

The Institute of Scientific and Industrial Research is making constant efforts toward higher level contribution to science and industries.

Activity 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, arrangement of biomolecules on silicon substrates, 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 on Si surfaces and thermal deformation of Si trenches
- Dvelopment of bio/chemical imaging sensor and nano-patterning of biomolecules
- Crystal growth, characterization and device application of new semiconductors including Tl-III-V, III-V nitrides, magnetic III-V semiconductors and quantum nanostructures
- Control of the physical properties of carbon nanotibes and the fabrication of single electron transistor
- Prediction of new functional materials, high efficient energy conversion materials and fabrication processes by first principles electronic structure calculations
- Materials 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:	Tatsuo YOSHINOBU
Research Associates:	Toshiyuki ADACHI, Koichi SUDOH
Post Doctoral Fellow:	Hongwen LIU, Shanmugam KUMARAN
Graduate Students:	Hitoshi KURIBAYASHI, Hideaki FUJIMURA, Hiroomi GOTO, Koji MIYAZATO, Yuki MORIKAGE
Support Staff:	Fumi TOGAI

Outlines

The Department of Quantum Molecular Devices is engaged in development of novel devices that integrate the quantum mechanical features of semiconductors and molecular functions of biomolecules including DNA and protein. We are also developing the Scanning Chemical Microscope for visualization of chemical and biological specimens.

Current Research Programs

Kinetics of Step Flattening on $SrTiO_3$(001) Surfaces

Kinetics of step flattening on $SrTiO_3$(001) surfaces have been studied, using ultrahigh vacuum scanning tunneling microscopy (STM). By examining the wavelength dependence of Fourier components of step edges during thermal flattening, the dominant mechanism for step motion was determined to be attachment/detachment of adatoms migrating on terraces. It was also found that the repulsive interactions between steps accelerate decay of large wavelength components of step edge structures.

Shape Transformation of Si Trenches by Hydrogen Annealing

Thermal relaxation of micron-sized trench structures fabricated on Si(001) by high temperature hydrogen annealing has been studied. Morphology of trench sidewalls has been observed by atomic force microscopy (AFM). It was found that, during trench corner rounding, step instability occurs, leading to drastic morphological changes of sidewall surfaces. Performing numerical simulations based on a one-dimensional step flow model, we have shown that the observed step instability occurs when the mass transport on each terrace obeys a local mass conservation low.

Patterning of Biomolecules on Si by AFM Anodic Oxidation

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

Observation of Protein by AFM, STM and Spectroscopic Ellipsometry

AFM, STM and (scanning) spectroscopic ellipsometry were applied to observation and detection of protein molecules on solid surfaces.

Study of Luminescent Organic Films by STM-induced Luminescence

The molecular luminescence of porphyrin film on a nanometer region has been observed in air for the first time. The spectra excited by tunneling electron injected from STM shows peaks which are nearly identical to photo luminescence peaks.

Application of the Chemical Imaging Sensor to Microfluidic Devices

A flow channel was microfabricated on the surface of the chemicalimaging sensor, which allows visualization of ion distributions inside the channel.

Publications

Original Papers

Fractal Aggregation of DNA after Therma Denaturation, L. Yan and H. Iwasaki: Chaos, Solitons and Fractals., 20 (2004) 877-881.

Immobilization of Urease and Cholinesterase on the Surface of Semiconductor Transducer for the Development of Light-Addressable Potentiometric Sensors, I. G. Mourzina, T. Yoshinobu, Yu. E. Ermolenko, Yu. G. Vlasov, M. J. Schöning and H. Iwasaki: Microchim. Acta., 144 (2004) 41-50.

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Yoshinobu, W.-C. Moon, A. Nishikawa, J. Suzuki and H. Iwasaki: Sensors and Materials, 16 (2004) 421-428.

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Analysis of Cu Silicides by Atom Probe Field Ion Microscope, T. Adachi: J. Vac. Soc. Jpn. 47 (2004) 567-573.

Growth of SiC Nanodots on Si(111) by Exposure to Ferrocene and Annealing Studied by Scanning Tunneling Microscopy, K. Kametani, K. Sudoh, and H. Iwasaki: Thin Solid Films 467 (2004) 50-53.

International Conferences

Surface Morphological Evolution During Protein Crystal Growth from Solutions, K. Kimura, T. Yoshinobu, K. Sudoh and *H. Iwasaki, 2004 Scanning Probe Microscopy, Sensors and Nanostructures, Beijing - TEDA, China, May. 23 – 27, 2004.

Interaction between Steps on $SrTiO_3$(001) Vicinal Surfaces, K. Sudoh and *H. Iwasaki, 2004 Scanning Probe Microscopy, Sensors and Nanostructures, Beijing - TEDA, China, May. 23 – 27, 2004.

Island Nucleation during Submonolayer Growth of CaF_2 on Vicinal Si(111), Y. Miyata, K. Sudoh, and *H. Iwasaki, 2004 Scanning Probe Microscopy, Sensors and Nanostructures, Beijing - TEDA, China, May. 23 – 27, 2004.

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Micropatterning of Biomolecules on Silicon by AFM Anodic Oxidation (Poster), * T. Yoshinobu, W. Moon, A. Nishikawa, J. Suzuki and H. Iwasaki, International Symposium on Cellular Engineering and Nanosensors (part of the 38th Annual Congress on Biomedical Engineering), Ilmenau, Germany, September. 21 2004.

Immobilization of DNA on Arrayed SiO_2 Dots Prepared by AFM Anodic Oxidation (Poster), * T. Yoshinobu, W. Moon, A. Nishikawa and H. Iwasaki, 5th International Symposium on Electrochemical Micro& Nanosystem Technologies (EMT2004), Tokyo, Japan, September. 28 – October. 1 2004.

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Patterning of Biomolecules on Silicon by AFM Oxidation, *T. Yoshinobu, W. C. Moon, A. Nishikawa, J. Suzuki and H. Iwasaki, 2004 International Microprocesses and Nanotechnology Conference (MNC 2004), Osaka, Japan, October. 26 - 29, 2004.

STM-Excited Fluorescence from Organic Films, *H. W. Liu, R. Nishitani, T. Yoshinobu, H. Iwasaki and T. Matsumura-Inoue, Korea Japan Joint Forum 2004 "Organic Materials for Electronics and Photonics", Okinawa, Japan, November. 3 - 6, 2004.

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Portable Multi-Sensor LAPS (Light-Addressable Potentiometric Sensor) for Ion Sensing, T. Wagner, R. Otto, H. Iwasaki, *T. Yoshinobu and M.J. Schöning, Shanghai International Conference on Physiological Biophysics (Shanghai ICPB'04), Shanghai, China, November. 9 - 13, 2004.

AFM Micropatterning of Protein and DNA Molecules on Si, *T. Yoshinobu, W.-C. Moon, A. Nishikawa, J. Suzuki and H. Iwasaki, Shanghai International Conference on Physiological Biophysics (Shanghai ICPB'04), Shanghai, China, November. 9 - 13, 2004.

STM-Excited Luminescence from Organic Materials on Au(111) (Poster), *H. W. Liu, R. Nishitani, Y. Ie, T. Yoshinobu , Y. Aso and H. Iwasaki, SANKEN International Symposium on Scientific and Industrial Nanotechnology - Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing (8th SANKEN International Symposium & 3rd International Symposium on Scientific and Industrial Nanotechnology), Osaka, Japan, December. 6 - 7, 2004.

STM Study on Scaling Property of 2D Island Density in CaF_2 Growth on Vicinal Si(111) (Poster), *K. Sudoh, Y. Miyata, K. Kametani and H. Iwasaki, SANKEN International Symposium on Scientific and Industrial Nanotechnology - Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing (8th SANKEN International Symposium & 3rd International Symposium on Scientific and Industrial Nanotechnology), Osaka, Japan, December. 6 - 7, 2004.

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AFM Micropatterning of Biomolecules on Silicon (Invited), *T. Yoshinobu, Molecule-Based Information Transmission and Reception - Application of Membrane Protein Biofunction - (MB-ITR2005), Okazaki, March. 3 - 7 2005.

Study of Porphyrin Molecules Adsorbed on Conductive Substrates by STL (Poster), *H. W. Liu, R. Nishitani, Y. Ie, T. Yoshinobu, Y. Aso and H. Iwasaki, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium (ISCOE-2005), Shiga, March. 9 - 10 2005.

Positive Patterning of Ferritin Molecules on Silicon (Poster), *K. Shanmugam, S. Iida, T. Yoshinobu and H. Iwasaki, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium (ISCOE-2005), Shiga, March. 9 - 10 2005.

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

Publications in Domestic Meetings

The Japan Society of Applied Physics	2 papers
The Physical Society of Japan	2 papers
The Vacuum Society of Japan	2 papers
The Surface Science Society of Japan	1 paper
The Electrochemical Society of Japan	1 paper
The Chemical Society of Japan	1 paper

Academic Degrees

Master Degree of Engineering

Hideaki FUJIMURA	Behavior of Steps during Relaxation of Micro-Structures on Crystalline Surfaces

Sponsorship

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

T. YOSHINOBU	Development of Multiple Ion Imaging Sensor and its Application to Biological Specimens	¥1,200,000

Other Research Fund

H. IWASAKI	Foundation for Biomedical Research and Innovation 2,3-D Display of Cells and Its Application to Next Generation Analysis System	¥4,437,500

Department of Photonic and Electronic Materials

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Support Staff:	Noriko KIKUMOTO

Outlines

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

Current Research Programs

Crystal Growth and Properties of Diluted Magnetic Semiconductors

Diluted magnetic semiconductors, which have two characters of semiconductors and magnetic materials, are gathering interest as a candidate for new functional materials. In 2001, we succeeded in the growth of GaCrN and observed the room temperature ferromagnetism as well as the PL emission. We also observed the room temperature ferromagnetism together with sharp PL emission for the rare-earth doped GaN, GaGdN and GaEuN. By the EXAFS measurement, we confirmed that the Cr, Gd and Eu atoms occupy the Ga site. Great advances in 2004 are the fabrication/demonstration of the magnetic spin tunnel characteristics in DyN/GaN superlattice structure diodes as well as the fabrication/demonstration of the vertical magneto-resistance characteristics in GaCrN/GaN/GaCrN ferromagnetic/nonmagnetic/ferromagnetic trilayer structure diodes.

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 succeeded in the growth of TlInGaAs by MBE and already realized the pulsed-current injection laser operation in TlInGaAs/InP DH laser diodes (LDs) at room temperature and confirmed the small temperature variation of lasing peak wavelength as small as 0.06 nm/K. We also confirmed the small temperature variation of the refractive index of TlInGaAs. In 2004, we have proposed the TlInGaAsN/AlGaAs for both temperature-stable wavelength and threshold current LDs and succeeded in the growth of TlInGaAs/GaAs heterostructures. We also achieved the current injection laser operation in TlInGaAs/GaAs LDs. To further improve the TlInGaAs/InP LD characteristics, we proposed the insertion of TlInP cladding layer. We have measured the refractive index of TlInP and confirmed the effectiveness of the TlInP cladding layer.

Crystal Growth and Characteristics of Nitride Semiconductor Mixed Crystals

III-V nitride semiconductors gather much interest from the viewpoint of application to light emitting devices as well as devices used in harsh environment. We have observed the strong PL emission from the grown polycrystalline GaN and proposed the wide variety of device applications. We also obtained the good electric field emission characteristics of electrons from GaN/metal samples, which is promising to fabricate the field emission electron source devices. In 2003, we formed the GaN nano-rod structures on Si substrate and obtained the very small threshold voltage of 1.1 V/μm for the electron emission. In 2004, we confirmed the improvement in field emission threshold voltage by the growth of thin AlN layer on the nano-rod top surfaces because of small electron affinity of AlN. We also showed the existence of the optimum nano-rod size.

Self-Formation and Properties of Semiconductor Quantum Structures

By growing GaAs/InAs short period superlattices on InP (411)A substrates, we succeeded in the fabrication of QDs showing the controlled PL emission at wavelengths of 1.3-1.6 μm, which is very important wavelength region in the optical information communication systems. In 2004, by using these QDs together with the InAlAs current blocking layer we have realized the current injection lasing operation.

Nano-Observation and Characterization of Short-Channel MOSFET

The nano-structural and physical properties of the short-channel MOSFETs are studying with STM from various viewpoints. In 2004, we have succeeded in the visualization of the device nano-structures for the samples with different cross section angle and position.

Publications

Original Papers

Observation of photoluminescence emission in ferromagnetic semiconductor GaCrN, M. Hashimoto, H. Tanaka, R. Asano, S. Hasegawa, and H. Asahi: Appl. Phys. Lett. 84 (21) (2004) 4191-4193.

Growth and characterization of new III-V-based magnetic semiconductors for

application to semiconductor spintronics devices (Invited), H. Asahi, Y.K. Zhou, M. Hashimoto, H. Tanaka and S. Emura: Proceedings of 12th International Workshop on The Physics of Semiconductor Devices (Eds. by K.N. Bhat and A. DasGupta, 2004 Narosa Publishing House, New Delhi, India) 1095-1100.

Migration enhanced epitaxy (MEE) growth of five-layer asymmetric coupled quantum well (FACQW) and its cross-sectional STM observation, J.H. Noh, S. Hasegawa, T. Suzuki, T. Arakawa, K. Tada and H. Asahi: Physica E 23 (2004) 482-486.

Wavelength control of 1.3 –1 .6 μm light emission from the quantum dots self-formed in GaAs/InAs short-period superlattices grown on InP (411)A substrates, *J. Mori, T. Nakano, T. Shimada, S. Hasegawa and H. Asahi: J. Appl. Phys. 96 (3) (2004) 1373-1375.

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GaN-based magnetic semiconductors for nanospintronics (Invited), H. Asahi, Y.K. Zhou, M. Hashimoto, M.S. Kim, X.J. Li, S. Emura and S. Hasegawa: J. Phys.: Condens. Matter. 16 (48) (2004) S5555-S5562.

Optical properties of GaN-based magnetic semiconductors, Y.K. Zhou, M.S. Kim, X.J. Li, S. Kimura, A. Kaneta, Y. Kawakami, Sg. Fujita, S. Emura, S. Hasegawa and H. Asahi: J. Phys.: Condens. Matter. 16 (48) (2004) S5743-S5748.

Magnetic, optical and transport properties of GaN-based ferromagnetic/nonmagnetic heterostructurtes, M.S. Kim, Y.K. Zhou, X.J. Li and H. Asahi: J. Phys.: Condens. Matter. 16 (48) (2004) S5711-S5716.

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Local structural change in GaCrN grown by radio frequency plasma-assisted molecular-beam epitaxy, M. Hashimoto, H. Tanaka, S. Emura, M.S. Kim, T. Honma, N. Umesaki, Y.K. Zhou, S. Hasegawa and H. Asahi: J. Cryst. Growth 273 (2004) 149-155.

Two-dimensional characterization of carrier concentration in metal-oxide-

semiconductor field-effect transistors with the use of scanning tunneling microscopy, H. Fukutome, H. Arimoto, S. Hasegawa, and H. Nakashima: J. Vac. Sci. Technol. B22 (2004) 358-363.

Accelerated decay of the 31-yr isomer of Hf-178 induced by low-energy photons and electrons, C. B. Collins, N. C. Zoita, F. Davanloo, S. Emura, Y. Yoda, T. Uruga, B. Patterson, B. Schmitt, J. M. Pouvesle, I. I. Popescu, V. I. Kirischuk and N. V. Strilchuk: Laser Physics, 14 (2004) 154-165.

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Ferromagnetic semiconductors and their synthesis, H. Asahi: in *From Introduction to Magnetism to Spintronics Materials and Devices*, Introductory Seminar to Spintronics 3 (2004) 53-61.

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Temperature-stability of lasing wavelength for TlInGaAs/InP DH laser diodes and 77K CW operation, *A. Fujiwara, H.J. Lee, A. Imada, K. Mukai, S. Hasegawa and H. Asahi, Second 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" and 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, January 13-14, 2004.

Luminescence from Gd Site in Dilute Magnetic Semiconductor GaGdN, *S. Emura, Y.K. Zhou, M. Hashimoto, H. Tanaka, M.S. Kim, S. Kimura, S. Shanthi, X.J. Li, N. Teraguchi, A. Suzuki, A. Yanase, and H. Asahi, Second 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" and 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, January 13-14, 2004.

Tunneling magnetoresistance effect in magnetic semiconductor heterostructure DyN/GaN, *M.S. Kim, Y.K. Zhou, X.J. Li and H. Asahi, Second 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" and 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, January 13-14, 2004.

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Optical properties of GaN-based magnetic semiconductors, *Y.K. Zhou, M.S. Kim, X.J. Li, S. Kimura, A. Kaneta, Y. Kawakami, Sg. Fujita, S. Emura, S. Hasegawa and H. Asahi, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

Magnetic, optical and transport properties of GaN-based ferromagnetic/nonmagnetic semiconductor heterostructures, *M.S. Kim, Y.K. Zhou, X.J. Li and H. Asahi, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

Raman scattering characterization of GaN-based spintronics materials, *H. Fukumura, N. Hasuike, H. Harima, K. Kisoda, M. Hashimoto, Y.K. Zhou and H. Asahi, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

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Reduced temperature dependence of refractive index in TlInGaAs by addition of Tl, A. Imada, A. Fujiwara, H.J. Lee, *T. Mukai, S. Hasegawa and H. Asahi, 16th International

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GaN-based diluted magnetic semiconductors for spintronics (Invited), *H. Asahi, Y.K. Zhou, M.S. Kim, S. Emura, S. Shanthi, S. Kimura and S. Hasegawa, 31st International Symposium on Compound Semiconductors, Seoul, Korea, September 12-15, 2004.

Polycrystalline GaN for field electron emitter application (Invited), *S. Hasegawa, S. Nishida, T. Yamashita and H. Asahi, International Conference on Polycrystalline Semiconductors 2004, Potsdam, Germany, September 5-10, 2004.

Formation of local ferromagnetic area on GaAs by focused Mn ion beam implantation, *M. Kasai, J. Yanagisawa, H. Tanaka, S. Hasegawa, H. Asahi, K. Gamo, and Y. Akasaka, 14th International Conference on Ion Beam Modification of Materials, Monterey, California, USA, September 5 - 10, 2004.

Magnetoresistance in GaCrN-based ferromagnet/nonmagnet/ferromagnet trilayer structures, *Y.K. Zhou, M.S. Kim, H. Kimura, S. Emura, S. Hasegawa and H. Asahi, 13th Semiconducting and Insulating Materials Conference, Beijing, China, September 20-25, 2004.

Magnetic, electric and optical properties of AlN and GaN doped with rare-earth element Gd, *S.W. Choi, Y.K. Zhou, M.S. Kim, S. Kimura, S. Shanthi, S. Emura, S. Hasegawa and H. Asahi, 3rd Asian International Symposium on the Science of Engineering Ceramics, Osaka, Japan, October 31-November 3, 2004.

Optical properties of Cr-doped GaN/AlN quantum dots, *H. Munakata, S. Matsuno, S. Hasegawa and H. Asahi, 3rd Asian International Symposium on the Science of Engineering Ceramics, Osaka, Japan, October 31-November 3, 2004.

Emission spectra from AlN and GaN doped with rare earth elements, (Invitrd) S. Emura, *S.W. Choi, S. Kimura, M.S. Kim, Y.K. Zhou, N. Teraguchi, A. Suzuki, A. Yanase, and H. Asahi, International Conference on Rare Earths in Nara, Nara, Japan, November 7-12, 2004.

Electron field emission from polycrystalline GaN nanorods (Invited), *S. Hasegawa and H. Asahi, 2004 Fall International Symposium on Crystal Growth and Devices, Seoul, Korea, November 10-13, 2004.

Evaluation of device configurations through different cross-sectional planes of 0.1 μm MOSFETs by scanning tunneling microscopy/spectroscopy, *S. Hasegawa, W. Doi, A. Yabuuchi and H. Asahi, 12th International Colloquium on Scanning Probe Microscopy, Izu-Atagawa, Shizuoka, December 9-11, 2004.

Luminescence properties of GaN and AlN doped by rare earth elements, *S. Emura, S.W. Choi, S. Kimura, S. Kobayashi, M.S. Kim, S. Shanthi, Y.K. Zhou, N. Teraguchi, A. Suzuki and H. Asahi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, December 6-7, 2004.

Effect of chromium doping on the luminescence properties of GaCrN on sapphire, *S. Shanthi, M. Hashimoto, S. Kimura, Y. K. Zhou, S.W. Choi, M. S. Kim, S. Emura, S. Hasegawa and H. Asahi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, December 6-7, 2004.

Cross-sectional scanning tunneling microscopy study of 100 nm MOSFETs through the different cross sections, *W. Doi, A. Yabuuchi, S. Hasegawa and H. Asahi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, December 6-7, 2004.

The use of selected monochromatic X-rays to induce a cascade of gamma transitions from the 31-year nuclear isomer to the 4 second isomeric state of Hf-178, *N.C. Zoita, F. Davanloo, C.B. Collins, J.M. Pouvesle, S. Emura, I.I. Popescu, V.I. Kirischuk, N.V. Strilchuk, T. Uruga and Y. Yoda, UVX2004, St. Etienne, France, June 7 – 11, 2004.

Li De-intercalate mechanism of the layered $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$, *H. Kobayashi, Y. Arachi, S. Emura, H. Kageyama, K. Tatsumi and T.Kamiyama, 12th International Meeting on Lithium Batteries, Nara, Japan, June 27 – July 2, 2004.

Crystal structure and feasibility for 16x DVD-rewritable media of In-Sb phase-change material, *H. Miura, E. Suzuki, H. Tashiro, M. Harigaya, K. Ito, N. Iwata, A. Watada, K. Tani, Y. Nakata and S. Emura, PCOS symposium, Osaka, Japan, Novembre 18 – 19, 2004.

Contributions to International Conferences and Journals

H. Asahi	16th International Conference on Indium Phosphide and Related Materials (International Steering Committee member)
H. Asahi	International Conference on Nanospintronics Design and Realization (Organizing Committee member)
H. Asahi	International Workshop on Nitride Semiconductors 2004 (International Advisory Committee member)
H. Asahi	12th International Colloquim on Scanning Probe Microscopy (Steering Committee member, Publication Committee member)
H. Asahi	14th International Conference on Molecular Beam Epitaxy (Organizing Committee Vice-Chair, Program Committee Chair)
H. Asahi	17th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	SANKEN International Symposium on Scientific and Industrial Nano-Technology 2004 (Organizing Committee member, Local Arrangement Chair)
H. Asahi	Third International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" (Organizing Committee member, Publicity and Publication Chair)
H. Asahi	International Workshop on Nitride Semiconductors 2006 (International Advisory Committee member)
H. Asahi	SpinTech III (Organizing Committee member)
H. Asahi	2005 International Conference on Solid State Devices and Materials (Program Committee member)
S. Hasegawa	16th International Conference on Indium Phosphide and Related Materials (Conference Arrangements Committee member)
S. Hasegawa	14th International Conference on Molecular Beam Epitaxy (Program Committee member, Treasures Committee member)
S. Hasegawa	SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004 (Executive Committee member)
H. Asahi	Japan. J. Appl. Phys. (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	22 papers
Electronic Materials Symposium	2 papers
Symposium on PASPS	3 papers

Academic Degrees

Master Degree of Engineering

S. Kimura	Crystal Growth and Characterization of GaN-Based Diluted Magnetic Semiconductors

T. Mukai Study on Crystal Growth, Characterization and Device Application of TlInGaAsN/GaAs by Gas Source MBE

Master Degree of Science

T. Shimada Study on III-V Semiconductor Quantum Dots

W. Doi Study on Nano-Characterization of Nano-Structure Devices by Scanning Tunneling Spectroscopy

H. Munakata Study on Fabrication and Characterization of Cr-Doped GaN/AlN Quantum Dots

T. Yamashita Field Emission from GaN Nano-Rods Formed on SiO2/Si

Sponsorship

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

H. Asahi	Study on Applications of Polycrystalline Nitride Semiconductors to Field Emission Electron Source and Visible Fluorescent Substance	¥4,200,000
S. Hasegawa	Nano-Magnetic Characterization of Diluted Magnetic Semiconductors by Spin-Polarized Scanning Tunnel Spectroscopy	¥3,500,000

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

S. Emura	Study on the Local Atomic Arrangement and the Origin of Magnetism of GaN-Based Ferromagnetic Semiconductors by XAFS and XMCD	¥500,000

Entrusted Research

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

Other Research Fund

H. Asahi	MEXT Special Coordination Funds for Promoting Science and Technology (H. Kasai)	Design and Invention of Spintronics ¥18,717,000

Department of Semiconductor Electronics

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Supporting Staff:	Ayumi OKANO

Outlines

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

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

Current Research Programs

Chirality Selected Growth of Carbon Nanotubes Using a Laser CVD Method

It is important to grow carbon nanotubues with the chirality suitable for the application to quantum devices. Last year, carbon nanotubes with the specific chirality could be removed from the other nanotubes by the laser irradiation with the resonant wavelength in atmosphere. Conversely this year, we have developed a laser CVD method in which carbon nanotubes are grown under specific laser irradiation, and in this method, it may be possible to promote the growth of carbon nanotubes with the specific chirality by the resonance effect.

Raman Scattering Spectra of Oxygen Ion-Implanted Carbon Nanotubes

It is known that carbon nanotubes usually shows p-type character in atmosphere. In order to obtain n-type carbon nanotubes, oxygen ions have been implanted into carbon nanotubes at 25 eV which is near to the exchange energy of C atoms in the graphene. In resonant Raman scattering spectra of the implanted carbon nanotubes, the characteristic shift of the resonant energies has been observed. It has been concluded that O atoms are stable at the substitutional site in carbon nanotubes by the 1st principle calculations. The shift of resonant energies can be explained due to the change of electronic band

structures in carbon nanotubes doped with substitutional O atoms.

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

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

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

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

Publications

Original Papers

Effects of Ultra Low Energy Nitrogen Ion Irradiation on Carbon Nanotube Channel Single-Electron Transistor, T. Kamimura, K. Yamamoto and K. Matsumoto: Jpn. J. Appl. Phys., Vol. 43, No. 5A, (2004) 2771-2773.

Reduction of Hysteresis by Refining Process to Carbon Nanotube Field-Effect Transistors, T. Kamimura and K. Matsumoto: IEICE TRANS. ELECTRON, E87-C, (2004) 1795-1798.

Chirality Selection of Single-Walled Carbon Nanotubes by Laser Resonance Chirality Selection Method, K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto: Appl. Phys. Lett. 85 (2004) 858-860.

Field emission characteristics from CNT field emitter arrays grown on silicon emitters, T. Yoshimoto, D. Kamimaru, H. Iwasaki, T. Iwata, and K. Matsumoto: J. Vac. Sci. Technol. B 22(3), 1338 (2004).

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Growth Control of Carbon Nanotube for Electron Device Applications, M. Maeda, T. Kamimura, C. K. Hyon, A. Kojima, K. Matsumoto: Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials SSDM, pp.346 - 347.

Ballistic Transport of Hole in p Type Semiconductive Carbon Nanotube, T. Kamimura, K. Matsumoto: Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials SSDM, (Tokyo) pp. 344-345.

Chirality Selection of Single-Walled Carbon Nanotubes by Laser Resonance Chirality Selection Method, K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto: Virtual Journal of Nanoscale Science & Technology, VOL10, August 16, (2004), http://www.vjnano.org.

International Conferences

Coherent Transport of Hole in p Type Semiconductive Carbon Nanotube, *T. Kamimura, C. K. Hyon, A. Kojima, M. Maeda, and K. Matsumoto, Device Research Conference(DRC) Notre Dame University, Jun. 22, 2004.

Carbon Nanotube Quantum Devices and its Applications with Ultra-High Charge Sensitivity (Invited), *K. Matsumoto, Japan-Switzerland Nanoscience Workshop, Nara, Jun.23, 2004.

Control of Electrical Property of Carbon Nanotube by Oxygen Ion Implantation with Ultra-low Energy of 25eV, *T. Kawai, T. Kamimura, C. K. Hyon, A. Kojima, M. Maeda, K. Matsumoto, The Electronic Materials Conference (EMC), Notre Dame University, Jun. 24. 2004.

P type Semiconductive Carbon nanotube for Quantum Wire, *T. Kamimura, C. K. Hyon, A. Kojima, M. Maeda, K. Matsumoto, The Electronic Materials Conference (EMC), Notre Dame University, Jun. 24. 2004.

Growth Control of Carbon Nanotube by Applied Electric Field, *M. Maeda, T. Kamimura, C. K. Hyon, A. Kojima, K. Kurachi, T. Kawai, M. Torigoe, K. Matumoto, Electronic Material Conference Notre Dame University, Jun. 24, 2004.

Application of Ultra-High Sensitive Electrometer by Carbon Nanotube Quantum Dot Single Electron Transistor at Room Temperature, *K. Matsumoto, NANO 8, Venice, Jul. 1, 2004.

High Sensitivity of Carbon Nanotube Single Electron Transistor Sensor, *K. Matsumoto, T. Kamimura, A. Kojima, Y. Nagamune, Asia-Pacific Conference on Transducer and Micro-Nano Technology (APCOT MNT2004), Sapporo, Jul. 6, 2004.

Coexistence of Ballistic Transport and Coulomb Blockade Effect of Hole in 4mm Carbon Nanotube Channel Transistor, *K. Matsumoto, T. Kamimura, 27th Int. Conf. on

Physics of Semiconductors Flagstaff, Arizona, USA, Jul. 26-30, 2004.

Chirality Selection of Single-Walled Carbon Nanotubes by Laser Resonance Chirality Selection Method, *K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto, 27th Int. Conf. on the Physics of Semiconductors, Flagstaff, Arizona, USA, Jul. 26-30, 2004.

Transport Properties of Charge Carriers in Single-Walled Carbon Nanotubes by Pulse-Radiolysis Time-Resolved Microwave Conductivity Technique, *Y. Ohno, K. Maehashi, K. Inoue, K. Matsumoto, A. Saeki, S. Seki, and S. Tagawa, 27th Int. Conf. on the Physics of Semiconductors, Flagstaff, Arizona, USA, Jul. 26-30, 2004

The Application of AFM Electrical Manipulation to the Fabrication of Room Temperature Operating Carbon Nanotube SET, *C. K. Hyon, T. Kamimura, A. Kojima, M. Maeda, K. Matsumoto, NANO KOREA 2004 Symposium and Exhibition, Seoul, Aug. 24, 2004.

Field-Emission Characteristics from Carbon Nanotube Single Emitter Grown on Si Cone, *T. Yoshimoto, T. Iwata, K. Matsumoto, 15th European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, Nitrides & Silicon Carbide, Sept. 12-17, Riva Del Garda, Italy, Sep. 12-17, 2004.

Carbon Nanotube Devices and Bio-Sensor Applications with Ultra-High Charge Sensitivity (Invited), *K. Matsumoto, JAIST International Symposium on Nano Technology 2004, Kanazawa, Sep. 9, 2004.

Ballistic Transport of Hole in p Type Semiconductive Carbon Nanotubes, *T. Kamimura, and K. Matsumoto, The 2004 International Conference on Solid State Devices and Materials (SSDM), Tower Hall Funabori, Tokyo, Sep. 16, 2004.

Growth Control of Carbon Nanotube for Electron Device Applications, *M. Maeda, T. Kamimura, C. K. Hyon, A. Kojima, K. Matsumoto, The 2004 International Conference on Solid State Devices and Materials (SSDM), Tower Hall Funabori, Tokyo, Sep.16, 2004.

Ballistic Transport of Hole in 4μmm Carbon Nanotube Channel Transistor with Coulomb Blockade Effect, *K. Matsumoto, 51th American Vacuum Society Meeting, Anaheim USA, Nov. 15, 2004.

Carbon Nanotube Applications for Nanoelectronic Devices (Invited), *K. Matsumoto, The 1st International Symposium on the Functionality of Organized Nanostructures (FON'04) Tsukuba, Dec. 2, 2004.

Laser-Resonance Chirality Selection in Single-Walled Carbon Nanotubes, *K. Maehashi, Y. Ohno, K. Inoue, and K. Matsumoto, Sanken Int. Symp. on Scientific and Industrial Nanotechnology 2004: Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, Dec. 6-7, 2004.

Carbon Nanotube Field-Effect Transistors with Si3N4 Passivation Films Formed by Catalytic Chemical Vapor Deposition Method, *H. Ozaki, D. Kaminishi, Y. Ohno, K. Maehashi, K. Inoue, K. Matsumoto, Y. Seri, A. Masuda, and H. Matsumura, Sanken Int. Symp. on Scientific and Industrial Nanotechnology 2004: Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan Dec. 6-7, 2004.

Laser-Irradiated Chemical Vapor Deposition for Position-Controlled Growth of Single-Walled Carbon Nanotubes, *Y. Fujiwara, K. Maehashi, Y. Ohno, K. Inoue and K. Matsumoto, Sanken Int. Symp. on Scientific and Industrial Nanotechnology 2004: Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan Dec. 6-7, 2004.

Flash-photolysis Time-resolved Microwave Conductivity Measurements of Single-Walled Carbon Nanotubes, *Y. Ohno, K. Maehashi, K. Inoue, K. Matsumoto, A. Saeki, S. Seki, and S. Tagawa, Sanken Int. Symp. on Scientific and Industrial Nanotechnology 2004: Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, Dec. 6-7, 2004.

Carbon Nanotube Devices and Applications, *K. Matsumoto, Advanced Hetero Workshop, Hawaii, Dec. 10, 2004.

Carbon Nanotube Quantum Devices and its Application to Bio-Sensor with Ultra-High Sensitivity (Invited), *K. Matsumoto, The 6th International Conference on Nano-Molecular Electronics (ICNME 2004), International Conference Center Kobe, Dec. 17, 2004.

Contributions to International Conference and Journals

K. Matsumoto	2004 Advanced Heterostructure Workshop (co-chairperson)
K. Matsumoto	The 2nd international conference on Quantum Sensing: Evolution and Revolution from Past to Future at the SPIE Optoelectronics （Organizing committee）
K. Matsumoto	Seventh International Conference on New Phenomena in Mesoscopic Structures (Organizing committee)
K. Matsumoto	Fifth International Conference on Surfaces and Interfaces of Mesoscopic Devices (Organizing committee）

Publications in Domestic Meetings

The Japan Society of Applied Physics 28 papers

Cooperative Research

K. Matsumoto	Mitsubishi Chemical Corporation	Bio-sensor by carbon nanotube single electron transistor at room temperature	¥20,000,000

Other Research Fund

K.Matsumoto	Japan Science and Technology Agency	Carbon nanotube single electron single spin measurement systems	¥120,000,000

Department of Condensed Matter Physics

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Support Staff:	Mika ASADA

Outlines

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

Current Research Programs

Ab 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. We have simulated the enhancement of the atomic diffusion of boron (B), hydrogen (H), and oxygen (O) in silicon under the electronic excitation.

Materials Design for the High-efficient Amorphous Silicon Solar Cells.

We have proposed a mechanism of photo-induced degradation for amorphous silicon solar cells based upon *ab initio* molecular dynamics simulation. In this mechanism, the conversion from the negative effective U dangling bond to the positive effective U dangling bond is the key point to understand the mechanism. We proposed

a new mechanism of the CN treatment to avoid the photo-induced degradation in silicon-based solar cells.

Spintronics and Materials Design Using Semiconductor Nanostructures.

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 (Tc) and 3d transition atom dependence of Tc in above diluted ferromagnetic semiconductors. New functional 4d-transition-metal (*4d*-TM)-doped K_2S diluted magnetic semiconductors with transparent and half-metallic ferromagnetism are designed based upon the first principles calculations. We have systematically investigated the magnetism in *4d*-TM-doped K_2S DMSs. K_2S is a transparent semiconductor with anti-CaF_2 crystal structure and has large lattice spacing due to its large ionic radius of K. It is found that Zr-, Nb-, Tc-, Ru- and Rh-doped K_2S show the half-metallic and high-spin ferromagnetism and that Zr- or Nb-doped K_2S are promising candidate for high-Tc ferromagnetic DMSs with transparecy and large magneto-optical effect.

We have designed the transparent and half-metallic ferromagnetic oxide in C and N-doped BaO, CaO, MgO, SrO, and SiO_2.

We have proposed a new methodology to calculate the Curie temperature (Tc) by using the exchange interaction as a function of the distance of the magnetic atoms and Monte Carlo calculation. We obtained the reasonable agreement between the design ed Tc and the experimental data in homogeneous systems such as (Ga,Mn)As and (Zn,Cr)Te.

We also designed the Delafossite $CuAlO_2$-based transparent and half-metallic ferromagnetic semiconductors.

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 $CuAlO_2$.

Materials Design of Spin and Charge Control Method in Heme-protein.

We proposed a new model to describe the spin (high-spin vs. low-spin ground state) and charge control (multiple charged states) in heme protein. We have studied the magnetic interaction of spins in this system and proposed a materials design for biological sensors.

Fermiology of Highly Correlated Electron Systems by FLAPW-LSDA+U Method

The new *ab initio* method for the electric structure calculation of highly correlated electron systems are developed by using the FLAPW-LSDA+U method and taking into account the spin-orbit interactions. We have calculated the Fermi surface of

ferromagnetic CeSb and $CeRh_3B_2$, and analyzed the Fermi surfaces and compared with detail of the experimental data. We have understood the complex Fermi surfaces of these highly correlated electron systems.

Electronic Structures of Newly Reported Superconductors

Electronic bandstructures have been calculated for new superconductors Y_2C_3 and KOs_2O_6. From the result, in Y_2C_3, C-p electrons should play a significant role in its superconductivity.

n-Alkane and Metal Surface Interaction

The interaction between n-alkane and metal surfaces has been studied by means of density-functional theoretical calculations within a generalized gradient approximation GGA. We demonstrate that although the GGA cannot reproduce the physisorption energy well, our calculations can reproduce the experimentally observed work-function change and softening of the CH stretching mode reasonably well. We also show that the most significant factor determining their dependence on metal substrates is the distance between the molecule and the substrate.

Chiral Structure of Glycinate on Cu(001)

We have examined the stability of self-assembled monolayers of glycinate on the Cu(001) surface by density functional theoretical calculations. We found that a c(2x4) homochiral structure is as stable as a (2x4)-pg heterochiral (pseudo-2x2) structure, strongly suggesting the co-existence of the both phases. Calculated STM images agree well with the experimentally observed ones.

Adsorption States of Au on TiO_2(110)

The atomic and electronic structures of Au/TiO_2s110d systems have been investigated theoretically based on the density-functional theory. The adhesive energies between the Au layer and the TiO_2 surface for the nonstoichiometric surfaces are much larger than that for the stoichiometric surface. The charge transfer between the Au ad atom and the substrate is negligible for the stoichiometric surface, in accordance with its smaller adhesive energy. The electron transfer occurs from the six fold Ti atom to the Au atom for the Ti-rich surface, while from the Au atom to the in-plane and inner oxygen atoms for the O-rich surface. It can be said that the TiO_2 surface conditions such as defects or nonstoichiometry strongly affect the adsorption energy and the electronic structure of the Au adlayer. This point should be closely related to the catalytic property of the Au/TiO_2 system.

Origin for the Stability of the Ge/Si(105) Surface

We studied stability and electronic structure of the Ge(105)1x2 surface by density functional theory (DFT) calculations. We show that the (001) surface is more stable than the (105) surface if the in-plane lattice constant is equal to the equilibrium lattice constant of Ge (a-Ge), while (105) becomes much more stable than (001) when the in-plane lattice constant is compressed to aSi. This stability change is in agreement with experimental observations that Ge(105) is stable on the Si substrate, and the reason can be explained from the differences in the surface bond lengths of the two surfaces. Because the Ge-Ge bond length is considerably elongated near the Ge(105) surface, the

surface bond lengths approach their equilibriumvalues by compressing the in-plane lattice constant from aGe to aSi, and (105) becomes fairly stable. Band calculations revealed that the gap between occupied and unoccupied surface states is quite large, suggesting the stability of the surface.

Atomic Geometries and the Electronic Properties of Alq_3/Al Interfaces

We have studied the atomic geometries and the electronic properties of the Alq_3/Al interface by using density functional theoretical calculations. We examined three surfaces, the close packed Al(111) surface, the Al(332) stepped surface, and the Al adatom adsorbed Al(111) surface to investigate the effect of the surface roughness on the electronic properties of the interfaces. The calculated interface dipoles agree reasonably well with the experimental results and we found that the origin of the interface dipole formation mainly comes from the permanent dipole moment of Alq_3 molecules. Although we have examined various possible structures, an interface gap state observed experimentally could not be reproduced by the present calculations.

Chemical Reactions between Alq_3 and Al Atoms

In the actual production process of organic electroluminescent (EL) devices, electrode metals are deposited onto organic EL materials such as Alq_3. In order to clarify the chemical reactions at the metal-organic interfaces, we have examined the deposition process of Al onto Alq_3 by using density functional theoretical simulations. We found that the first Al interacts strongly with Alq_3 molecule while the second one interact with Alq_3-Al complex quite weakly. Currently, we are investigating the electronic origin for the reactivity.

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Bandstructure Calculations and Fermi Surfaces of Ferromagnetic CeSb, *K. Yamauchi, A. Yanase, H. Harima and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Contributions to International Conferences and Journals

H. Katayama-Yoshida	3rd International Conference on Physics and Application of Spin-related Phenomena in Semiconductors: PASPS3 (International Advisory Committee and Program Committee)
H. Katayama-Yoshida	1st International Conference on Nanospintronics Design and Realization: ICNDR (Organizing Committee and Program Committee and Proceedings Editor)
H. Katayama-Yoshida	23rd International Conference on Defects in Semiconductors : ICDS23 (Conference Chair)
H. Katayama-Yoshida	The third international school and conference on spintronics and quantum information technology: Spintech III (Conference Chair)
H. Katayama-Yoshida	International Conference on Magnetism: ICM2006 (Organizing Committee)

Publications in Domestic Meetings

The Physical Society of Japan	20papers
The Japan Society of Applied Physics	5papers
Discussion meeting for molecular structures	1papers
The Membrane Society of Japan	1papers

Academic Degrees

Doctor Degree of Science

K. Yamauchi	Theoretical Study on Electronic Bandstructure of Ferromagnetic Ce Compounds

Master Degree of Science

M. Toyoda	Development of self-interaction corrected electronic structure calculation method and study on electronic and magnetic state in ZnO-based dilute magnetic semiconductors"
T. Fukushima	Theoretical Prediction of Curie temperature in (Zn,Cr)S, (Zn,Cr)Se and (Zn,Cr)Te by First Principles Calculations.

Master Degree of Engineering

H. Kizaki	First-principles materials design of $CuAlO_2$ based dilute magnetic semiconducting oxide
K. Kenmochi	Materials Design of Transparent and Half-Metallic Ferromagnetic Semiconductors without Transition Metal Elements

Sponsorship

Grant-in-Aid for Scientific Research on the Priority Area (M. Shirai)

H. Katayama-Yoshida Design for Opto-spintronics and Spin Prove

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

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

Entrusted Research

Special Coordination Funds for Promoting Science and Technology

H. Katayama-Yoshida	Design and Fabrication of Nanospintronics Computational Nanomaterials and Device Design	¥27,164,000

Ministry of Education, Culture, Sports, Science and Technology
Grant-in-Aid for the Creation of Innovations through Business-Academic-Public Sector Cooperation

H. Katayama-Yoshida	Research on selective and low-temperature impurity diffusion in semiconductor by infra-red laser excitation	¥4,500,000

Japan Science and Technology Corporation

H. Katayama-Yoshida Core Research for Evolutional Science and Technology (H. Kobayashi)

Silicon Thin Film Solar Cells with New Chemical Bonds

Japan Science and Technology Corporation

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

Japan Science and Technology Corporation

Y. Morikawa — Core Research for Evolutional Science and Technology
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Japan Science and Technology Corporation

H. Katayama-Yoshida — Research and development Applying Advanced Computational Science and Technology
(H. Akai)
Computational Nano-materials Design

New Energy and Industrial Technology Development Organization (NEDO)

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

Cooperative Research

H. Katayama-Yoshida	Institute for Materials Research, Tohoku Univ.	Spintronics in II-VI based ferromagnetic semiconductors
H. Katayama-Yoshida	SPring8	Mechanism of New Materials Fabrication Using Electronic Excitation
H. Katayama-Yoshida	International Institute of Advanced Study	Materials Science and System Design
H. Katayama-Yoshida	Jülich Institute (Germany)	Computational Materials and Devices Design for Nanospintronics
Y. Morikawa	School of Science, the University of Tokyo	Catalytic reactions on metal oxide surfaces
Y. Morikawa	National Institute of Advanced Industrial Science and Technology (AIST)	Simulation on Metal-Organic Interfaces and Electrochemical Reactions
Y. Morikawa	Institute of Materials Science, Univ. of Tsukuba	Reaction processes of formate on Cu catalysis
Y. Morikawa	Fuji Photo Film CO., LTD.	Electronic structure of inorganic optical materials
Y. Morikawa	The Institute for Solid State Physics, The Univ. of Tokyo	Origin for the stability of the Ge/Si(105) surface

and
Institute for Materials Research,
Tohoku Univ.

Division of Advanced Materials Science and Technology

Outline

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

Achievements

- Designing, prediction of atomic structure and properties of materials by computer simulation
- Local structural analysis of amorphous materials
- Fabrication and physical properties of nano-particles
- Fabrication of high-performance lotus-type porous metals and its application
- Diffusion in intermetallic compounds
- Observation and manipulation of DNA on inorganic substrate by SPM
- Construction and properties of functional artificial lattices by laser MBE and atomic layer controlled super-ferroelectric materials
- Design and development of brain mimetic memory and super five sensor
- Improvement of Si solar cell characteristics by use of new method of eliminating defect states
- Formation of dielectric films by use of new chemical reactions and the application to MOS devices
- Development and materials design of strong and tough ceramic-based nanocomposites
- Development of new functional ceramics from nanocomposite concept
- Preparation and design of atomic/molecular-level composites
- Laser-induced nano-processing of semiconductor surfaces
- Dynamics of photoinduced phase transitions in low-dimensional crystals

Department of Structural Characterization and Design

Professor:	Yoshihiko HIROTSU
Associate Professor:	Manabu ISHIMARU
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Outlines

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

Current Research Programs

Nanocrystallization Process in Fe-based Amorphous Alloys

We have examined a bcc-Fe nanocrystallization process in amorphous $Fe_{84}Nb_7B_9$ by means of transmission electron microscopy and electron diffraction with the help of reverse Monte Carlo (RMC) simulation. The RMC simulation for amorphous states indicated an existence of bcc-like local atomic arrangements around Fe atoms, even in an as-quenched state. In an annealing state, moreover, a development of the local bcc-Fe regions was revealed by high-resolution electron microscopy supported by image simulations, a radial distribution function analysis and a nanobeam diffraction technique. We concluded that the bcc-Fe nanocrystallization is ascribed to the appearance and development of the local bcc-Fe regions as a local structural fluctuation.

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) We established a determination process of the long-range order parameter for isolated $L1_0$-type nanoparticles by electron diffraction with the aid of intensity calculation taking the multiple scattering of electrons into consideration. (2) With this method long-range order parameters for individual FePd nanoparticle were determined by using nano-beam electron diffraction. As a result, particle size dependence of the order

parameter was firstly revealed and the decrease of the order parameter was observed with particle size reduction below about 8 nm in diameter. (3) 10-nm-sized Fe-Pt-Cu nanoparticles with orientation and high-density dispersion were fabricated by rf-magnetron sputtering under the lower substrate temperature as low as 340^{o}C. Large coercivities as large as 1.4 and 5.3 kOe were obtained for these FePtCu nanoparticles at 300 and 10 K, respectively.

Local Structure Analysis of Amorphous Materials

We analyzed atomistic structures of functional amorphous materials by transmission electron microscopy and computer simulations. The following results were obtained. (1) Thermally-induced SiO_2 as a gate insulator layer was characterized by high-resolution electron microscopy. It was found that medium-range ordered regions exists in the amorphous matrix. (2) Structural relaxation in amorphous Si-Ge alloys was examined by a molecular-dynamics approach. On the basis of the results obtained by the present simulations, we found that major changes in topological short-range order upon annealing occurred within the second coordination shell, while chemical short-range order was not altered. (3) A local atomic structure of an amorphous Ge-Sb-Te thin film in a rewritable optical recording disk was studied using cross-sectional nano-beam electron diffraction and HREM techniques. Atomistic structures of medium range order observed in the amorphous matrix were examined in detail, and the mechanism of functional rapid crystallization in the optical recording was discussed.

Publications

Original Papers

Nanoscale Phase Separation in an $Fe_{70}Nb_{10}B_{20}$ Glass Studied by Advanced Electron Microscopy Techniques, T. Hanada, Y. Hirotsu and T. Ohkubo: Mater. Trans. 45 (2004) 1194-1198.

Prominent Nanocrystallization of $25KO•25Nb_2O_5•50GeO_2$ Glass, K. Narita, Y. Takahashi, Y. Benino, T. Fujiwara, T. Komatsu, T. Hanada and Y. Hirotsu: J. Am. Ceram. Soc. 87 (2004) 113-118.

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Fabrication of Exchange-coupled α-Fe/$L1_0$-FePd Nanocomposite Isolated Particles, J. Kawamura, K. Sato and Y. Hirotsu: J. Appl. Phys. 96 (2004) 3906-3911.

Magnetoanisotropy, Long-range Order Parameter and Thermal Stability of Isolated $L1_0$ FePt Nanoparticles with Mutual Fixed Orientation, K. Sato and Y. Hirotsu: J. Magn.

Magn. Mater. 272-276 (2004) 1497-1499.

The Investigation of Multiply Twinned $L1_0$-type FePt Nanoparticles by Transmission Electron Microscopy, A. Kovács, K. Sato, G. Sáfrán, P. B. Barna and Y. Hirotsu: Philos. Mag. 84 (2004) 2075-2081.

Structural Relaxation of Amorphous Silicon-Germanium Alloys: Molecular-Dynamics Study, M. Ishimaru, M. Yamaguchi and Y. Hirotsu: Jpn. J. Appl. Phys. 43 (2004) 7966-7970.

Local Structure Analysis of Ge-Sb-Te Phase Change Materials Using High-resolution Electron Microscopy and Nanobeam Diffraction, M. Naito, M. Ishimaru, Y. Hirotsu and M. Takashima: J. Appl. Phys. 95 (2004) 8130-8135.

Local Structural Change of Amorphous Ge-Sb-Te Thin Film during Annealing, M. Naito, M. Ishimaru, Y. Hirotsu and M. Takashima: J. Non-Cryst. Solids 345/346 (2004) 112-115.

Solid Phase Epitaxy of Amorphous Silicon Carbide: Ion Fluence Dependence, I.-T. Bae, M. Ishimaru, Y. Hirotsu and K. E. Sickafus: J. Appl. Phys. 96 (2004) 1451-1457.

Molecular-dynamics study on amorphous structures of $Si_{1-x}Ge_x$ alloys, M. Yamaguchi, M. Ishimaru and Y. Hirotsu, J. Jpn. Inst, Met. 68 (2004) 70-73 (in Japanese).

Crystallographic Correspondence between the bcc and C14-type Structures in the Fe-Ti Alloy System, A. Hirata and Y. Koyama: Mater. Sci. Eng. A 374 (2004) 72-76.

Kinetic Process of the Phase Separation in the Alloy $Ni_3Al_{0.52}V_{0.48}$, M. Tanimura, A. Hirata and Y. Koyama: Phys. Rev. B 70 (2004) 094111(1)-094111(7).

Disordered Atomic Column State in Fe-Mo Alloys, A. Hirata and Y. Koyama: Phys. Rev. B 70 (2004) 134203(1)-134203(7).

Atomistic Structures of Amorphous $Si_{1-x}Ge_x$ Alloys: A Molecular-dynamics Study, M. Yamaguchi, M. Ishimaru and Y. Hirotsu: Trans. Mater. Res. Soc. Jpn. 29 (2004) 3771-3774.

Structural Characterization of Oriented $L1_0$-FePd Nanoparticles, K. Sato and Y. Hirotsu: Trans. Mater. Res. Soc. Jpn. 29 (2004) 1647-1650.

Local Structure Analysis of Metallic Glasses Using HREM and Electron Diffraction (invited), Y. Hirotsu, T. Ohkubo and T. Hanada: Proc. 8th Asia-Pacific Conf. on Electron Microscopy (2004) 589-590.

Structural Analysis of As-sputterd and Melt-quenched Ge-Sb-Te Thin Film, M. Naito, M. Ishimaru, Y. Hirotsu and M. Takashima: Proc. 8th Asia-Pacific Conf. on Electron Microscopy (2004) 608-609.

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Characterization of Isolated Fe-Pd Alloy Nanoparticles with Orientation, K. Sato, J. Kawamura and Y. Hirotsu: Proc. 8th Asia-Pacific Conf. on Electron Microscopy (2004) 524-525.

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Crystallographic Feature of Laves Phase Formation in Fe-Mo Alloy, A. Hirata and Y. Koyama: Proc. 8th Asia-Pacific Conf. on Electron Microscopy (2004) 608-609.

Fabrication and Characterization of $FeSi_2$ Nanoparticles on Si(100) Substrate, J. H. Won, K. Sato, M. Ishimaru and Y. Hirotsu: Proc. Int'l Conf. New Frontiers of Process Science and Engineering in Advanced Materials (2004) 47-51.

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Nanoscale Phase Separation in Amorphous Fe-B alloys, T. Hanada, A. Hirata, Y. Hirotsu, T. Ohkubo and V. Bengus, Materia Japan 43 (2004) 1002 (in Japanese).

Structure and Order Parameter of $L1_0$-type Alloy Nanoparticles, K. Sato and Y. Hirotsu: Microscope 39 (2004) 144-149 (in Japanese).

Books

Nanostructure of Amorphous Alloys, Y. Hirotsu, T. Ohkubo and M. Matsushita: "Novel Nanocrystalline Alloys and Magnetic Nanomaterials", Edited by B. Cantor, Series in Materials Science and Engineering, Institute of Physics Publishing, Bristol, 2004, p 16-41.

International Conferences

Characterization of Exchange-Coupled Fe/L1o-FePd Nanoparticles (Poster), *K. Sato, J. Kawamura and Y. Hirotsu, 2nd 21st Century COE & 7th SANKEN Int'l Symposium on Hybridization of Chemistry, Biology and Material Science, Osaka, Jan. 13-14, 2004.

Characterization of Isolated Fe-Pd Nanoparticles with Orientation, *K. Sato, J. Kawamura and Y. Hirotsu, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Effects of Amorphous Structures on Recrystallization of Silicon Carbide, I.-T. Bae, *M. Ishimaru, Y. Hirotsu, and K. E. Sickafus, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Structural Analysis of As-Sputterd and Melt-Quenched Ge-Sb-Te Thin Film (Poster), *M. Naito, M. Ishimaru, Y. Hirotsu, and M. Takashima, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Epitaxially-grown α-$FeSi_2$ Nano-particle Synthesized by Electron Beam Deposition (Poster), *J. H. Won, K. Sato, M. Ishimaru, and Y. Hirotsu, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Crystallographic Feature of Laves Phase Formation in Fe-Mo Alloy (Poster), *A. Hirata and Y. Koyama, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Structure and Metallurgy of Alloy Nanoparticles in Fe-Pd System (Invited), *Y. Hirotsu and K. Sato, $L1_0$ Ordered Intermetallic and Related Phases for Permanent Magnet and Recording Applications, Colorado, August 15-20, 2004.

Determination of Long-Range Order Parameter of $L1_0$-FePt and FePd Nanoparticles by Electron Diffraction (Poster), *K. Sato and Y. Hirotsu, $L1_0$ Ordered Intermetallic and Related Phases for Permanent Magnet and Recording Applications, Colorado, Aug.15-20, 2004.

Local Structures and Nanocrystallization in Fe-Nb-B Amorphous Alloys (Poster), *E. Matsubara, T. Ichitsubo, S. Tanaka, A. Hirata, Y. Hirotsu and A. Makino, 11th International Symposium on Metastable, Mechanically Alloyed and Nanocrystalline Materials, Sendai, Aug. 22-26, 2004.

Transmission Electron Microscopy Study on $FeSi_2$ Nanoparticles Synthesized by Electron Beam Deposition (Poster), *J. H. Won, K. Sato, M. Ishimaru, and Y. Hirotsu, 11th International Symposium on Metastable, Mechanically Alloyed and Nanocrystalline Materials, Sendai, Aug. 22-26, 2004.

Nanostructure and Long-Range Order Parameter of $L1_0$-FePd Particles, *K. Sato and Y. Hirotsu, 5th Polish-Japanese Symposium on Advanced Methods of Materials Characterization, Niedizca, Aug. 29-Sept.1, 2004.

Chemical Short-range Order in Ion-beam-induced Amorphous SiC, *M. Ishimaru, I.-T. Bae, Y. Hirotsu, J. A. Valdez, and K. E. Sickafus, 14th International Conference on Ion Beam Modification of Materials, Monterey, USA, Sep. 5-10, 2004.

Fabrication and Structural Analysis of Oriented $L1_0$-FePt and FePd Nanoparticles (Invited), *Y. Hirotsu and K. Sato, The First Asia Forum on Magnetics, Okinawa, Sept.21-24, 2004.

Growth and atomic ordering of hard magnetic $L1_0$-FePt, FePd and CoPt alloy nanoparticles studied by transmission electron microscopy (Invited), *Y. Hirotsu and K.

Sato, 2004 International Symposium on Crystal Growth and Devices, Seoul, Korea, Nov. 10-13, 2004.

Solid Phase Epitaxy of Amorphous SiC Induced by Ion-beam-bombardment (Invited), *M. Ishimaru, I.-T. Bae, and Y. Hirotsu, 2004 International Symposium on Crystal Growth and Devices, Seoul, Korea, Nov. 10-13, 2004.

Two dimensionally dispersed Fe/FePd nanocomposite particles synthesized by electron beam deposition (Invited), *Y. Hirotsu, K. Sato and J. Kawamura, International Conference on New Frontiers of Process Science and Engineering in Advanced Materials, Kyoto, Nov. 24-26, 2004.

Fabrication and Characterization of $FeSi_2$ Nanoparticles on Si(100) Substrate (Poster), *J. H. Won, K. Sato, M. Ishimaru, and Y. Hirotsu, International Conference on New Frontiers of Process Science and Engineering in Advanced Materials, Kyoto, Nov. 24-26, 2004.

Effects of Amorphous Structures on Solid Phase Epitaxy of SiC (Poster), *M. Ishimaru, I.-T. Bae, and Y. Hirotsu, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 – Advance Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Dec. 6-7, 2004.

Electron Diffraction and High-Resolution Electron Microscopy Studies of Amorphous $Fe_{80}B_{20}$ and $Fe_{70}Nb_{10}B_{20}$ Alloys (Poster), *Akihiko Hirata, Takeshi Hanada, Yoshihiko Hirotsu, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 – Advance Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Dec. 6-7, 2004.

Determination of Order Parameter of $L1_0$-FePt and FePd Nanoparticles by Electron Diffraction (Poster), *K. Sato and Y. Hirotsu, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 – Advance Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Dec. 6-7, 2004.

Contributions to International Conferences and Journals

Y. Hirotsu	8th Asia-Pacific Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	16th International Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Advisory Committee)
Y. Hirotsu	5th Japan-Polish Joint Seminar on Materials Analysis (Organizing Committee)
Y. Hirotsu	11th International Symposium on Metastable, Mechanically Alloyed and Nanocrystalline Materials (Advisory Committee)

Publications in Domestic Meetings

The Japan Institute of Metals	12 papers
The Japan Society of Applied Physics	2 papers
The Magnetic Society of Japan	1 papers
Others	11 papers

Academic Degrees

Master Degree of Engineering

Takeshi Kotera	Structure and magnetic properties of Co-Pt thin films and Fe-Pt-Cu nanoparticles
Keisuke Yagi	Structural analysis of thermally-oxidized Si by high-resolution transmission electron microscopy

Sponsorship

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

Y. Hirotsu	In situ observation of atomistic structures in metallic liquid and metallic glass	¥30,100,000

Grant-in-Aid for Scientific Research (S)

Y. Hirotsu	Fabrication and characterization of hard magnetic alloy nanoparticles produced by vapor quenching	¥33,400,000

Grant-in-Aid for Scientific Research (C)

M. Ishimaru	Amorphous structures of phase-change recording materials and their rapid crystallization mechanisms	¥2,100,000

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

K. Sato	Characterization of atomic ordering process and epitaxial growth mechanism for FePt and FePd nanoparticles with hard magnetic properties	¥1,800,000

Entrusted Research

Y. Hirotsu	Special Coordination Funds for Promoting Science and Technology on “Nanohetero Metallic Materials” from the Ministry of Education, Culture, Sports, Science and Technology, Japan	Electron Diffraction Local Structure Analysis of Nanohetero Metallic Materials	¥15,057,000
Y. Hirotsu	NEDO (Advanced Materials Technology Utilizing Glassy Metals for Commercial Uses)	Nano-structure Analysis for the Evaluation of Mechanical Properties in Glassy Metals	¥3,150,000

Other Research Funds

M. Ishimaru	Hosokawa Powder Technology Foundation	Fabrication of Environment-friendly Semiconductor β-$FeSi_2$ Nanoparticles and Their Ordered Array	¥800,000

Department of Metallic Materials Process

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Outlines

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

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

Current Research Programs

Fabrication of Lotus-type Porous Metals and Alloys

In our research group, porous metals with cylindrical pores extending in one direction have been fabricated by unidirectional solidification under pressurized gas atmosphere utilizing the solubility gaps of gas atoms in metals at melting points. Lotus-type porous metals are superior in mechanical strength to conventional sphere-type porous metals, since the stress concentration around pores does not occur by the stress parallel to the pore growth direction. In this year, we have fabricated lotus-type porous Ni_3Al intermetallic compounds, aluminium and Nitinol and have established the fabrication technique for continuous casting.

Lotus-type porous Ni_3Al intermetallics whose long cylindrical pores are aligned in one direction have been fabricated by unidirectional solidification of the melt in a pressurized hydrogen gas. The porosity and the pore size are decreased with increasing aluminum content.

Since the hydrogen solubility in molten aluminium is much lower than that in molten metals such as iron, copper and nickel, it had been considered to be difficult to fabricate the lotus-type porous aluminium with high porosity such as 10 % or more. We tried to control of solidification velocity to raise the porosity and fabricated porous aluminium with 20% porosity.

Electrical conductivity of lotus-type porous metals

We proposed the method for calculating the anisotropic electrical conductivity of lotus-type porous metals on the basis of the mean-field theory, and applied the method to lotus-type porous nickel. The results by calculation agree well with those of measurements, which indicates that electrical conductivity of lotus metals can be predicted quantitatively by using the proposed method.

Vibration-damping capacity of lotus-type porous magnesium

We measured the vibration-damping capacity of lotus-type porous magnesium with hammering-vibration-damping test. For lotus magnesium, the vibration excited by the hammering decreases more rapidly than that for nonporous magnesium, which indicates that the damping capacity of lotus magnesium is higher than that of nonporous magnesium.

Corrosion Behavior of Lotus-type Porous Stainless Steel.

Corrosion resistance of lotus-type porous stainless steel was investigated. The current density of lotus-type porous SUS304L was higher than that of non-porous SUS304L at around -100mV (-100mV peak), while it was similar to that of non-porous stainless steel in the passive and trans-passive region. In the case of lotus-type porous SUS316L, corrosion behavior was similar to that of SUS304L.

Publications

Original Papers

Fabrication of Lotus-type Porous Metals and their Physical Properties, H. Nakajima, T. Ikeda and S.K. Hyun: Adv. Eng. Mater., 6 [6] (2004) 377-384.

Measurement and Analysis of Effective Thermal Conductivities of Lotus-type Porous Copper, T. Ogushi, H. Chiba, H. Nakajima and T. Ikeda: J. Appl. Phys., 95 [10] (2004) 5843-5847.

Fabrication of Lotus-type Porous Iron and its Mechanical Properties, S.K. Hyun, T. Ikeda and H. Nakajima: Sci. Tech. Adv. Mater. 5 (2004) 201-205.

Heat Transfer Capacity of Lotus-type Porous Copper Heat Sink, H. Chiba, T. Ogushi, H. Nakajima and T. Ikeda: JSME Int. J. Series B-Fluids and Thermal Eng., 47 [3] (2004) 516-517.

Elastic Properties of Lotus-type Porous Iron: Acoustic Measurement and Extended Effective-mean-field Theory, M. Tane, T. Ichitubo, H. Nakajima, S.K. Hyun and M. Hirao: Acta Mater., 52 [17] (2004) 5195-5201.

Fabrication of Lotus-type Porous Silicon by Unidirectional Solidification in Hydrogen, T. Nakahata and H. Nakajima: Mater. Sci. Eng., A384 [1-2] (2004) 373-376.

Bending Properties of Porous Copper Fabricated by Unidirectional Solidification, S.K. Hyun, H. Nakajima, L.V. Boyko and V.I. Shapovalov: Mater. Lett., 58 (2004) 1082-1086.

Tracer Diffusion in Pt_3Fe Ordered Alloys, Y. Nose, T. Ikeda, H. Nakajima and H. Numakura: Z. Metalkd., 95 (2004) 904-912.

Elastic Constants of Lotus–type Porous Magnesium: Comparison with Effective-mean-field Theory, M. Tane, T. Ichitubo, M. Hirao, T. Ikeda and H. Nakajima: J. Appl. Phys., 96 (2004) 3696-3701.

Temperature Dependence of Elastic Constants of Lotus-type Porous Copper, M. Tane, T. Ichitsubo, M. Hirao, R. Takeda, T. Ikeda and H. Nakajima: Mater. Lett., 58 (2004) 1819-1824.

Characteristics of Sound Absorption in Lotus-type Porous Magnesium, Z.K. Xie, T. Ikeda, Y. Okuda and H. Nakajima: Japanese J. Appl. Phys., 43[10] (2004) 7315-7319.

Effective-mean-field Approach for Macroscopic Elastic Constants of Composites, M. Tane and T. Ichitsubo: Appl. Phys. Lett., 85 (2004) 197-199.

Titanium Coating of Lotus-type Porous Stainless Steel by Vapor Deposition Technique, T. Ikeda and H. Nakajima: Mater. Lett., 58 [29] (2004) 3807-3811.

Sound Absorption Characteristics of Lotus-type Porous Copper Fabricated by Unidirectional Solidification, Z.K. Xie, T. Ikeda, Y. Okuda and H. Nakajima: Mater. Sci. Eng., A386 [1-2] (2004) 390-393.

Measurement and Analysis of Sound Absorption of Porous Magnesium, Z.K. Xie, T. Ikeda, Y. Okuda and H. Nakajima: Mater. Sci. Forum, 449-452 (2004) 661-664.

Fabrication of Lotus-type Porous Ni-Al Intermetallics by Continuous Zone Melting Method, S.K. Hyun, M. Tane and H. Nakajima, Proc. Int. Conf. on New Frontiers of Process Sci. and Eng. in Adv. Mater., High Temperature Society of Japan, (2004) 415-418.

Elastic and Plastic Properties of Lotus-type Porous Iron, M. Tane, S.K. Hyun H. Nakajima, T. Ichitsubo and M. Hirao: Proc. Int. Conf. on New Frontiers of Process Sci. and Eng. in Adv. Mater., High Temperature Society of Japan, (2004) 86-91.

Investigation on Pore Morphology in Lotus-type Porous Nickel, H. Onishi, S.K. Hyun and H. Nakajima: Proc. Int. Conf. on New Frontiers of Process Sci. and Eng. in Adv. Mater., High Temperature Society of Japan, (2004) 116-119.

Corrosion Behavior of Lotus-type Porous SUS304L Stainless Steel, M. Fuseya, T. Nakahata, S.K. Hyun, S. Fujimoto and H. Nakajima: Proc. Int. Conf. on New Frontiers of Process Sci. and Eng. in Adv. Mater., High Temperature Society of Japan, (2004) 287-292.

Fabrication of Lotus-type Porous Carbon Steel by Continuous Zone Melting Method and its Mechanical Properties, T. Kujime, S.K. Hyun, T. Ikeda and H. Nakajima: Proc. of Modeling of Casting and Solidification Processes, (2004) 379-384.

Fabrication of Lotus-type Porous Ni_3Al Intermetallics, S.K. Hyun, T. Ikeda and H. Nakajima: Journal of the Japan Institute of Metals, 68 [2] (2004) 39-42.

Characteristic of Absorbing Sound in Lotus-type Porous Copper Fabricated by Unidirectional Solidification, Z.K. Xie, T. Ikeda, Y. Okuda, H. Nakajima: Journal of the Japan Institute of Metals, 68 [3] (2004) 185-190.

Fabrication of Lotus-type Porous Nickel Using Moisture, Y. Suematsu, S.K. Hyun and H. Nakajima: Journal of the Japan Institute of Metals, 68 (2004) 257-261.

Fabrication of Lotus-type Porous Stainless Steel by Continuous Zone Melting Technique, T. Ikeda, T. Aoki and H. Nakajima: Tetsu to Hagane, 90 [1] (2004) 9-16.

Structure, Mechanical Properties and Thermal Conductivity of Thermal Sprayed Nickel Coatings, K. Murakami, H. Matsumoto and H. Nakajima: J. of High Temp. 30 (2004) 336-341.

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Recent Development in Research of Porous Metals, H. Nakajima: The Production & Technique, 56 [1] (2004) 55-57.

Porous Metals Containing a Number of Unidirectionally Elongated Pores, S.K.Hyun, T.Ikeda and H.Nakajima: Mater.Integration, 17[1] (2004) 35-40.

Fabrication and Mechanical Properties of Lotus-type Porous Magnesium and its Alloys, T.Ikeda, H.Yoshiyama and H.Nakajima: J.Japan Light Metals, 54[9] (2004) 388-393.

Fabrication of Lotus-type Porous Metals and its Application, H. Nakajima: Journal of the JRIC, 43 [1] (2004) 12-16.

Development of Light Structural Materials Using Lotus-type Porous Steel, H. Nakajima, T. Ikeda, K. Murakami and K. Ota: Bulletin of the Iron and Steel Inst. of Japan, 9 [11] (2004) 56-58.

Development of Porous Metals, H. Nakajima: Mater. Sci. & Tech., 74 [7] (2004) 646-647.

Fabrication of Porous Stainless Steel with Unidirectional Pores by Continuous Zone Melting Method, T. Ikeda, T. Aoki and H. Nakajima: Mater. Sci. & Tech., 74 [7] (2004) 647-651.

Development of Lotus-type Porous Ni_3Al Intermetallics, S.K. Hyun and H. Nakajima: Mater. Sci. & Tech., 74 [7] (2004) 667-670.

Books

Utilization of Hydrogen towards 21th Century, H. Nakajima, Kurapro Corp., (2004) 26-37.

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Patents

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Contributions to International Conferences and Journals

H. Nakajima	Materials Letters (Principal Editor)
H. Nakajima	Fourth International Conference on Porous Metals and Metal Foaming Technology (MetFoam2005) (Organizing Committee Chairman)
H. Nakajima	High Temperature Materials and Process (Editorial Board)
H. Nakajima	Diffusion and Defect Data (Editorial Advisory Board)
H. Nakajima	Materials Science Foundations (Editorial Advisory Board)
H. Nakajima	Pacific Rim International Conference on Materials (Organizing Committee Member)
H. Nakajima	International Symposium on Advanced Structural and Functional Materials Design (Organizing Committee Member)
H. Nakajima	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Organizing Committee Member)
H. Nakajima	THEMEC'2006 Symposium on Metallic Foams (Organizing Committee Member)

H. Nakajima	International Conference on Diffusion in Materials (Organizing Committee Member)
H. Nakajima	International Symposium on Eco-Materials Processing & Design (Organizing Committee Member)
H. Nakajima	The 3rd NIMS International Conference on Materials for Human Safety (International Advisory Board)

Publications in Domestic Meetings

The Japan Institute of Metals	32 Papers
The Society of Materials Science	1 Paper
High Temperature Society of Japan	2 Papers
The Japan Copper and Copper Alloys Research Association	1 Paper

Academic Degrees

Doctor Degree of Engineering

Z.K. Xie	Sound Absorption and Vibration Damping Characteristic of Lotus-type Porous Magnesium and Copper

Master Degree of Engineering

T. Ide	Compressive Properties of Lotus-type Porous Stainless Steel
H. Onishi	Fabrication of Lotus-type Porous Nickel Using Moisture and their Pore Morphology
M. Fuseya	Corrosion Behavior of Lotus-type Porous Stainless Steel

Sponsorship

Grant-in-Aid for Scientific Research on Exploratory Research

H. Nakajima	Fabrication of the light iron with 4 times higher strength than iron	¥1,600,000
H. Nakajima	Biomaterials	¥9,700,000
S.K. Hyun	Fabrication and mechanical properties of Lotus-type porous intermetallics	¥2,900,000

Entrusted Research

H. Nakajima	Engineering Research Association for Supersonic Transport Propulsion System Development of Innovative Multifunctional Foundry Process	￥23,000,000

Other Research Funds

H. Nakajima	The Ministry of Education, Culture, Sports, Science and Technology Grant-in-Aid for Development of Innovative Collaboration between University and Industry	¥63,700,000

	Commercialization of lotus-type porous metals	
H. Nakajima	The Iron and Steel Institute of Japan	¥1,000,000
	Database of porous metals	
H. Nakajima	Mori Seiki Co. Ltd.	¥7,000,000
	Development of machine parts	
H. Nakajima	Hosokawa Powder Engineering Foundation	¥300,000
	Conference of MetFoam2005	
H. Nakajima	Mitsubishi Electric Co. Ltd.	¥500,000
	Development of heat sinks	
H. Nakajima	Light Metals Scholarship	¥250,000
	Development of light metals	
M. Tane	Tanigawa Heat Technical Foundation	¥300,000
	Development of pore morphorgy control	

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Outlines

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

Current Research Programs and Achievements

Function Harmonised Superlattices.

・ Electric field control of ferromagnetism at room temperature was realized in

transition metal oxide nano-heterostructure so as to newly propose the novel Magnetic Random Access Memory (MRAM).

- A new method to evaluate its interfacial electronic/magnetic structure was also developed by bulk sensitive Hard X-ray Photoemission Spectroscopy in SPring-8.
- At the thickness around 40nm, the $La_{0.8}Ba_{0.2}MnO_3$ thin films possessed high TCR value and low noise amplitude at room temperature, showing higher potential as an uncooled bolometer than the ordinary VO_x-based IR sensor.

Nano-science by Using of Scanning Probe Microscopes.

- By using scanning tunneling microscopy (STM), we obtained submolecular-resolution STM images of a single molecule of DNA labeled with the fluorescein isothiocyanate (FITC), which can be a good molecular marker even in STM.
- Using the atomic force microscopy (AFM), we found the valuable information to identify the solution for the rate-limiting step of small-scale protein synthesis system by analyzing the reaction process.
- Using the base recognition function of the immobilized ribosome, the base sequencing process of mRNA was detectable with the optical technique, which did not need any special purifications.

Development of Electrochemical Nano-biochip/Sensor.

- Developing highsensitive electrochemical DNA chip utilizing highly-specific bindings on nano-sized electrode arrays.
- Confirmation of SNPs feasibility with label-free oligonucletides by using electric signal transducer.
- Developing novel nano-immunosensor on functional lipid vesicle modified nanowell-electrode surface by fabricated e-beam lithography.

Development of Bio-molecular Device Constructed from DNA.

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

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Construction of ZnO Devices: Electric and Magnetic Properties, *Hitoshi Tabata, Satoshi Masuda, Hiroaki Matsui, Hiromasa Saeki and Tomoji Kawai, The 12th Gallium Arsenide and other Compound Semiconductors Application Symposium(GAAS 2004) , Amsterdam(the RAI Exhibition & Congress Centre), Netherland 2004.10.11-12.

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Measurements of Contactless Microwave Conductivity and Infrared Absorption in Poly(dG)-Poly(dC) and Poly(dA)-Poly(dT) DNA Molecules, *Hiroshi Matsui, Toshiori Yanagimachi, Koudai Abe, Toshihiro Suzuki, Masateru Taniguchi, Shinichi. Tanaka, Tomoji Kawai, Hasanudin, Noriyoshi Kuroda, Naoki Toyota: The 5th International Conference on Biological Physics, Gothenburg, Sweden, 2004.8.23-27.

Contributions to International Conferences and Journals

T. Kawai	Nanotech (Edit committee Chairman)
T. Kawai	Electronics society (Edit committee Chairman)
T. Kawai	IEICE (Institute of Electronics, Information and Communication Engineers) Electronics Express (Edit committee)
T. Kawai	e-JSSNT (e-Journal of Surface Science and Nanotechnology) (Adviser lee board)

Publications in Domestic Meetings

The Japan Society of Applied Physics	31 papers
The Surface Science Society of Japan	5 papers
The Molecular Biology Society of Japan	4 papers
The Chemical Society of Japan	3 papers
The Magnetic Society of Japan	3 papers
Others	41 papers

Academic Degrees

Master Degree of Science

R. Yamasaski	The quantitative Analysis of the Interaction between Streptavidin and biotinylated DNA on the substrate modified by streptavidin

Master Degree of Engineering Science

M. Kataoka	I-V characterization of electron-transfer metalloprotein "Cytochrome

	c" at a few molecular level
M. Hirooka	The Phase Transition of Manganite Nanowires Fabricated by AFM Lithography

Doctor Degree of Science

M. Seki	Cluster-Glass Nature and Photoinduced Magnetization in Spinel and Garnet Ferrite Thin Films

Sponsorship

21st Century Center of Excellence

T. Kawai	Toward Creating New Industries Based on Inter-Nanoscience	¥274,000,000

Grant-in-Aid for Scientific Research (B)

Hide. Tanaka	Construction of room temperature spin electronics devices by strongly correlated oxide nano-structure	¥5,900,000

Grant-in-Aid for Scientific Research (A)

Hide. Tanaka	Creation of opt-magnetic materials by programmed self-assembly using DNA molecules and nano-particles	¥7,700,000

Fund for JSPS Research fellowships for Young Scientist

B. Vilquin	Growth of novel materials using ferroelectric thin films	¥1,200,000
T. Yanagida	Fabrication of functional harmonic artificial lattice by controlling surface structures towards realization of biomimic sensors	¥1,100,000
M. Seki	Creation of room temperature photomagnetic materials and elucidation of photoinduced magnetization	¥1,000,000
Y. Otsuka	Controlling the structure and sequences of DNA and the elucidation of the charge transport phenomenon in nanoscale	¥1,000,000
F. Yamada	Arrangement of nano-magnet-particles using programmed self-organization system and investigation of novel magnetic properties	¥1,000,000
A. Hossain (COE)	Construction of novel magnetic materials constructed from oxide artificial lattices	¥400,000

Entrusted Research

T. Kawai	Core Research for Evolutional Science and Technology (CREST), Japan Science and Technology Agency	Creation of bio-mimetic intellectual material based on programmed self-assembly	amount of acceptance ¥157,280,000

T. Kawai	NEDO: Focus 21 Advanced nanobiodevice project	〔 TORAY 〕 Research and Development of High Through Put Protein Chip: Analysis of Protein Synthesis Mechanism	amount of acceptance: ¥8,890,000
		〔Matsushita Electric Industrial Co., Ltd. 〕 Research and Development of Immobilization Method of Biomolecules	amount of acceptance: ¥9,240,000
		〔Shimadzu Co.〕Development of Single Molecular DNA Analysis System	amount of acceptance: ¥8,132,000

Other Research Funds

Hidekazu Tanaka	PRESTO21-JST	Construction of room temperature spin electronics devices by nano-scale function harmonized artificial lattices	¥6,000,000
Hidekazu Tanaka	Research fund for young scientist (Sanken)	An organization of the knowledge of various materials fields using Ontology Engineering	¥2,000,000
Hiroyuki Tanaka	21 COE	Fabrication and characterization on DNA of various local electronics states	¥1,000,000
Yoichi Otsuka	Research Association of Industry and Science Foundation	Structure and electrical property of DNA molecules immobilized on the patterned self-assembled monolayers	¥164,000

Department of Functional Ceramic Materials

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Outlines

The modern society is based on semiconductor technology. Our research is aiming to improve the characteristics of semiconductor devices and to develop semiconductor devices with new structure. For this purpose, we have developed new methods of the low temperature formation of insulating layers, a method for the observation of semiconductor interfaces with high sensitivity, and a method of controlling semiconductor interfacial properties. Semiconductor devices studied in this department are as follows: 1) solar cells, 2) metal-oxide-semiconductor (MOS) devices for LSI, 3) thin film transistors (TFT) for display devices.

Current Research Programs

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 oxygen atoms 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.

Low Temperature Fabrication of Thick SiO_2/SiC Structure by Use of Chemical Method and its Application to SiC-MOS Devices

Due to the chemical stability of SiC, oxidation of SiC to form SiO_2 layers requires high temperature heat treatments at ~1100 °C. High temperature heat treatments degrade the interfacial characteristics, and thus good device characteristics expected from bulk SiC physical properties have not been achieved.

We have succeeded in the fabrication of SiO_2/SiC structure with a SiO_2 layer thicker than 10 nm at ~120 °C by use of the two-step nitric acid oxidation method. TEM observation has shown that the SiO_2/SiC interfaces formed by the two-step nitric acid oxidation method are atomically flat. We have also developed the "bias-applied nitric acid oxidation method" to form 0.5~1 μm SiO_2 layers at room temperature. SiO_2 layers formed by the two-step nitric acid oxidation method is expected to be applied to gate oxide layers in SiC-MOS devices, and the bias-applied nitric acid oxidation method is expected to be applied to device separation.

Developement 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.

Publications

Original Papers

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

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Contributions to International Journals

H. Kobayashi Applied Surface Science, Editor

Publications in Domestic Meetings

The Physical Society of Japan	5 papers
The Japan Society of Applied Physics	5 papers
Surface Electronics Society	1 paper
The Japan Vacuum Society	1 paper
Seminar on spectroscopic investigation for adsorbed molecules	1 paper

Academic Degrees

Master Degree of Science

A. Okafuji Fabrication of the High-Efficiency a-Si Solar Cells with Light Trapping Structure by the Use of Al_2O_3 Fine Particles.

Doctor Degree of Science

T. Kobayashi Control of Band Bending of Si-based Metal-Oxide-Semiconductor Diodes and p-n Junction Si Solar Cell

Sponsorship

Grant-in-Aid for Scientific Research (B)

O. Maida	Control of threshold voltage of MOSFET by inclusion of fixed charges in insulators	¥1,200,000

Grant-in-Aid for Scientific Research

Asuha	Low temperature formation of SiO_2/Si structure and decrease in leakage current density	¥1,200,000

Entrusted Research

H. Kobayashi	Japan Science and Technology Organization	Development of semiconductor cleaning solutions with defect passivation effect	¥29,600,000
H. Kobayashi	Japan Science and Technology Organization	Silicon Thin Film Solar Cells with New Chemical Bonds	¥2,500,000
H. Kobayashi	Kansai Bureau of Economy, Trade and	Development of apparatus for low temperature	¥74,826,000

	Industry	oxidation of silicon by use of nitric acid oxidation method	
M. Takahashi	Japan Science and Technology Corporation	Suppression of Charge Carrier Recombination in Polycrystalline Si by Cyanide Treatment	¥500,000
H. Kobayashi	Kansai Bureau of Economy, Trade and Industry	Practical study of defect passivation etch-less semiconductor cleaning technology	¥20,000,000

Other Research Funds

H. Kobayashi	Core Research for Evolutional Science and Technology	Silicon Thin Film Solar Cells with New Chemical Bonds	¥54,110,000

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Outlines

Ceramics material is one of the most promising key materials for supporting the science and technology of the coming 21st century. It is now required to be a multi-functional material to meet the future demand. It is over 15 years since we proposed a new materials design concept "nanocomposite technology", that realizes the dominant improvement of mechanical properties of ceramics by controlling nano- and atomic-scale structure of the polycrystalline ceramics. Based on this concept, this department has been focusing mainly on the basic researches for developing high-performance ceramic-based materials with multiple functionalities over the decade. Special emphasis is placed on the understanding of the relation between the nanostructures and mechanical properties. Systematic researches have revealed that the mechanical properties of these nanocomposite ceramics are remarkably enhanced even at high temperatures. In addition excellent functional properties, such as machinability, superplasticity, electric/magnetic properties and so on, are also found to be consistent with the improved mechanical property. Recent studies suggest that the nanocomposite concept is also applicable to metal and organic materials. Thus the target of these researches is to develop new materials, named "intermaterials" which ranges ceramic, metal and organic materials.

Current Research Programs

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

To develop high performance ceramic-based materials we focused on the microstructural control of ceramics in nanometer-scale. It realizes "Nanocomposite" in which nanometer-sized second phase exists within several oxide and nonoxide ceramics. These composite materials exhibit superior mechanical properties, i.e., high fracture strength, toughness, creep resistance, thermal shock resistance and so on, not only at room temperature but also at elevated temperature. Development of new ceramic nanocomposites possessing superplasticity, machinability are also achieved by synthesizing nanostructured and nanocomposite powders, and/or by using conventional

sintering method, novel in-situ sintering, reaction sintering and spark plasma sintering methods. In this study preparation process, micro/nano/interface structure, and properties relation have been investigated. Roles of nanostructures on properties enhancements are also studied in detail.

Development of Non-oxide Nanocomposites.

Most non-oxide ceramics such as silicon nitride are sintered by assisting of liquid phase during heating, due to the small amount of additives and oxide impurities at the powder surfaces. Sintered bodies thus have grain boundary glassy phases that decrease mechanical performances at elevated temperature. In this study passive control of additives and resultant grain boundary structures, micro- and nano-structures as well are investigated. Selecting suitable additives and sintering methods resulted in high-performance and low-cost non-oxide ceramic nanocomposites, which enlarges the industrial applications of the materials. Relationships between processing-structure-properties are systematically investigated.

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 so on. 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.

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

Nanocomposite technology is also applicable to the functional ceramics such as ferroelectric, piezoelectric, varistor and ion-conducting materials. Incorporation of 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 a severe environmental condition. In addition, electric properties can also be enhanced by dispersing nanoparticles. Relationships between nano- and interface-structure, mechanical properties and electric properties have been investigated in detail. Also the nanocomposite technology can be used to the magnetic materials. For the hard magnet materials, nanostructural control has found to realize great improvement of the magnetic properties, which is used to practical application.

Design and Development of Atomic/Molecular-Level Composites.

We have proposed new materials design concept which is consisted of structural control in atomic and molecular level. These materials can be prepared by incorporating very small amount of additive into ceramics. The additive segregates at the grain boundary with gradient concentration, or precipitates molecular or cluster seized particles within the grains or at the grain boundaries. In this study relation between preparation process - structural development mechanisms - properties have been investigated by means of detailed TEM observations.

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

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

Development and Properties of Layer by Layer Lattice Composites with Bulky Form.

Addition of small amount of oxides was found to form superlattice structure with cyclic period of several angstrom in lithium niobate. In this study bulky sintered body of this material has successively prepared by controlling powder processing and sintering procedure. Detailed TEM investigations revealed that the periodicity of superstructure was varied depending on the amount of additive and sintering condition, and some insulating layer was formed at the phase boundary of each superlattices. Temperature dependence of dielectric constant was performed up to high-temperature and some dielectric relaxation phenomena due to the 1st or 2nd order phase transformation were observed. This is found to be relating with its characteristic superstructure. Present study thus revealed that realizing novel electric properties could be achieved in a bulk material when layer-by-layered superstructures are controlled in an atomic scale.

Development of High Performance Organic Polymers by Nanocompositie 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. More recently, we are introducing nano technology in polymer/ceramic system to investigate the electrical property relationship with microstructure for practical applications, resulted in successive development of novel tactile sensor material.

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Sasaki, K. Niihara, T. Kusunose, Tokkyo 3586784.

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Fabrication of Transparent Polycrystalline Silicon Nitride Ceramic, R. Sung, T. Kusunose, T. Nakayama, T. Sekino, *S. Lee, and K. Niihara, 106th Annual Meeting & Exposition of The American Ceramic Society, Indiana Convention Center & RCA Dome, Indianapolis, Indiana, USA Apr. 18-21, 2004.

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Fabrication and Characterization of Zirconia-based New Ceramic Composite for Thermal Barrier Coatings, *A. T. Hirvonen, Y. Yamamoto, T. Sekino, R. Nowak, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

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Multifunctionalization of Natural Rubber by Sonochemical Silver Nanoparticle (Poster), *Y. Saijo, Y. Hayashi, R. Ramaseshan, T. Sekino, T. Kusunose, T. Nakayama, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Preparation and Electrical Properties of Carbon Nanotubes Dispersed Zirconia Nanocomposite (Poster), *T. Ukai, T. Sekino, T. Kusunose, T. Nakayama, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Mechanical and Thermal Properties of Silicon Nitride Ceramics with Rare-Earth Oxide Addition (Poster), *D.-H. Choi, S.-W. Lee, R.-J. Sung, S.-H. Kim, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

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Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Tribological Properties of Al_2O_3/SiC Nanocomposites (Poster), *S.-H. Kim, T. Kusunose, T. Nakayama, T. Sekino, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Silicon Nitride Ceramics with Ionic and Electronic Conductivity, Y.-H. Kim*, T. Sekino, T. Kusunose, T. Nakayama, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

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The Effects of Nitrogen and Annealing on the Electrical and Structure Properties of the DLC Films Deposited by RF-PECVD System (Poster), The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Application to Nanoparticle Filteration Using Anodic Aluminium Oxide (Poster), *Y.-H. Choa, S.-H. Kim, D.-J. Park, J.-K. Yang, T. Sekino, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Fabrication and Applications of Nano-metal Particle Composites by Ultrasonic Eco-process (Poster), *Y. Hayashi, Y. Saijo, T. Sekino, K. Suganuma, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

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Preparation and Evaluation of Metal/Ceramic Nanocomposites for High Frequency Inductor (Poster), *J.-K. Yang, D.-J. Park, J. Kim, T. Sekino, K. Niihara, and Y.-H.Choa, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

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Gamma-ray Synthesis of Gold/Iron-Oxide Nanocomposite Particles for Biomedical Applications (Poster), *S. Seino, T. Kinoshita, Y. Otome, T. Nakagawa, K. Okitsu, Y. Mizukoshi, T. Nakayama, T. Sekino1, K. Niihara, and T. A. Yamamoto, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31- Nov. 3, 2004.

Electrical and Mechanical Properties of Conducting Polymer/Clay Nanocomposite Sensors, *R. Rajagopalan, T. Sekino and K. Niihara The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31-Nov. 3, 2004.

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Multifunctionalization of Structural Oxide-ceramics by Microstructure and Grain Boundary Control in Nano-scale (Invited), *T. Sekino, A. Hirvonen, N. Tanaka, H. Wang, T. Nakayama, T. Kusunose, and K. Niihara, The 3rd International Symposium on the Engineering Ceramics (EnCera 04), Senri-Hankyu Hotel, Osaka, Japan, Oct. 31-Nov. 3, 2004.

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Fabrication of Single Nano Sized Composites by Modified Vapor Deposition Technique (Invited), *T. Nakayama, T. Shigaki, S. Seino, M. Nagashima, M. Fujikane, S. Yamanaka, T. A. Yamamoto, Y. Hayashi, T. Kusunose, T. Sekino and K. Niihara, International Technical Forum Inspiring Powder Technology, 2004(ITFIPT2004), Makuhari Messe, Chiba, Japan, Nov. 10-11, 2004.

Novel Nanostructured Materials with Multi Functionality (Invited), K. Niihara, T. Sekino, R. Ramaseshan, T. Kusunose, T. Nakayama, and Y. Hayashi, International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (PSEA'04), Kyoto International Conference Hall, Kyoto, Japan, November 24-26, 2004.

Fabrication and Properties of Multifunctional Ceramic/Metal Nanocomposites by Novel Gel-casting and Gel-coating Process, T. Sekino, B.-S. Kim, N. Tanaka, A. Hirvonen, T. Nakayama, T. Kusunose, and K. Niihara, International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (PSEA'04), Kyoto International Conference Hall, Kyoto, Japan, November 24-26, 2004.

Electrically Conductive Aluminum Nitride with High Thermal Conductivity (Poster), *T. Kusunose, T. Sekino, T. Nakayama, and K. Niihara, 8th SANKEN International Symposium & 3rd International Symposium on Scientific and Industrial Nanotechnology, Convention Center, Suita Campus, Osaka University, Japan, December 6-7, 2004.

Formation of 3D Charge Transfer Network in Bulk Ceramics by Carbon Nanotube Dispersion and Its Characterization (Poster), *T. Sekino, T. Okamoto, and K. Niihara, 8th SANKEN International Symposium & 3rd International Symposium on Scientific and Industrial Nanotechnology, Convention Center, Suita Campus, Osaka University, Japan, December 6-7, 2004.

Nanocomposite Sensors for Various Engineering Applications, *T. Sekino, The 1st IMAGINE International Forum on Venture-Business, Hotel Hankyu Expo Park, Osaka, Japan, Dec. 15 - 17, 2004.

The High-performance Catalyst with the Unique Nanocomposite Structure (Poster), *T. Nakayama, The 1st IMAGINE International Forum on Venture-Business, Hotel Hankyu Expo Park, Osaka, Japan, Dec. 15 - 17, 2004.

Development and Industrial Application of the TiO_2 Nanotube (Poster), *T. Sekino, The 1st IMAGINE International Forum on Venture-Business, Hotel Hankyu Expo Park, Osaka, Japan, Dec. 15 - 17, 2004.

Development of Electrically Conductive AlN by Grain Boundary Control and Its Applications (Poster), *T. Kusunose, The 1st IMAGINE International Forum on Venture-Business, Hotel Hankyu Expo Park, Osaka, Japan, Dec. 15 - 17, 2004.

Development of Machinable Nanocomposites with Multi-functionality and Their

Industrial Applications, *T. Kusunose, The 1st IMAGINE International Forum on Venture-Business, Hotel Hankyu Expo Park, Osaka, Japan, Dec. 15 - 17, 2004.

Contributions to International Conferences and Journals

Koichi Niihara	The International Nano Ceramic Forum and The International Symposium on Internationals (NCF & IMA) （Co-Chairman）
Koichi Niihara	Seminar on Core University Program between Japan and Korea （Chairman）
Koichi Niihara	International Symposium on Eco-materials Processing and Design （Chairman）
Koichi Niihara	The 3rd International Symposium on the Science of Engineering Ceramics（Chairman）
Koichi Niihara	International Symposium on Nanostructured Materials（Organizing Committee）
Koichi Niihara	Journal of Korean Ceramics Society（Organizing Committee）
Koichi Niihara	Advances in technology of Materials and Materials Processing Journal (ATM)（Organizing Committee）
Koichi Niihara	Journal of Nanoscience and Nano Technology（Editorial Board）
Koichi Niihara	Materials Integration（Editor）
Koichi Niihara	Journal of the Chinese Ceramic Society（Editorial Board）
Koichi Niihara	Journal of Ceramic Processing Research（Editorial Board）
Koichi Niihara	11th International Conference on Fracture (ICF11)（Organizing Committee）
Koichi Niihara	International Conference on Novel and Emerging Ceramics and Composites（Organizing Committee）
Tohru Sekino	The 3rd International Symposium on the Science of Engineering Ceramics（Organizing Committee）
Tohru Sekino	International Conference on New Frontiers of Processing Science and Engineering in Advanced Materials (PSEA'04)（Organizing Committee）
Tohru Sekino	The 7th international symposium on Eco-Materials Processing and Design (Organizing Committee)
Tohru Sekino	11th International Conferences on Modern Materials and Technologies (CIMTEC 2006) (Organizing Committee)
Tohru Sekino	Materials Integration（Organizing Committee）
Takafumi Kusunose	The 3rd International Symposium on the Science of Engineering Ceramics（Sterring Committee）
Tadachika Nakayama	The 3rd International Symposium on the Science of Engineering Ceramics（Sterring Committee）

Publications in Domestic Meetings

The Ceramic Society of Japan	15 papers
Japan Society of Powder and Powder Metallurgy	6 papers
The Japan Institute of Metals	1 paper
Sciety of Nano Science and Technology	3 papers
Others	3 papers

Academic Degrees

Bachelor Degree of Engineering

Shin-ya Itano	Multi-functionalization of Al_2O_3 Based Nanocomposite by Coating of Carbon Nanotube
Hideaki Fujiwara	Development of AlN/BN Nanocomposite with Multi-functionality

Master Degree of Engineering

Takeshi Ukai	Development of Carbon Nanotube Dispersed Zirconia Ceramics with High Fracture Toughness and Electrical Conductivity
Takumi Okamoto	Highly Functionalized Titania Nanotubes
Masahiro Sasaki	Fabrication and Property Evaluation of New Thermoelectric Complex Oxides

Doctor Degree of Engineering

Seung-Ho Kim	Wear Mechanism of Al_2O_3/SiC Nanocomposites
Yoon-Ho Kim	Multifunctionali Silicon Nitride Ceramics Through Nanostructure Control of Grain Boundary
Rak-Joo Sung	Fabrication and Characterization of Transparent Polycrystalline Silicon Nitride Ceramics

Sponsorship

Grant-in-Aid for Scientific Research on Exploratory Research

Tadachika Nakayama	Hydrogen Storage Property of Nano Cluster Level Oxide Composites	¥500,000

Grant-in-Aid for Scientific Research on Special Research Fellow

Satoshi Seino	Radiation-Induced Synthesis of Single-Nanosized Composite Nanoparticles with Improved Functionality.	¥1,100,000
Yoon-Ho Kim	Fabrication of Grain-Boundary Controlled Electric Conductive Ceramic Nanocomposite	¥1,000,000

Entrusted Research

Tohru Sekino	NEDO (Materials Nanotechnology Program, Nanocoating Project)	Development of Nanocomposite Coating by In-situ Structuralization.	¥5,565,000

Cooperative Research

Koichi Niihara	Fine Ceramics Technology Cooperative Association	Studies on Remote Sensing of Micro-fractures and Stresses by Nanocomposite Technology	¥30,000,000
Koichi Niihara Takafumi Kusunose	Tokuyama Corporatin	Development of AlN/BN Nanocomposites with High Fracture Toughness and High Strength	¥3,000,000
Takafumi Kusunose	Sumitomo Electric Industries, Ltd.	Synthesis of Phosphor Exited by Electron or Electric Field	¥2,625,000
Koichi Niihara Takafumi Kusunose	Sumitomo Electric Industries, Ltd.	Research on Nanostructured Ceramic Materials	¥3,000,000

Other Research Funds

Tohru Sekino	NEDO (Industrial Technology Research Grant Program in 2004)	Hyper-functionalization of Oxide Nanotube and Its Application for Environmentally-harmonized Systems	¥31,850,000
Takafumi Kusunose	NEDO (Industrial Technology Research Grant Program in 2001)	Application of BN Dispersed Nanocomposites in Fields of Semiconductor Mnufacturing Equipment and Biomaterial	¥27,508,000
Tadachika Nakayama	NEDO (Industrial Technology Research Grant Program in 2002)	Fabrication of the Novel Single Nano Composites Catalysts with High Efficiency	¥10,010,000
Tohru Sekino	Hosokawa Powder Technology Foundation	Highly-functionalization of Self-organized Oxide Nanotubes by Lattice	¥800,000
Tohru Sekino	Kansai Research Foundation for Technology Promotion	Functionalization of Oxide Nanotube by Highly-Structure Control Aiming for Energy Creation	¥2,600,000

Department of Advanced-Energy Material

Professor:	Katsumi TANIMURA
Associate Professor:	Shin'ichiro TANAKA
Graduate Students:	Ei'ichi INAMI, Junzi TSURUTA
Support Staff:	Sachoyo NOZAWA, Masanobu NUNOGAKI

Outlines

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

1) the primary processes of the structural changes induced at solid excited state,
2) laser-induced structural changes of semiconductor surfaces,

As topics in the first category, we have studied the primary processes of Frenkel-pair formation by electronic excitation in ionic crystals, the initial process of photoinduced polymerization of diacetylene crystals, and the dynamics of the photoinduced phase transition in quasi-one dimensional organic crystals. As topics of the second categories, we have studied laser-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 femtoseconds

Current Research Programs

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

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

1) The primary process of photo-induced polymerization of diacetylene crystals

For one of typical diacetylene crystals that show photo-induced polymerization, mechanism of selective polymerizationof 5,7-dodecadiyne-1,12-diol bis[phenyl carbamate] (TCDU) has been stidied by means of resonance Raman scattering spectroscopy. We have found that the polymerization pathways into A and B phases are induced in chain-propagation reactions at the stage of forming origomers in the two-types of monomer crystals where diacetylene molecules have different crystalline orientations. This is the first clear demonstration of the primary process of selective photo-polymerization of diacetylene crystals.

2) The dynamics of neutral-to-ionic phase transition in tetrathiafulvalen-p-chloranil

crystals

As a series of studies for this topic, we studied excitation-dependent dependent features of the dynamics of the phase transition. Among the three distinctive steps of the precursor-forming step, local proliferation, and neutral-phase forming step in the transition, the first step is the key step that shows the strong dependence on the excitation density. Fie the densities below a critical value, the local proliferation which follows the first step cannot be induced, thus showing strong intensity-dependent dynamics of the process. Also, two different modes of coherent phonons can be generated in the transition process; one is generated at the first step of precursor formation, and the other is generated at the beginning of the second step of local proliferation. The force constant of the later mode is weakened significantly, and the amplitude depends super-linearly on the excitation density.

These results have revealed an important feature of non-linearity of the phase-transition process following optical excitation to generate charge-transfer excitons in this crystal.

Excitation-Induced Instability on Semiconductor Surfaces

By using STM for revealing the structural changes on surfaces from atomic level, together with the femtosecond non-resonant ionization spectroscopy, which enables us to detect desorbed neutral species simultaneously with high sensitivity, we have studied the laser-induced electronic processes of structural changes and desorption for Si(111)-(7x7), Si(001)-(2x1), Si(111)-(2x1), GaAs(110)-(1x1) and InP(110)-(1x1) surfaces. For all surfaces studied, the laser-induced electronic excitation results in surface structural changes associated with bond breaking of constituent atoms incorporated in the intrinsic surface structures. Main results are summarized as follows.

1) The morphology of defects generated by laser-induced bond breaking depends critically on the Fermi level of crystals in III-V semiconductors. On the InP(110)-(1x1) surfaces, P-vacancy clusters are formed predominantly on n-type surfaces, while isolated P-monovacancies are formed exclusively on p-type surfaces. In view of the fact that surface P-monovacancies are charged positively (negatively) on p-type (n-type) surfaces, this anomalous Fermi-level effect has revealed the crucial role of surface holes in the structural instability on the surfaces.

2) The role of two-hole localization in anion-vacancy formation on the (110) surfaces of III-V semiconductors at the third regime of Langmuir evaporation

We have studied theoretically the significant Fermi-level effects on the formation rate of anion vacancies on vacuum-cleaved III-V semiconductor surfaces revealed by STM observations, by applying the two-hole localization mechanism of bond rupture on semiconductor surfaces. The increasing rate of vacancy formation with hole concentration results from the enhanced rate of two-hole localization at surface anion sites due to reduced energy separations between the Fermi energy and the energy level of the surface state composed of occupied anion dangling bonds.

Thus, the phenomena under laser excitation and those under thermal equilibrium can be understood on the same basis in terms of carrier localization at surface sites.

3) Photoinduced structural instability on the Si(111)-(2x1) surface

We have shown that the top-most Si atoms on the Si(111)-(2x1) surface have been removed electronically under valence excitation of Si crystals. The mechanism of two-hole localization has been proposed for the bond rupture, based on the studies under

valence excitation. Here we have shown that the instability is in fact induced under infrared-laser excitation that results only in the surface specific optical transitions without inducing any bulk valence excitations of Si crystals. The results have revealed the crucial role of holes generated in the surface valence state of semiconductor surfaces.

4) Structural instability of Si(111)-(7x7) induced by low-energy electron beam irradiation

The instability of surface structures under low-energy electron excitation has been studied for the Si(111)-(7x7) surface, for establishing new methods of nano-scale fabrication of semiconductor surfaces. The excitation of the surface with electron beams with primary energies less than 50 eV induces site-sensitive bond breaking of adatoms on the surface; the center adatoms are removed three times more efficiently than the corner adatoms, similar to the case of laser excitation. The cross-section of adatom removal depends strongly on the primary energy of incident electron; it decreases from the highest value at 15 eV with increasing primary energy. Inspection of electron-energy loss spectra for this surface suggest strongly the important role played by surface-plasmon excitation on the bond-breaking event.

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

We have studied the electron dynamics on the surfaces by means of two-photon photoelectron spectroscopy in order to elucidate the dynamics of photogenerated surface carriers, which play crucial roles in the excitation-induced instability. Use of femtosecond laser pulses for pump and probe pulses has a strong advantage for resolving the carrier dynamics directly. On the Si(001)-(2x1) surface, we show that the lifetime of the surface D_{down} state is shorter than at most 20 ps, and that the transition from bulk-to-surface states is rate-determining of the surface-state population. Consequently, apparent decay of electrons at surface un-occupied state of D_{down} shows a strong excitation-wavelength dependent feature.

The Primary Processes of Photoinduced Structural Instabilities in Insulating Solids

Temperature-dependent yield of Frenkel pairs generated by valence excitation in alkali halides

The dynamics of formation of self-trapped excitons (STEs) and Frenkel pairs upon band-gap excitation have been studied in several alkali halide crystals by femtosecond time-resolved spectroscopy at temperatures ranging from 6 to 330 K. We found that the primary yield of Frenkel pairs was governed by the process of exciton relaxation that terminated within 20 ps of excitation in all alkali halides at all temperature regimes studied. The yield increases with temperature, and is anti-correlated with the yield of triplet STEs, showing a strong effect of temperature on branching during exciton relaxation. We discuss the mechanism of the temperature-dependent branching of excitons based on the present results and knowledge accumulated from studies of other crystals.

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 given a reasonable performance in intensity and in stability.

Publications

Original Papers

Role of two-hole localization in anion-vacancy formation on the (110) surfaces of InP and GaAs at the third regime of Langmuir evaporation, K. Tanimura, Phys. Rev. B 69, (2004) 033301-1-4.

Temperature-dependent yield of Frenkel pairs generated by valence excitation in NaCl, Katsumi Tanimura and Wayne P. Hess, Phys. Rev. B 69, (2004) 155102-1-7.

Electronic bond rupture of Si dimers on the Si(001)-(2x1), J. Kanasaki, K. Katoh, Y. Imanishi, and K. Tanimura, Appl. Phys. A79, (2004) 865-868.

Photoinduced structural instability of the InP(110)-(1x1) surface, T. Gotoh, S. Kotake, K. Ishikawa, J. Kanasaki, and K. Tanimura, Phys. Rev. Lett. 93, (2004) 117401-1-4.

Femtosecond time-resolved reflection spectroscopy of photoinduced ionic-to-neutral phase transition in tetrathiafulvalen-p-chloranil crystals, Katsumi Tanimura, Phys. Rev. B 70, (2004) 144112-1-11.

Books

Time-resolved spectroscopy of the dynamics of photoinduced ionic-to-neutral phase transition in the trathiafulvalen-p-chloranil crystals, K. Tanimura, “Photoinduced Phase Transition”, edited by K. Nasu, (World-Scientific, Singapore, 2004), 71-115.

International Conferences

Ultrafast time-resolved spectroscopic study on photo-induced structural phase transitions in quasi one-dimensional organic crystals (Invited), K. Tanimura, 6th International Conference on Excitonic Processes in Condensed Matter, Cracow, Poland, July 2004.

Ultrafast Dynamics of Excitation-Induced Atomic Processes in Insulating Solids (Invited), T.Tanimura, 15th International Conference on Defects in Insulating Crystals, Riga, Lativia, July 2004.

Surface carrier dynamics and excitation-induced structural instability on semiconductor surfaces (Invited), K. Tanimura, Gordon Research Conference on Laser Interactions

with Materials, Andover, USA, August 2004.

Time-resolved two-photon photoelectron spectroscopy on the Si(001)-(2x1) surface, S.Tanaka, 10th International Workshop on Desorption Induced by Electronic Transitions, Susono, Japan, November 2004.

Photoinduced structural instability on Si(111)-(2x1), E. Inami and K. Tanimura, 10th International Workshop on Desorption Induced by Electronic Transitions, Susono, Japan, November 2004.

Structural instability of Si(111)-(7x7) induced by low-energy electron irradiation, Y. Sugita, J. Kanasaki, and K. Tanimura, 10th International Workshop on Desorption Induced by Electronic Transitions, Susono, Japan, November 2004.

Publications in Domestic Meetings

Physical Society of Japan 12 papers

Academic Degrees

Bachelor Degree of Engineering

K.Ichihashi	Excitation-induced structural reconstruction of Si surfaces
T. Ichibayashi	Surface carrier dynamics on semiconductor surfaces by tunable femtosecond 2ppe technique

Sponsorship

Grand-in-Aid for Scientific Research (B)

K. Tanimura	Mechanisms of photoinduced structural phase transitions of quasi one-dimensional organic crystals studied by time-resolved Raman-scattering spectroscopy	¥5,300,000

Grand-in-Aid for Scientific Research (C)

S. Tanaka	Ultra-fast carrier dynamics on semiconductor surfaces by means of time-resolved femtosecond 2ppe technique	¥3,200,000

Division of Organic Molecular Science

Outline

Division of Organic Molecular Science has five departments: Dep. of Organometallic Compounds (changed to Department of Regulatory Bioorganic Chemistry from July 2004), 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, organometallic chemistry, physical organic chemistry and photochemistry. In each department research on own original subject is going on and in some cases joint projects between several departments are carried out. A special project "Energy and Environment Friendly Materials," supported by the Ministry of Education, Culture, Sports, Science and Technology, Japan, was performed for the past five years.

Achievements

- Synthesis of helical-chiral poly(isocyanide)s in which the metal-porphyrin pendants are regularly arranged around the helical main chain
- Synthesis of helical-chiral poly(isocyanide)s having ferrocenyl pendants which exhibit reversible conformational change in response to external electric stimulus
- Ru-catalyzed carbonylation of allenyl-alcohols and –amines giving lactones and lactams, respectively, with atom economy of 100%
- Stereoselective reactions of planar-chiral cyclopentadienyl-ruthenium complexes
- Self-Assembly of transition metal ions with bipyridine ligands
- Synthesis of β-strand peptidomimetics bearing an epoxide cross-linker
- Synthesis of branch-type nano-scale conjugated molecules and their application to molecular electronics
- Synthesis of imidazolium-containing molecular wires with switching function
- Development of molecular wires insulated completely with bulky substituents
- 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 new asymmetric ligands
- Immobilization of multicomponent consisting asymmetric catalysts
- Functionalized nanoparticle as an asymmetric catalyst
- Elucidation and design of organic reactions
- Analysis of functional molecular materials with ultra small quantity and high sensitivity
- Basic concept for the appearance of functions of molecules and molecular materials.

Department of Regulatory Bioorganic Chemistry

Associate Professor: Kiyotaka ONITSUKA
Research Associate: Da-Yang ZHOU
Research Assistant: Fumie TAKEI

Outlines

The main projects of this department are the synthesis of new organometallic complexes and their application for selective organic synthesis and controlled polymerization with low impact for the environment as well as for the novel hybrid materials having unique functions. Current works are focused on the synthesis of optically active transition-metal complexes with planar and helical chirality, and the precise synthesis of organometallic polymers with characteristic molecular structures. Property and reactivity of these new complexes are investigated for the development of novel homogeneous catalysts and functional materials.

Current Research Programs

1. Stereoselective Reactions with Planar-Chiral Cyclopentadienyl Complexes

(1) The reaction of planar-chiral cyclopentadienyl-ruthenium complexes with Bu_4NI resulted in the formation of iodo complexes with high diastereoselectivity (up to >99 %de). The stereochemistry of the ruthenium center in the starting material did not influence the diastereoselectivity of the products. Epimerization of a diastereomerically pure sample gave a mixture of two diastereomers in the same ratio as with the ligand-exchange reaction, suggesting that the selectivity is determined by the difference in thermodynamic stability between the diastereomeric pair of iodo complexes.

(2) The treatment of planar-chiral cyclopentadienyl-ruthenium complexes with prochiral dienes led to the ligand-exchange reaction that gave η^4-diene complexes with high enantioface selectivity (up to >99%de). The selectivity of the reaction is under thermodynamic control of the resulting η^4-diene complexes and is affected by the substituents on both the cyclopentadienyl ligand and the diene.

(3) The reaction of planar-chiral cyclopentadienyl-ruthenium complexes with allyl chloride at room temperature resulted in the diastereoselective formation of π-allyl-ruthenium complexes, in which the chirality at the Ru center depended on the substituent at the 4-position of the cyclopentadienyl group. Epimerization at the Ru center of π-allyl complexes at 90 ˚C suggested that the diastereoselectivity was under kinetic control.

2. Precise Polymerization with Transition-Metal Complexes

Multinuclear acetylide complexes containing two or three Pd–Pt μ-ethynediyl units were prepared as multifunctional initiators for the living polymerization of aryl isocyanides. The polymerization smoothly proceeded to give two- or three-armed polymers with narrow polydispersity indexes in quantitative yields. Trace experiments using gel permeation chromatography and ^{31}P NMR spectroscopy as well as kinetics revealed that all the Pd–Pt μ-ethynediyl units acted as initiators for the living

polymerization.

3. Homogeneous Catalysis for Organic Synthesis

(1) Carbonylation of norbornene in the presence of rhodium carbonyl catalyst under water–gas-shift reaction conditions gave norbornene and carbon monoxide co-dimer having an enol–lactone structure in a high yield.

(2) Rhodium-catalyzed carbonylation of 2-alkynylbenzylamine under water–gas shift reaction conditions produced 2,4-disubstituted-1,4-dihydrobenz[c]azepin-3-one in a good yield.

(3) Carbonylation of azobenzene derivatives catalyzed by rhodium carbonyl in the presence of nitrobenzene as a hydrogen acceptor gave a four-ring heterocyclic product, indazolo[2,1-a]indazole-6,12-dione, in a good yield, which is derived from a novel cyclocarbonylation with C–H bond activation and CO insertion at each benzene nucleus of azobenzene.

4. Synthesis and Properties of Organometallic Macromolecules

An efficient convergent route to the main chain type of organometallic dendrimers in which platinum moieties are linked by 1,3,5-triethynylbenzene has been developed. The synthesis of platinum-acetylide dendrons involved the use of two types of trialkylsilyl groups for protection of the terminal acetylene. The platinum-acetylide dendrimers were prepared up to the third generation by reacting dendrons with a triplatinum core and a tetraplatinum core.

Publications

Original Papers

Rhodium-Catalyzed Carbonylation of Norbornene under Water-Gas-Shift Reaction Conditions. Selective Formation of Co-dimeres with Lactone Terminus, D.-Y. Zhou, S.-W. Zhang, K. Onitsuka and S. Takahashi: Chem. Lett., 33 (2004), 70–71.

Stereoselective Ligand-Exchange Reaction of Planar-Chiral Cyclopentadienyl-Ruthenium Complexes: Thermodynamic Control of Configuration at a Stereogenic Metal Center, Y. Matsushima: K. Onitsuka and S. Takahashi: Dalton Trans., (2004), 547–553.

Rhodium-Catalyzed Carbonylation of 2-Alkynylbenzylamine: A New Route to the Synthesis of Benzazepinones, T. Shiba, D.-Y. Zhou, K. Onitsuka and S. Takahashi: Tetrahedron Lett., 45 (2004), 3211–3213.

Enantioface-Selective Coordination of Prochiral 1,3-Dienes to Planar-Chiral Cyclopentadienyl-Ruthenium Complexes, Y. Matsushima, K. Onitsuka and S. Takahashi: Organometallics, 23 (2004), 2439–2446.

Quasi-Octahedral Complexes of Pentamethylcyclopentadienyliridium(III) Bearing Bis(diphenylphosphinomethyl)phenylphosphine (dpmp), Y. Yamamoto, Y. Kosaka, Y. Tsutsumi, Y. Sunada, K. Tatsumi, F. Takei and S. Takahashi: Dalton Trans., (2004),

2969–2978.

Rhodium-Catalyzed Cyclocarbonylation of Azobenzene, D.-Y. Zhou, T. Koike, S. Suetsugu, K. Onitsuka and S. Takahashi: Inorg. Chim. Acta, 357 (2004), 3057–3063.

Diastereoselective Oxidative Addition of Allyl Chloride to Planar-Chiral Cyclopentadienyl-Ruthenium Complexes, Y. Matsushima, K. Onitsuka and S. Takahashi: Organometallics, 23 (2004), 3763–3765.

Rapid Exciton Migration and Fluorescent Energy Transfer in Helical Polyisocyanides with Regularly Arranged Porphyrin Pendants, M. Fujitsuka, A. Okada, S. Tojo, F. Takei, K. Onitsuka, S. Takahashi and T. Majima: J. Phys. Chem. B., 108 (2004), 11935–11941.

Di- and Trifunctional Initiators Containing Pt–Pd μ-Ethynediyl Units for Living Polymerization of Aryl Isocyanides, K. Onitsuka, K. Yabe, N. Ohshiro, A. Shimizu, R. Okumura, F. Takei and S. Takahashi: Macromolecules, 37 (2004), 8204–8211.

Unexpected Formation of Vinyl-Phosphonio Complex $[CpRu(PPh_3)(C_6H_4PPh_2CH{=}CH_2)][PF_6]$ from Vinylidene Complex via Nucleophilic Addition and *ortho*-Metalation of Triphenylphosphine, K. Onitsuka, M. Nishii, Y. Matsushima and S. Takahashi: Organometallics, 23 (2004), 5630–5632.

Convergent Synthesis of Platinum-Acetylide Dendrimers, K. Onitsuka, M. Fujimoto, H. Kitajima, N. Ohshiro, F. Takei and S. Takahashi: Chem. Eur. J., 10 (2004), 6433–6446.

Review Papers

Helical polyisocyanide - Discovery of new catalyst, development of precise polymerization, and creation of new function (in Japanese), S. Takahashi, K. Onitsuka and F. Takei: Mirai Zairyo, 4(8) (2004), 8–15.

Helical Structure of Polyisocyanides (in Japanese), K. Onitsuka, Koubunshi, 53 (2004), 922–925.

Books

Synthesis of Organometallic Supra Moleculer Complexes (in Japanese), S. Takahashi and K. Onitsuka, In Zikken Kagaku Kouza 5th Ed. Vol. 12 Organotransition-metal Complexes and Supra Molecular Complexes, Chem. Soc. Jpn. Ed., Maruzen, pp 417–460.

International Conferences

Stereoselective Reactions of Planar-Chiral Cyclopentadienyl–Ruthenium Complexes (Poster), *K. Onitsuka and S. Takahashi, XXIst International Conference on Organometallic Chemistry, The University of British Columbia, Vancouver, Canada, July 25-30, 2004.

Novel Redox-Active Organometallic Dendrimers Composed of Ruthenium-Acetylide Units (Poster), *K. Onitsuka, N. Ohara, F. Takei and S. Takahashi, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004) -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Cyclic Aminocarbonylation of Alkynylimines with Cobalt-Catalyst (Poster), *D.-Y. Zhou, S. Suetsugu, K. Onitsuka and S. Takahashi, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004) -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Synthesis and Electrochemical Behavior of Organo-Ruthenium Dendrimers with Tri(4-ethynylphenyl)amine Bridges (Poster), *K. Onitsuka, N. Ohara, F. Takei and S. Takahashi, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Publications in National Meetings

The Chemical Society of Japan	1 paper
The Society of Polymer Science, Japan	1 paper
Division of Organometallic Chemistry, Kinki Chemical Society, Japan	2 papers

Sponsorship

Grant-in-Aid for Young Scientist (B)

F. Takei	Synthesis and Properties of Helical Poly(isocyanide)s	¥ 1,500,000

Department of Organic Fine Chemicals

Professor:	Nobuo KATO
Research Associates:	Hajime NITTA, Tomikazu KAWANO
Research Assistant:	Naoto TAJIMA
Graduate Students:	Masamitu HIRAOKA, Erika KAJITANI, Hitoshi KAJIYA, Akinobu TAKEDA, Yoshimi YANO, Takahiko YOSHINO
Research Student:	Masahide ANADA
Support Staff:	Mikako NAKASHIMA, Misuzu TANNO

Outlines

The object of this department is to create lead compounds for drug development, based on chemical proteomic approaches. Currently, we are focusing on the investigation of small organic molecules that can modulate protein-protein interactions in intracellular signal transductions. The stereoselective synthesis of biologically active compounds and the construction of biomimetic supramolecular systems are also investigated.

Current Research Programs

1. Synergetic Effects of Cotylenin A and Interferon-α on Ovarian Cancer Cells

We have found that cotylenin A and IFN-α synergistically inhibited growth both in vitro and in vivo, and induced apoptosis in human cancer cells. In the analysis of 39 cancer cell lines, ovarian cancer cells were highly sensitive to combined treatment with cotylenin A and IFN. This treatment was also effective toward ovarian cancer cells from the patients in primary cultures.

2. 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 differentiation of HL-60 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 and have succeeded in obtaining FC derivatives having CN-like activities on HL-60 cells.

3. Synthesis of a Stable Analogue of Autoinducer-2 in Bacterial Quorum-Sensing

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

4. Triple-Stranded Helicates as a Synthetic Template

We desiged and synthesized triple-stranded helicates possessing polyether side chains and investigated their potential as a synthetic template for creation of novel organic

molecular science. Ring-closing metathesis of our helicates have proceeded smoothly to yield pridine-containing macrocyclic (for instance, 288-membered ring) compounds.

Publications

Original Papers

Semi-wet peptide/protein array using supramolecular hydrogel, S. Kiyonaka, K. Sada, I. Yoshimura, S. Shinkai, N. Kato, and I. Hamachi: Nature Materials, 3 (2004) 58-64.

Effects of benzoyl group substituents on the mesomorphic properties of 5-alkoxy-2-benzoylamino- tropones, A. Mori, K. Uno, K. Kubo, N. Kato, H. Takeshita, K. Hirayama, and S. Ujiie: Liquid Crystals, 31 (2004) 285-294.

Novel Fusicoccins R and S, and Fusicoccin S Aglycone (Phomopsiol) from *Phomopsis amygdali* Niigata 2-A, and Their Seed Germination-stimulating Activity in the Presence of Abscisic Acid, N. Tajima, M. Nukina, N. Kato, and T. Sassa: Biosci. Biotechnol. Biochem., 68 (2004) 1125-1130.

Identification of (+)-Phyllocladene, (-)-Sandracopimaradiene, and (+)-Kaurene as New Fungal Metabolites from Fusicoccin-producing *Phomopsis amygdali* F6, H. Kenmoku, M. Tanaka, K. Ogiyama, N. Kato, and T. Sassa: Biosci. Biotechnol. Biochem., 68 (2004) 1574-1577.

Fusicocca-3(16),10(14)-diene, and β- and δ-Araneosenes, New Fusicoccin Biosynthesis-related Diterpene Hydrocarbons from *Phomopsis amygdali*, T. Sassa, H. Kenmoku, K. Nakayama, and N. Kato: Biosci. Biotechnol. Biochem., 68 (2004) 1608-1610.

Erinacol (Cyatha-3,12-dien-14β-ol) and 11-*O*-Acetylcyathin A3, New Cyathane Metabolites from an Erinacine Q-Producing *Hericium erinaceum*, H. Kenmoku, K. Tanaka, K. Okada, N. Kato, and T. Sassa: Biosci. Biotechnol. Biochem., 68 (2004) 1786-1789.

International Conferences

Indole Sensing Mechanisms that Control Growth Phase-dependent Expression of Xenobiotic Exporter Genes (Poster), *H. Hirakawa, A. Kobayashi, T. Hirata, H. Nitta, N. Kato and A. Yamaguchi, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Synthesis of a Stable Analogue of Autoinducer-2 in Bacterial Quorum-Sensing (Poster), *M. Hiraoka, Y. Yano, T. Kawano, H. Hirakawa, A. Kobayashi, T. Hirata, A. Yamaguchi, and N. Kato, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10,

2005.
Fusicoccane Diterpenoids Having Differentiation-inducing Activity on Human Myeloid Leukemia Cells: Studies on Structural Requirements (Poster), *V. Bulbule, T. Yoshino, H. Nitta, N. Tajima, Y. Honma, T. Sassa, and N. Kato, 21st 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Publications in Domestic Meetings

Japanese Cancer Association	2 papers
The Japanese Society of Hematology	1 paper
Japan Society for Bioscience, Biotechnology, and Agrochemistry	1 paper

Sponsorship

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

N.Kato	Chemogenomic Approach to Clarify the Intracellular Signal Transductions	¥3,300,000

Grant-in-Aid for Scientific Research (A) (1)

N.Kato	Gene-Cloning of Fungal and Plant Terpene Synthases and Its Usage for the Production of Useful Compounds	¥1,600,000

Department of Organic Molecular Materials

Professor:	Yoshio ASO
Associate Professor:	Takahiro KANEDA
Research Associate:	Yutaka IE
Research Assistant:	Kaori ASANO
Post Doctoral Fellow:	Aihong HAN
Graduate Students:	Nobukazu Negishi, Wakana YAMAMOTO, Tetsuro KAWABATA, Susumu TSUDA
Under Graduate Students:	Setsuko ISHIOKA, Masaru ENDO
Research Student:	Liu FENG
Support Staff:	Misayo IMAI

Outlines

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

Current Research Programs

1. Molecular Electronics Materials

We have developed a novel conjugated oligomeric system, which incorporated with the switching unit. The synthesis and properties of molecular wires bearing an imidazolium salt have been investigated. The shifts of oxidation potential with different counter anion have been observed. This result indicates that the control of electronic state has been achieved by the influence of counter anions.

We have synthesized the blanched oligothiophenes with the juncture of 1,3,5-trisubstituted benzene ring. The NMR spectra of the compounds with several junctures showed the significant dependence of chemical shifts of the aromatic protons on both the concentration and the temperature. Moreover, MALDI-TOF MS revealed a series of clear ion peaks of the associated species together with the strong molecular-ion peak. These results indicate the potentiality of the highly blanched oligothiophenes with several junctures for the construction of π-stacked structures.

2. Molecular Wires

We have been preparing molecular wires for building up nanoelectronic devices, with

the use of the 24-mer of oligothiophenes (24T) with ca. 10 nm in length having insulating coverage around the oligomer chain. We firstly prepared the thiophene-monomer unit with bukly t-butyldiphenylsilyl groups, and then a series of its oligomers was synthesized by repeated oxidative coupling reactions. Their electronic absorptions and redox potentials indicated that the π-conjugated backbone preserves good coplanarity. This was proved by the X-ray analysis of 4T, which also revealed that the oligomeric backbone of 4T is completely insulated by the bukly t-butyldiphenylsilyl groups. Moreover, it is highly important to connect each molecular wire to the bulk electrode and we have succeeded in synthesis of 4T, 8T, and 24T with terminal ethynyl anchor groups for silicon electrodes

3. Molecular Machines

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

Publications

Original Papers

α,ω-Bis(quinquethienyl)alkanes as a π-Dimer Model of Polythiophenes, T. Satou, T. Sakai, T. Kaikawa, K. Takimiya, T. Otsubo, and Y. Aso: Org. Lett., 6 (2004) 997-1000.

Vapour Deposited Films of Quinoidal Biselenophene and Bithiophene Derivatives as Active Layers of n-Channel Organic Field-Effect Transistors, Y. Kunugi, K. Takimiya, Y. Toyoshima, K. Yamashita, Y. Aso, and T. Otsubo: J. Mater. Chem., 14 (2004) 1367-1369.

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Photoinduced Electron Transfer in Porphyrin-Oligothiophene-Fullerene Linked Triads by Excitation of a Porphyrin Moiety, T. Nakamura, M. Fujitsuka, Y. Araki, O. Ito, J. Ikemoto, K. Takimiya, Y. Aso, and T. Otsubo: J. Phys. Chem. B, 108 (2004) 10700-

10710.

Dendrimer-Encapsulated Oligothiophenes, T. Otsubo, S. Ueno, K. Takimiya, and Y. Aso: Chem. Lett., 33 (2004) 1154-1155.

An Ambipolar Organic Field-Effect Transistor Using Oligothiophene Incorporated with two [60]Fullerenes, Y. Kunugi, K. Takimiya, N. Negishi, T. Otsubo, and Y. Aso: J. Mater. Chem., 14 (2004) 2840-2841.

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The Chemical Society of Japan	11 papers
Symposium on Fundamental Organic Chemistry	1paper
The Society of Polymer Science, Japan	2 papers
Symposium on Heteroatom Chemistry	2 papers

Sponsorship

Grant-in-Aid for Scientific Research (B)

Y. Aso	Function-Accumulated Extended-Conjugation Systems Based on Oligothiophenes and Their Novel Functions	¥9,700,000

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

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

Entrusted Research

Y. Aso	Japan Science and Technology Agency	Synthesis of Insulated Molecular Wires	¥871,000

Department of Molecular Excitation Chemistry

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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 Programs

1. Multi-beam Chemistry

Multi-beam chemistry has been studied using pulse radiolysis-laser flash photolysis combined method, two-color two-laser photolysis and three-color three-laser photolysis. Photochemistry of reaction intermediates and short-lived chemical species generated from the reaction induced by the first beam excitation of a starting molecule (two-step excitation method), and moreover, photochemistry of other chemical species generated from the reaction of the short-lived intermediate induced by the second beam excitation (three-step excitation method) can be studied. We clarified the properties of the higher triplet excited states of various organic compounds such as benzophenone and naphthalene using two-color two-laser flash photolysis. Furthermore, bond cleavage specific to the higher triplet excited states was found for the first time with a series of dyad molecules of benzophenone and naphthalene. Direct observation of the higher triplet excited state and excited radical cations became possible using a picosecond laser as the second laser. Stepwise photocleavage of two C-O bonds of 1,8-bis[(4-

benzoylphenoxy)-methyl]naphthalene was performed with three-step excitation by three-color three-laser irradiation. In addition, one electron oxidation, hole migration, and bimolecular reactions of aromatic hydrocarbon radical cations were elucidated from the formation and decay during the resonant two-photon ionization of such aromatic hydrocarbons in dendrimers and in cyclodextrins.

2. TiO_2 Photocatalytic Reactions

One-electron oxidation of various aromatic compounds such as aromatic sulfides and biphenyl derivatives, adsorbed on the surface of TiO_2 powder slurried in acetonitrile has been investigated by time-resolved diffuse reflectance spectroscopy. We directly observed the formation of $MV^{\bullet+}$ generated from the one-electron reduction reactions with carbon dioxide radical anion ($CO_2^{\bullet-}$), which is generated from the one-electron reduction reactions of HCO_2^- with the photogenerated h^+, in the colloidal TiO_2 aqueous solution. It is indicated that the $CO_2^{\bullet-}$, which is desorbed from the surface, reacts with MV^{2+} via a homogeneous electron transfer process in the bulk solution. We also studied the photocatalytic oxidation reactivities of the photogenerated h^+ during the UV or Vis laser flash photolysis of S- and C-doped TiO_2 powders. The oxidation reactions of substrates by h^+ generated during the 355-nm laser photolysis of the TiO_2 powders increased in the order of the pure > S-doped > C-doped TiO_2. On the other hand, no oxidation reaction was observed during the 430-nm laser photolysis of the S- and C-doped TiO_2 powders, although charge carriers were sufficiently generated under excitation. The mobility and potential energy of h^+ trapped at the doping sites would have significant influence on the efficiency of the one-electron oxidation reactions of organic molecules adsorbed on the S- and C-doped TiO_2 powders.

3. Photochemistry of DNA

To develop highly efficient photodynamic therapy (PDT) and a new method preventing aging and carcinogenesis originated from the photosensitized DNA damage processes, various DNA covalently attached with photosensitizer were synthesized and laser flash photolysis (LFP) of these photosensitizer-modified DNA was performed. DNA may serve as an excellent molecule to store information in nano-electronic devices, if the electronic readout of the sequence became possible. The measurement of the kinetics of the hole transfer in DNA may open the way for it. So far, there are many experimental and theoretical studies for the mechanism of “one-dimensional” conductivity in the double helix. Gel electrophoretic analysis showed the hole transfer over 100 Å, while the kinetics of single-step hole transfer was studied by time-resolved measurements. We succeeded direct observation of the long-distance hole transfer over 100 Å in DNA which depends upon the distance and DNA sequence. The hole transfer process occurred in the time scale of microseconds to milliseconds. Hole transfer kinetics was highly dependent upon the DNA sequence and base stacking. Given a certain sequence and length of DNA, an unique hole transfer kinetic will be obtained. The direct measurements of long-range hole transfer though DNA may allow high throughput readout of the stored information.

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Contribution to International Conferences

T. Majima, 14th International Congress on Photobiology (Session organizer)
T. Majima, 11th Symposium of Intelligent Electrophotonic Materials and Molecular Electronics (SIEMME'11) (Organizing member)
T. Majima, 2004 Korea-Japan Symposium on Frontier Photoscience "Photochemsitry and Nanotechnology" (Chairperson)

Publications in Domestic Meetings

Photochemistry Meeting	14 papers
Radiation Chemistry Meeting	2 papers
Basic Organic Chemistry Meeting	3 paper
Japan Photomedical Science and Photobiology	1 paper
85th Japan Chemical Society Meeting	12 papers
Oxidation Reaction Meeting	3 papers
Annual Conference of Japan Radiation Research Society	1 papers

Academic Degrees

Doctor Degree of Engineering

T. Takada, Mechanistic Studies on Charge Separation and Charge Transfer in DNA
K. Nakayama, Studies on Expression of Protein Functions by Photochemical Regulation of the Structure

Master Degree of Engineering

S. Uegaki, DNA Supramolecules Using Cross-linked Oligonucleotides
S. Samori, Resonant Two-Photon Ionization of Stilbene Derivatives
H. Yoshida, DNA Dynamics Studied by Formation of Pyrene Dimer Radical Cation

Sponsorship

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

T. Majima	Molecular Devices by Function-control of Conjugated DNA	¥1,300,000

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

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

Grand-in-Aid for Scientific Research (C) (2)

S. Tojo	Decomposition of Organic Compounds by Photocatalysts -Multi-photon Excitation Methods-	¥900,000

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

K. Kawai	High Efficient DNA Damage using Two-color Two-laser Irradiation	¥1,000,000

Grand-in-Aid for Scientific Research for Young Scientist

X. Cai	Development of Multi-laser Chemistry to Molecular Devices, Medical Treatment, and Environmental Science	¥1,000,000

Grand-in-Aid for Scientific Research for Young Scientist

T. Takada	High Efficient Formation of Long-lifetime Charge Separated State in DNA and its Application to DNA Molecular Devices	¥1,000,000

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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 Programs

1. Development Multifunctional Asymmetric Catalysts

Multifunctional asymmetric catalysts such as La-Li_3-tris(binaphthoxide) (LLB) complex and Al-Li-bis(binaphthoxide) complex (ALB) function like an enzyme by activating two different substrates to facilitate a chemical reaction. In a similar manner, a homo-dinuclear catalyst should be able to activate two identical substrates in a homolytic coupling reaction. Chiral dinuclear vanadium(IV) complexes with axial skeletons have been synthesized and found to promote the enantioselective oxidative coupling of 2-naphthol derivatives through a dual activation mechanism affording the product with up to 94% ee. The dual activation mechanism in this system was supported by the kinetic analysis and catalyst loading effects.

A new double-activation catalysis for the Morita-Baylis-Hillman (MBH) reaction of an α,β-unsaturated ketone and an aldehyde has also been established by the combined use of multifunctional asymmetric complexes and tributylphosphine ($(n\text{-Bu})_3P$). The above asymmetric catalysis is found to accelerate the enantioselective MBH reaction to afford the adduct in good chemical yield with up to 99% ee.

2. New Asymmetric Spiro-type Ligands

So far we have developed a new type of chiral bis(isoxazoline) ligand with

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

3. Chiral Ionic Liquids and Organocatalysts

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.

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 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. 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.

4. Highly Effective Synthesis of Functionalized Particles

Spherical particle such as a dendrimer has attracted much attention due to the great potential of applications in material science.

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-*i*-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.

5. Solvent-free Catalytic Epoxidation Using Green Solid Disperse Phase

Recently we have developed a new reaction system using the polyoxometalate catalyst and a harmless solid disperse phase as an environmentally benign oxidation system. Using the solid phase system of cetylpyridinium dodecatungstate ((CetylPy)$_{10}$[$H_2W_{12}O_{42}$]) catalyst / fluorapatite phase (FAp)/ urea-H_2O_2 without organic solvents, the epoxidations of alkenes and allylic alcohols proceed smoothly at ambient

temperature and pressure to afford the corresponding epoxides in good yields. We found that the similar solid-phase-system, Keggin-type of phosphomolybdate catalyst ($(Bu_4N)_3[PMo_{12}O_{40}]$)/ FAp/ urea-H_2O_2, was effective for selective oxidation of sulfides to the sulfoxides and the sulfones. Our solid phase system is a convenient green process; a solvent-free catalytic reaction, using a harmless solid disperse phase and reusable solid catalyst phase, without heating or cooling, without special apparatus.

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Design and Synthesis of Novel Spiro-type Ligands (Poster), *T. Tsujihara, K. Wakita, T. Kato, A. Shimomoto, M. L. Patil, C. V. L. Rao, T. Shinohara, M. A. Arai, S. Takizawa, and H. Sasai, 17th French-Japanese Symposium on Medicinal and Fine Chemistry (FJS-2004), Miyagi, Japan, May 17-20, 2004.

Dual Activation in a Homolytic Coupling Reaction Promoted by an Enantioselective Dinuclear Vanadium(IV) Catalyst (Poster), H. Somei, Y. Asano, *T. Yoshida, S. Takizawa, H. Yamataka, and H. Sasai, 17th French-Japanese Symposium on Medicinal and Fine Chemistry (FJS-2004), Miyagi, Japan, May 17-20, 2004.

The aza-Morita-Baylis-Hillman Reaction Catalyzed by Chiral Phosphine-Binol as an Organocatalyst, *K. Matsui, S. Takizawa, and H. Sasai, 16th International Symposium on Chirality (ISCD 16), New York, USA, July 11-14, 2004.

Development of Novel Chiral Spiro-type Ligands, *H. Sasai, K. Wakita, T. Kato, Y. Honda, M. A. Arai, T. Shinohara, C. Muthiah, T. Tsujihara, and S. Takizawa, The 36th International Conference on Coordination Chemistry (ICCC-36), Mérida Yucatán, México, July 18-23, 2004.

Dual Activation in a Homolytic Coupling Reaction Promoted by an Enantioselective Dinuclear Vanadium(IV) Catalyst (Poster), H. Somei, Y. Asano, *T. Yoshida, S. Takizawa, H. Yamataka, and H. Sasai, 15th International Conference on Organic Synthesis (ICOS-15), Aichi, Japan, Aug. 2-6, 2004.

The aza-Morita-Baylis-Hillman (aza-MBH) Reaction Promoted by Chiral Phosphine-BINOL as an Organocatalyst (Poster), *K. Matsui, S. Takizawa, and H. Sasai, 15th International Conference on Organic Synthesis (ICOS-15), Aichi, Japan, Aug. 2-6, 2004.

Novel Bifunctional Asymmetric Organocatalysts for aza-Morita-Baylis-Hillman (aza-MBH) Reaction, *K. Matsui, S. Takizawa, and H. Sasai, The 7th IUPAC International Conference on Heteroatom Chemistry (ICHAC-7), Shanghai, China, Aug. 20-25, 2004.

Catalytic Enantioselective Direct Henry Reaction, S. Takizawa, K. Murai, K. Wataguchi, T. Hara, and *H. Sasai, Rare Earths '04 in Nara, Nara, Japan, Nov. 7-12, 2004.

Novel Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman

(aza-MBH) Reaction (Poster), *K. Matsui, S. Takizawa, and H. Sasai, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Development and Application of Novel Immobilization Method for Multicomponent Asymmetric Catalysts (Poster), S. Takizawa, K. Marubayashi, *N. Inoue, and H. Sasai, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Environmentally benign solid-phase-reaction-system for aerobic oxidative dehydrogenation (Poster), *J. Ichihara, K. Iteya and Y. Sasaki, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Dual Activation in a Homolytic Coupling Reaction Promoted by an Enantioselective Dinuclear Vanadium Catalyst (Poster), T. Yoshida, *T. Katayama, H. Somei, Y. Asano, S. Takizawa, and H. Sasai, THE INTERNATIONAL SYMPOSIUM ON DYNAMIC COMPLEX (ISDC-2005), Nagoya, Japan, Jan. 9-10, 2005.

Development of Novel Spiro-type Ligands, T. Tsujihara, P. Koranne, C. Muthiah, K. Wakita, J. Yogo, S. Takizawa, and *H. Sasai, THE INTERNATIONAL SYMPOSIUM ON DYNAMIC COMPLEX (ISDC-2005), Nagoya, Japan, Jan. 9-10, 2005.

Development and Application of a Novel Method for the Immobilization of Multicomponent Asymmetric Catalysts (Poster), *K. Marubayashi, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Development of Artificial Enzymes with Relevance to Bioluminescence (Poster), *T. Kawase, D. Jayaprakash, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Design and Synthesis of Novel Chiral Spiro Ligands and Ionic Liquids (Poster), *C. V. L. Rao, M. L. Patil, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Study of Novel Chiral Ligands Bearing Spiro Skeleton and their Applications to Asymmetric Cyclizations (Poster), *C. V. L. Rao, M. L. Patil, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Development of Novel Chiral Spiro-type Ligands (Poster), *T. Tsujihara, P. Koranne, K.

Wakita, C. Muthiah, J. Yogo, S. Takizawa, and H. Sasai, 229th ACS National Meeting, San Diego, CA, USA, Mar. 13-17, 2005

Publications in Domestic Meetings

National Meeting of Chemical Society of Japan	12 papers
Symposium on Progress in Organic Reactions and Syntheses	1 paper
Congress of Organic Chemistry	5 papers
Symposium on Organic Synthesis	1 paper
Symposium on Organometallic Chemistry	1 paper
Congress of Heterocyclic Chemistry	1 paper
Perspective in Nano-supramolecule as Catalysts	2 papers
Symposium of Organic Synthesis for Young Scientists	2 papers
Japan Research Institute of Material Technology	1 paper

Academic Degrees

Master Degree of Science

T. Tsujihara	Development of Catalytic Enantioselective Aminocarbonylation
T. Yoshida	Development and Application of Chiral Dinuclear Complex with Dual Activation
K. Wataguchi	Design and Synthesis of Novel Chiral Ionic Liquids with Spiro Skeleton

Doctor Degree of Science

K. Marubayashi	Immobilization of Asymmetric Catalysts onto Spherical Nanoparticles

Sponsorship

Grant-in-Aid for Scientific Research (2)

H. Sasai	Development of Artificial Enzyme with Synergistic Multi-cooperation in Active Sites	¥2,000,000

Grant-in-Aid for JSPS Fellows

H. Sasai	Novel Asymmetric Catalytic Synthesis	¥400,000

Department of Analytical Molecular Chemistry

Professor: Tetsuro MAJIMA
Research Associate: Yoshio TAKAI

Outlines

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

Current Research Programs

1. TiO_2 photocatalytic reaction studied by solid-state high-resolution NMR

With collaboration to materials analysis center of ISIR, solid-state high-resolution NMR measurement was applied for elucidation of properties of substrates adsorbed on TiO_2 surface and the TiO_2 photocatalytic reaction mechanism. ^{1}H and ^{13}C solid-state high-resolution NMR spectra of several catechols adsorbed on the TiO_2 surface was measured before and after photoirradiation at the wavelength of the CT band.

2. Chiral Recognition Mass Spectrometry

With collaboration to materials analysis center of ISIR, electrospry ionization mass spectroscopy was applied for detecting host-guest chiral recognition properties.

Publications

Original Paper

Three papers were published with collaboration to materials analysis center of ISIR.

International Conferences

Four papers were presented with collaboration to materials analysis center of ISIR.

Publications in Domestic Meetings

Several papers were presented with collaboration to materials analysis center of ISIR.

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

Distributed ontology development environment
Systematization of functional knowledge using ontological engineering and its deployment
Advanced knowledge management and learning support
Analysis of collaborative learning interaction and meta-cognitive skill modeling
Authoring task ontology and an innovative architecture of an authoring system
3D modeling and visualization
Omnidirectiomal surveillance system and human behavior analysis

- Predicate Invention
- Constructive adaptive user interfaces
- Adaptive agents
- Web-based learning environments
- Sharing navigation knowledge
- Meta cognition in hyperspace
- Instructional design support for collaborative learning
- Knowledge acquisition from human experts

Knowledge discovery from graph structured data
Information retrieval under various data format
Discovery of time dependent law equations from data
Derivation of association rules for data with numeric attributes

Department of Knowledge Systems

Professor:	Riichiro MIZOGUCHI
Associate Professor:	Yoshinobu KITAMURA
Research Associates:	Akiko INABA(to Jan. 31), Munehiko SASAJIMA (from Jan. 1)
Post Doctoral Fellow:	Daniele Allard(from Nov.28)
Graduate Students:	Jonathan Touitou, Eiichi SUNAGAWA, Masataka TAKEUCHI, Yusuke TAKEUCHI, Yohei TANAKA, Shinya TARUMI
Undergraduates:	Mesbahy Houda, Shota YOSHIKAWA, Naoya WASHIO
Support Staff:	Naomi BANO

Outlines

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

Current Research Programs

1. Ontology : Theoretical Foundation of Knowledge Engineering

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

theorized about the fundamental issues on ontology from both scientific and engineering viewpoints. As a result, we published three enlightening papers which describe drawbacks of the current research, importance of ontological engineering, definitions of an ontology, its functions and roles, its classification and research topics. We further published some research results based on ontological engineering to show concrete examples of a new research direction. We have developed HOZO, an environment for ontology building/utilization based on our innovative theory on ontological engineering. HOZO 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.

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 2004, we developed a framework that transforms knowledge about functions based on mapping knowledge among ontologies. The framework enables integration of several conventional knowledge forms each of which represents context-dependent knowledge in a company. Furthermore, meta-data schema on semantic-web for annotation of functional knowledge has been investigated.

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 when 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 latest 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. In this year, we developed authoring task ontology and an architecture of an evolving authoring tool based on the task ontology. We also developed an authoring system for the collaborative learning and an innovative model of meta-cognitive skills with a framework 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' pro-found social intellectual awareness in organization. In this year, we developed a supporting system for designing a collaboration field optimized for both learning and practicing together with an explanation function of the design rationale of the field. Additionally we developed a knowledge management system for disclosure of the organizational knowledge to the outside world.

Publications

Original Papers

Ontology-based systematization of functional knowledge, Y. Kitamura, and R. Mizoguchi: Journal of Engineering Design, 15[4] (2004), 327-351.

Deployment of an Ontological Framework of Functional Design Knowledge, Y. Kitamura, M. Kashiwase, M. Fuse, R. Mizoguchi: Advanced Engineering Informatics, 18[2] (2004) 115-127.

A Design Environment to Articulate Design Intention of Learning Contents, Y. Hayashi, M. Ikeda, and R. Mizoguchi: International Journal of Continuing Engineering Education and Life Long Learning, 14[3] (2004) 276-296.

Le role de l'ingenierie ontologique dans le domaine des EIAH, R. Mizoguchi (Translated by: J. Bourdeau) : Sciences et Technologies de l'Information et de la

Communication pour l'Education et la Formation,11 (2004).

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Review Papers

Engineering Domain Ontologies, Kitamura,Y. Journal of the Japanese Society for Artificial Intelligence Vol.19 No.2 (2004) 179-186.

Tutorial on ontological engineering - Part 2: Ontology development, tools and languages, R. Mizoguchi: New Generation Computing 22[1] (2004) 61-96.

Tutorial on ontological engineering - Part 3: Advanced course of ontological engineering, R. Mizoguchi: New Generation Computing 22[2] (2004) 193-220.

Books

Leaner Model Ontology and leaner Model Agent, W. Chen, and R. Mizoguchi: Cognitive Support for Learning - Imagining the UnknownP. Kommers, Ed, IOS Press, (2004) 189-200.

International Conferences

Essentials of Ontological Engineering (Invited), *R. Mizoguchi, the Acfas Congress, Montreal Canada, May 11-12, 2004.

A Success Story of Ontological Engineering in a Japanese Company - Engineering Knowledge Management Based on Functional Ontology (Invited), *R. Mizoguchi, KEST04, Beijin, P.R.China, September 17-19, 2004

Ontological Engineering and ITS Research(Invited), *R. Mizoguchi, ITS2004, Maceio, Brazil, Aug.30-Sept.3, 2004.

Ontological integration of data models for cell signaling pathways, *T. Takai-Igarashi, and R. Mizoguchi, GIW2004, Tokyo, Dec.13-15, 2004.

Ontology-based Functional-Knowledge Modeling Methodology and its Deployment, *Kitamura, Y., Mizoguchi, R., The 14th International Conference on Knowledge Engineering and Knowledge Management EKAW 2004, Whittlebury Hall, Northamptonshire, UK, Oct. 5-8, 2004.

Coping with Unintended Behavior of Users and Products: Ontological Modelling of Product Functionality and Use Wilfred van der Vegte, *Y. Kitamura, Y. Koji, R. Mizoguchi, CIE 2004: ASME 2004 Design Engineering TechnicalConferences and Computers in Engineering Conference, Salt Lake City, Utah, Sep. 28 – Oct. 2, 2004.

Towards Modeling Design Rationale of Supplementary Functions in Conceptual Design, *Y. Koji, Y. Kitamura, and R. Mizoguchi, International Conference on Tools and Methods of Competitive Engineering - TMCE 2004 (TMCE2004), Lausanne, Switzerland, Apr. 13-17, 2004.

Learning Design Palette: An Ontology-aware Authoring System for Learning Design, *A. Inaba, and R. Mizoguchi, International Conference on Computers in Education (ICCE2004), Melbourne, Australia, Nov. 30-Dec. 3, 2004.

EASE: Evolutional Authoring Support Environment, *L. Aroyo, A. Inaba, L. Soldatova, and R. Mizoguchi, The seventh International Conference on Intelligent Tutoring Systems (ITS2004), Alagoas, Brazil, Aug. 30-Sep. 3, 2004.

Learners' Roles and Predictable Educational Benefits in Collaborative Learning - An Ontological Approach to Support Design and Analysis of CSCL, *A. Inaba and, R. Mizoguchi, The seventh International Conference on Intelligent Tutoring Systems (ITS2004), Alagoas, Brazil, Aug. 30-Sep. 3, 2004.

Towards Shared Understanding of Metacognitive Skill and Facilitating Its Development , *M. Kayashima, A. Inaba, and R. Mizoguchi, The seventh International Conference on Intelligent Tutoring Systems (ITS2004), Alagoas, Brazil, Aug. 30-Sep. 3, 2004.

What is Metacognitive Skill? - Collaborative Learning Strategy to Facilitate Development of Metacognitive Skill, *M. Kayashima, A. Inaba, and R. Mizoguchi, The sixteenth World Conference on Educational Mutimedia, Hypermedia & Telecommunications (ED-MEDIA 2004), Lugano, Switzerland, Jun. 21-26, 2004.

Development of a System that Provides Teachers with Useful Resources from Various Viewpoints Based on Ontology, *T. Kasai, H. Yamaguchi, K. Nagano, and R. Mizoguchi, The sixteenth World Conference on Educational Mutimedia, Hypermedia & Telecommunications (ED-MEDIA 2004), Lugano, Switzerland, Jun. 21-26, 2004.

Ontological Knowledge Base Reasoning with Sort-Hierarchy and Rigidity, *K. Kaneiwa, and R. Mizoguchi, The Ninth International Conference on the Principles of Knowledge Representation and Reasoning (KR2004), Canada, 278-288, June, 2004.

Intellect Transmission Support Based On Organizational Intellect Model, *M. Ikeda, Y. Hayashi, Y. Tanaka, M. Takeuchi, R. and Mizoguchi, SW-EL'04: Applications of Semantic Web Technologies for E-Learning, Hiroshima, Japan, Nov. 8, 2004.

A SW-based Framework for Disclosure of Organizational Knowledge to the Outside World (Poster), *Y. Tanaka, Y. Hayashi, M. Takeuchi, M. Ikeda, and R. Mizoguchi, 3rd International Semantic Web Conference (ISWC2004), Hiroshima, Japan, Nov. 7-11, 2004.

Contributions to International Conferences and Journals

Riichiro Mizoguchi	The 3rd International Semantic Web Conference (ISWC2004)(Organizing committee chair)
Riichiro Mizoguchi	European Project on SEKT(Steering committee member)

Riichiro Mizoguchi	International Conference on Intelligent Tutoring Systems(ITS2004)(PC member)
Riichiro Mizoguchi	The 9th Ibero-American Conference on Artificial Intelligence IBERAMIA'04(PC member)
Riichiro Mizoguchi	European Semantic Web Conference (ESWC2004) (PC member)
Riichiro Mizoguchi	The Fifth International Symposium on Tools and Methods of Competitive Engineering (TMCE 2004) (PC member)
Riichiro Mizoguchi	Workshop on Applications of Semantic Web Technologies for E-learning (Workshop Co-Chair)
Riichiro Mizoguchi	The 2004 IFIP International Conference on Intelligence in Communication Systems (INTELLCOMM 04) (PC member)
Riichiro Mizoguchi	The World Congress on Computers, AIAI2004 (PC member)
Riichiro Mizoguchi	European KAW Conference (EKAW 2004) (PC member)
Riichiro Mizoguchi	Secretary of International Artificial Intelligence in Education Society
Riichiro Mizoguchi	Asia-Pacific Society for Computer in Education (APSCE) (Board member)
Riichiro Mizoguchi	International Journal of Applied Ontology (Editorial board)
Riichiro Mizoguchi	International Journal of Artificial Intelligence in Education (Editorial board)
Riichiro Mizoguchi	International Journal of Advanced Engineering Informatics (Editorial board)
Riichiro Mizoguchi	International Journal of Web Semantics (Editorial board)
Riichiro Mizoguchi	International Journal of Computer and Engineering Management (Editorial board)
Riichiro Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)
Akiko Inaba	The Third International Semantic Web Conference 2004 (ISWC2004) (Publicity Chair)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	7 papers
Japanese Society for Information and Systems in Education	3 papers

Academic Degrees

Master Degree of Engineering

Youhei TANAKA	Design and development of a framework for disclosure of organizational knowledge to the outside world based on knowledge creation and inheritance model
Shinya TARUMI	Development of an Editing System of Integrated Knowledge Function/Manufacturing Process for Supporting Nano-Materials Design

Sponsorship

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

R. Mizoguchi	Management and Utilization of Knowledge Contents of Design and Manufacturing based on Function	¥4,900,000
A. Inaba	Constructing repositories of how we design effective collaborative learning to support instructional design process	¥3,600,000

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

R. Mizoguchi	Development of a Theory-Aware Authoring Workbench	¥15,600,000

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

Y. Kitamura	Research on functional ontologies for sharing functional design knowledge	¥1,200,000
A. Inaba	Modeling learner-to-learner interaction process in collaborative learning	¥1,100,000

Grant-in-Aid for JSPS Fellow

R. Mizoguchi	Ontological Modeling of Second Language Learning Interferences and an Experimental Computer Application	¥500,000

Other Allocations

R. Mizoguchi	Human-Centered Semantic Web	¥2,640,000

Entrusted Research

R. Mizoguchi	Galaxy Express Corporation	MEXT IT Program e-Science Project Building a support system for operating a large-scale system using advanced IT	¥1,050,000

Cooperative Research

R. Mizoguchi	The Society of Chemical Engineers, Japan	New Energy and Industrial Technology Development Organization Nanotechnology Materials Program "Structuralization of Materials Technology Know-How" Nanotechnology ontology studies and development of an ontology server	¥5,250,000
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	Japan Aerospace Exploration Agency	Research on Application of Ontology Engineering to Satellite Design Support	¥4,300,000
R. Mizoguchi	Sumitomo Electric Industries, Ltd.	Development of a tool for technical knowledge systematization	¥2,520,000

Department of Intelligent Media

Professor:	Yasushi YAGI
Associate Professor:	Yasuhiro MUKAIGAWA
Research Associate:	Ryusuke SAGAWA
Designated Researcher:	Tomio ECHIGO
Graduate Students:	Yu OHARA, Takuji MAEDA, Nobuya AOKI, Kazuaki KONDO, Hai VU, Tetsuji HAGA , Naoki KURITA, Kensuke UEDA, Suchit PONGNUMKUL, Masaya TAKATSUJI, Hiroyuki NOGUCHI
Undergraduates:	Nanaho OSAWA, Hidetoshi MANNAMI, Yuichiro KOJIMA
Support Staff:	Masako KAMURA, Noriko YASUI, Saiko ONISHI, Yuko NAKAZAWA

Outlines

The studies in this laboratory focus on theory and applications related to computer vision and media processing. Some of the major research projects undertaken in the laboratory involve the creation of novel vision sensors, including the omni-directional vision system, and the development of algorithms for modeling real environments. Our research projects are motivated by applications in the fields of digital archiving, surveillance, intelligent robots, human interfaces and visualization.

Current Research Programs

1. Compound Catadioptric Stereo Sensor for Omnidirectional Object Detection

We propose a novel system to detect objects close to our sensor. For real-time detection and easiness to carry, we develop a small sensor with multiple spherical mirrors. Since an object is projected on each mirror, our method computes the range by catadioptric stereo. Our method creates a lookup table of corresponding points for infinite range. If an object is close enough to the sensor, the projected points of the object are different from these corresponding points. Thus, our method can detect near objects by taking difference of intensity of the corresponding points between the images of mirrors. We show our experimental setup of our sensor and show effectiveness of our method by experiments of near object detection.

2. Calibration and Performance Evaluation of Omnidirectional Sensor with Compound Spherical Mirrors

A stereo system, which consists of a single camera with multiple omnidirectional mirrors, is proposed. This system offers omnidirectional observation, portability, and real-time detection of near objects. In order to detect near objects, we need to create a model of the shape and location of the mirrors. However, the accurate modeling is difficult, thus making the system calibration difficult as well. We propose a method of calibrating the multiple ominidirectional mirror sensor through observing the point light

source at an infinite range. The system performance was calculated only at each pixel. As a result, performance of the mirror proved to become higher near its center and lower near the edge.

3. Real Time 3D Environment Modeling for a Mobile Robot by Aligning Range Image Sequence

We propose real time 3D modeling of environment for a mobile robot by aligning range images. 3D modeling by mobile robot needs simultaneous localization and mapping (SLAM). We obtain range images by a real time laser range finder mounted on the robot and align them in real time for SLAM. Our method sequentially aligns range images by a variant of iterative closest point (ICP) method, therefore estimates the self-position of the robot without any external devices. Also we propose a new weighting scheme for an ICP method. In the experiment, we analyze the precision of the real time laser range finder and evaluate the accuracy of the estimation of robot's position. Finally we show the result of modeling and localization by the robot which mounts the real time range finder.

4. Wide Dynamic Range by Filtering with Transmissive Liquid Crystal

We propose a method to generate a wide dynamic range image (WDRI) with a liquid crystal filter. We have implemented a system that consists of a camera and a liquid crystal filter placed in front of the camera. Generating WDRI from image obtained by the method, we need relation between filter control and the radiance of the image. We experimentally determine the relation between transmittance and filter control and model the point spread function of the liquid crystal filter in advance. As a result, the scene radiance can be derived from filter controlling information and radiance obtained by the sensor. We have developed a prototype system and experimented in the scene which includes drastic change of lighting. The result shows WDRI can be obtained by the proposed method.

Publications

Original Papers

Real-time Omnidirectional Image Sensors, Y. Yagi, M. Yachida, International Journal of Computer Vision, 58[3] (2004) 173-207.

Super Wide Viewing for Tele-operation, H. Nagahara, Y. Yagi, M. Yachida, Transaction on Circuits and Systems, 3[3] (2004) 693-608.

Books

Image Processing Technologies: Algorithms, Sensors, and Applications, Y Yagi, Marcel Dekker Inc, (2004) Chapter 5, 116-141.

Patents

Endoscope and endoscopic system, Y. Yagi, T. Echigo, R. Sagawa, JP 2004-041209

System for detecting adjacent depth from compound mirrors, Y. Yagi, T. Echigo,

JP2004-043320

Attachment of omnidirectional mirrors for an endoscope, Y. Yagi, T. Echigo, R. Sagawa, JP2004-197355

International Conferences

Walking Person Identification Dealing With Resolution and Appearance Changes, *Y. Ohara, R. Sagawa, T. Echigo, Y. Yagi, "In Proc. of Korea-Japan Joint Workshop on Frontiers of Computer Vision, Fukuoka, Japan, Feb. 3-4, 2004.

Gait Volume : Spatio-Temporal Analysis of Walking, *Y. Ohara, R. Sagawa, T. Echigo, Y. Yagi, In The fifth Workshop on Omnidirectional Vision, Camera Networks and Non-classical cameras, Prague, Czech, May 16, 2004.

Evaluation of Iconic Memory-based ORP Navigation, *Y. Yagi, K. Tsuji, M. Yachida, In Proc. of the 2004 IEEE International Conference on Robotics & Automation, New Orleans, USA, Apr. 26-May. 1, 2004.

Super Wide Viewing for Tele-operation, *H. Nagahara, Y. Yagi, M. Yachida, In Proc . International Conference Instrumentation, Measurement, Control, Circuits and Systems, Miami, Florida, USA, Apr. 21-23, 2004.

Compound Catadioptric Stereo Sensor for Omnidirectional Object Detection, *R. Sagawa, N. Kurita, T. Echigo, Y. Yagi, In Proc. IEEE/RSJ International Conference on Intelligent Robots and Systems, Sendai, Japan, Sep. 28-Oct. 2, 2004.

Immersive Head Mounted Display, *H. Nagahara, Y. Yagi, M. Yachida, In Proc. International Conference Virtual System and Multimedia, Gifu, Japan, Nov. 17-19, 2004.

Human Detection in Outdoor Scene Using Spatio-Temporal Motion Analysis, *T. Haga, K. Sumi, Y. Yagi, In Proc. of 17th International Conference on Pattern Recognition, Aug. 23-26, 2004.

SpaceRelighter -Recording and Reproducing Illumination in a Real Scene-, *Y. Mukaigawa, H. Nagai, Y. Ohta, Proc. International Conference on Virtual Systems and Multimedia (VSMM2004), Nov.17-19, 2004.

Virtual Photometric Environment using Projector, *Y. Mukaigawa, M. Nishiyama, T. Shakunaga, Proc. International Conference on Virtual Systems and Multimedia (VSMM2004), pp.544-553, Nov. 17-19, 2004.

Free Viewpoint Browsing of Live Soccer Games, *Y. Kameda, T. Koyama, Y.

Mukaigawa, F. Yoshikawa, Y. Ohta, IEEE International Conference on Multimedia and Expo (ICME2004), Taipei, Taiwan, Jun. 27-30, 2004.

Contributions to International Conferences and Journals

Y. YAGI	OMNIVIS'04 The fifth Workshop on Omnidirectional Vision, Camera Networks and Non-classical cameras (Program Committee Members)
Y. YAGI	OMNIVIS'05 The Six Workshop on Omnidirectional Vision, Camera Networks and Non-classical cameras (Program Committee Members)
Y. YAGI	Robotics: Science and Systems（Program Committee Members）
Y. YAGI	Computer Vision and Pattern Recognition 2005 (Program Committee Members)
Y. YAGI	The International Journal of Automation and Computing (Editorial Board)
Y. YAGI	IEEE International Conference on Robotics and Automation 2004 (Best Vision Paper Evaluation Committee Members)
Y. YAGI	IEICE Transaction on Information and Systems, special section on **"Life-like Agent and its Communication" (**Guest Editors**)**
Y. YAGI	International Journal of Computer Vision, special issue on "Research in Japan on Omni-Directional Sensors and Their Applications", （Guest Editors）
Y. MUKAIGAWA	Computer Vision and Pattern Recognition 2005 (Program Committee Members)

Publications in Domestic Meetings

Information Processing Society of Japan	9 papers
The Institute of Electronics, Information and Communication Engineers	6 papers
The Robot Society of Japan	1 paper
The Society of Instrument and Control Engineering	1 paper

Academic Degrees

Doctor Degree for Information Science

Takuji Maeda　　Matrix Search Method for Biometrics Identification

Master Degree of Information Science

Naoki Kurita　　Proposal of Compound Catadioptric Omni-directional Stereo

Sponsorship

Grant-in-Aid for Scientific Research (B)

Y. Yagi	Basic research on task oriented ominidirectional image sensor	¥3,700,000

Grant-in-Aid for Young Scientists (B)

Y. Mukaigawa	Virtual Photometric Environment for Reproducing Photometric Properties of Real Objects	¥1,100,000
R. Sagawa	Research on 3-D Modeling of Deformable Tubes	¥1,800,000

Other Research Funds

Y. Yagi	Japan Science and Technology Agency (JST) Development of medical technology using omnidirectional vision	¥35,100,000
Y. Yagi	Strategic Information and Communications R&D Promotion Programme, Multimedia Information Search by Teleoperated Robot Network in a Disaster Site	¥1,950,000

Department of Architecture for Intelligence

Professor:	Masayuki NUMAO
Associate Professor:	Satoshi KURIHARA (From Oct.1)
Research Associate:	Cholwich NATTEE
COE Researcher:	Sukree SINTHUPINYO
Graduate Students:	Roberto LEGASPI, Kenji SHIMIZU, Yuya HASHIMONO, Kenichi FUKUI, Nagayoshi YAMASHITA
Special Research Students:	Yoshinobu SATO, Satoshi SUGAWARA, Hideki NAKAYAMA, Shinya MOTOYAMA
Research Student:	Md. Nazmul HUDA
Support Stuff:	Mayumi MIKI

Outlines

The main research objective is to explore basic technology for computer systems, which support human learning and understanding, beyond conventional artificial intelligence. We particularly focus on the process of human-computer interaction to discover and create architecture of intelligence for such systems. We try to produce highly original research with findings from cognitive science, psychology, education, and computer science. Principal issues addressed are as follows: 1. Constructive Adaptive User Interfaces, 2. Web-based Learning Environments, and 3. Instructional Design Support for Collaborative Learning.

Current Research Programs

1. Constructive Adaptive User Interfaces

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

2. Web-based Learning Environments

Web can be viewed as a promising learning platform that facilitates self-directed learning with hypermedia/hypertext-based learning resources. In particular, learners can deeply learn about a certain topic by navigating a number of learning resources dealing with the topic, and can navigate the Web pages to construct their own knowledge from the contents of the navigated pages. However, it is not so easy to learn web-based learning resources in a self-directed way. It is particularly difficult for learners to navigate hyperspace, which is a learning space provided by the learning resources, in a

constructive way. In order to overcome these problems, we address an issue of how to support meta-cognition in hyperspace.

(1) Adaptive Navigation Previewing

Web-based learning resources provide learners with hyperspace where they can navigate domain concepts/knowledge in a self-directed and a constructive way. However, learners often fail in making the navigation path since they reach an impasse due to a cognitive overload, which is caused by the complexity of hyperspace. In order to resolve this problem, we have developed an adaptive previewer, which is composed of hyperspace map, page previewer, and path previewer. The page previewer generates an overview of each WWW page in the map by extracting information from the HTML file according to the learning contexts. The path previewer helps learners make a sequence of the pages previewed as navigation path plan. These facilities help learners decide which page to visit and plan a navigation path without visiting hyperspace.

(2) Adaptive Reflection Support for Learning in Hyperspace

The main problem addressed here is how to help learners reflect on knowledge that they have constructed in navigating existing hypermedia/hypertext based learning resources on the Web. In order to resolve this problem, we have developed an adaptive postviewer that can identify and display the contents learners have learned in each page navigated. We have also developed history comparator and knowledge externalization environment for motivating learners to reflect their knowledge constructed in hyperspace.

3. Intelligent Ubiquitous Sensor-Networks

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

Publications

Original Papers

Inductive Logic Programming for Multiple-Part Data: Applications on Structure-Activity Relationship Studies, C. Nattee, S. Sinthupinyo and M. Numao, Transaction of Japanese Society for Artificial Intelligence. 20 (3). 2005. pp. 159--166.

International Conferences

Learning First-order Rules from Data with Multiple Parts: Applications on Mining Chemical Compound Data, *C. Nattee, S. Sinthupinyo, M. Numao, and T. Okada: the 21st International Conference on Machine Learning (ICML 2004). Alberta, Canada. July 2004.

Inductive Logic Programming for Structure-Activity Relationship Studies on Large Scale Data, *C. Nattee, S. Sinthupinyo, M. Numao, and T. Okada: International Workshop on Computer Intelligence for Exabyte Scale Data Explosion (CIESDE'05) in conjunction with the 2005 International Symposium on Applications and the Internet. Trento, Italy. January 2005.

A Category-based Self-improving Planning Module, *R. Legaspi, R. Sison, and M. Numao: the 7th International Conference on Intelligent Tutoring System (ITS2004). Alagoas, Brazil. August 2004.

A Multifaceted Self-improving Planner, *R. Legaspi, R. Sison, and M. Numao: the International Conference on Computers in Education (ICCE2004). Melbourne, Australia. November 2004.

Combining Partial Rules and Winnow Algorithm: Results on Classification of Dopamine Antagonist Molecules, *S. Sinthupinyo, C. Nattee, M. Numao, T. Okada, and B. Kijsirikul: the 3rd International Workshop on Active Mining (AM 2004). Kanazawa, Japan. 2004.

MSIP: Agents Embodying a Category-based Learning ess for the ITS Tutor to Self-improve Its Instructional Plans, *R. Legaspi, R. Sison, and M. Numao: the 8th Pacific Rim International Conference on Artificial Intelligence (PRICAI2004). Auckland, New Zealand. August 2004.

Multiple-Instance Learning Based Heuristics for Mining Chemical Compound Structure, *C. Nattee, S. Sinthupinyo, M. Numao, and T. Okada: Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ, and IEICE-SIGAI on Active Mining. Hanoi, Vietnam. December 2004.

Partial Rule Weighting Using Single-Layer Perceptron, *S. Sinthupinyo, C. Nattee, M. Numao, T. Okada, and Boonserm Kijsirikul: Joint Workshop of Vietnamese Society of

AI, SIGKBS-JSAI, ICS-IPSJ, and IEICE-SIGAI on Active Mining. Hanoi, Vietnam. December 2004.

Preprocessing Planning for Data Mining, *A. Shiro, M. Numao, and C. Nattee: Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ, and IEICE-SIGAI on Active Mining. Hanoi, Vietnam. December 2004.

SBSOM: Self-Organizing Map for visualizing structure in the time series of hot topics, *K. Fukui, Kazumi Saito, Masahiro Kimura , and M. Numao: Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ, and IEICE-SIGAI on Active Mining. Hanoi, Vietnam. December 2004.

Self-improving Instructional Plans on the Level of Student Categories. *R. Legaspi, R. Sison, and M. Numao: the 4th IEEE International Conference on Advanced Learning Technologies (ICALT2004). Joensuu, Finland. August 2004.

Using Neural Network to Weight the Partial Rules: Application to Classification of Dopamine Antagonist Molecules, *S. Sinthupinyo, C. Nattee, M. Numao, T. Okada, and B. Kijsirikul: Pacific Rim Knowledge Acquisition Workshop (PKAW04). Auckland, New Zealand. 2004.

Multi-Agent Human-Environment Interaction Framework for the Ubiquitous Environment, *S. Kurihara, K. Fukuda, T. Hirotsu, S. Aoyagi, T. Takada, T. Sugawara: International Workshop on Massively Multi-Agent Systems (MMAS2004).

Contributions to International Conferences and Journals

M. Numao	New Generation Computing (Area Editor)
M. Numao	8th Annual Symposium on Japanese-American Frontiers of Science (Co-chair of Planning Group)
M. Numao	7th Annual Symposium on Japanese-American Frontiers of Science (Planning Group Member)
M. Numao	The 4th International Joint Conference on Autonomous Agents and Multi Agent Systems (Program Committee)
M. Numao	The Ninth Pacific-Asia Conference on Knowledge Discovery and Data Mining (Program Committee)
M. Numao	The IEEE/WIC/ACM International Conference on Web Intelligence/Intelligent Agent Technology (Program Committee)
M. Numao	The Nineteenth International Joint Conference on Artificial Intelligence (Reviewer)
M. Numao	The 8th Pacific Rim International Conference on Artificial Intelligence (Program Committee)
M. Numao	The 22nd International Conference on Machine Learning (Program Committee)

S. Kurihara	The First International Workshop on Agent Network Dynamics and Intelligence (Program chair)
S. Kurihara	The Second International Workshop on Biologically Inspired Approaches to Advanced Information Technology (Program Committee)
S. Kurihara	The IEEE/WIC/ACM International Conference on Web Intelligence (Program Committee)
S. Kurihara	The Second International Workshop on Networked Sensing Systems (Program Committee)
S. Kurihara	International Workshop on Massively Multi-Agent Systems (Program Committee)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence:	5 papers
The Institute of Electronics, Information and Communication Engineers	1 paper

Academic Degrees

Master Degree of Engineering

Y. Sato	Knowledge discovery about hepatitis by using Inductive Logic Programming
S. Sugawara	Automated acquisition of personal feeling about melody
S. Motoyama	Knowledge discovery from time series data with irregular intervals
K. Shimizu	An Adaptive Support for Navigation on the Meta-Space in Learning on the Web

Sponsorship

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

M. Numao	Automatic Information Gathering and Preprocessing by using Multistage Learning Method	¥8,300,000

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

M. Numao	Data-gathering Apprentice for Data Mining	¥2,100,000

Department of Advanced Reasoning

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Post Doctoral Fellows:	Chien Phu NGUYEN, Alexandre TERMIER
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Research Student:	Hong Tao LU
Under Graduate Students:	Kiyoto TAKABAYASHI, Kotaro NAKANISHI
Supporting Staffs:	Kana KOYAGI, Hiroko OKADA

Outlines

Being able to reason is fundamental to the intelligent activities of human beings. We humans create new ideas and entities based on our internal knowledge resource acquired by both external facts and past experiences. However, there is a cognitive and psychological limit in our information processing capability. Humans are very good at reasoning and interpreting a small amount of data be it semantically or syntactically, but are very poor at extracting useful/meaningful information in a short period of time from a huge amount of data. Our laboratory's research focus is on exploring various methods of mining/discovering informative knowledge from massive data using mathematical constraints, heuristic and statistical search techniques. During this year, we have worked on 1) knowledge acquisition from human experts and data, 2) knowledge discovery from graph structured data, 3) information retrieval under various data format, 4) discovery of time dependent law equations from data, and 5) derivation of association rules for data with numeric attributes.

Current Research Programs

1. Knowledge acquisition from human experts and data

Human experts can justify a given example case when put in a right context, whereas they are not good at explicitly stating the knowledge used in the problem solving for the case. We have investigated the performance of ripple down rules (RDR) technique, which efficiently acquires and utilizes expertise cultivated by experienced users in real fields. This approach always ensures the integrity of the accumulated knowledge after every addition of new piece of knowledge. The main results obtained up to this year include the followings.

1. We found that which knowledge to use as the default strongly affects the efficiency of knowledge acquisition and the compactness of the final knowledge base, and proposed a measure that can select the best default knowledge. The measure is to select the knowledge whose minimum description length is maximum. We have tested this against 15 different datasets from UCI data repository and confirmed the usefulness of this measure.

2. We further investigated how to delete existing knowledge from the knowledge base that is no more valid due to environment change. This ensures that RDR is a useful technique of knowledge acquisition even in a dynamic changing environment.

3. We have extended the RDR approach to incorporate knowledge acquisition from existing data. The new method can construct an RDR tree using the minimum description length principle from data alone. Thus, it is now possible to acquire knowledge and build a single RDR tree from two different sources of knowledge, i.e., human experts and accumulated labeled data. Switching of knowledge acquisition from human expert to data and vive versa can be made at any time point of knowledge base development.

4. We investigated a method to accelerate the knowledge acquisition not only by waiting for a new piece of data coming but also by actively asking a human expert from RDR, and proposed a promising method that allows an expert to answer only the class labels when the prediction of RDR is not correct and yet yields a knowledge base which is as good as the one built by a standard RDR method in which an expert has to refine the knowledge base.

5. We integrated the mechanisms: extension to an environment change and knowledge acquisition from a human expert and data. The analysis confirmed that these two can work as expected in an integrated environment.

6. We added a function to prune the acquired knowledge in addition to the function to delete useless knowledge in order to enhance the generalization capability, and demonstrated its effectiveness by a large number of datasets.

This year we did an extensive study of performance evaluation for various combination of knowledge source and environment change comparing the case where we trust human expert decision and the case where we modify the expert's decision using the information available from data when both kinds of knowledge are available, and verified that the latter results in a better performance in general. We think that the major objectives of this research subject are accomplished.

2. Knowledge discovery from graph structured data

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

1. We have developed a learning mechanism called "graph-based induction (GBI)"

that discovers characteristic patterns in a graph based on a simple idea of repeated chunking of linked two nodes in the graph. We also have expanded the method to discover classification rules that can predict the root node of a tree-structured data, and applied this to command prediction which is one of the functions needed for friendly user interface and to browsing pattern discovery from WWW log data. This method has a pruning function to suppress the overfitting.

2. We have developed a framework of the conventional basket analysis to derive association rules among sub-graphs by appropriately pre-processing the graph-structured data to a standard transaction of the conventional basket analysis. This approach allows to use the well-known Apriori algorithm without any modification to a graph-structured data but it is limited to a graph where each node has a unique label.

3. We have succeeded in dropping the requirement of the uniqueness of each node by rebuilding a completely different method called "Apriori-based Graph Mining (AGM)" that allows to handle topological structure. Graph structure is represented by adjacency matrix and isomorphic structure is efficiently disambiguated by introducing a notion of canonical form. Unlike GBI which is very fast but can only obtain approximate solutions, AGM's search is complete and derives all frequent induced subgraphs. AGM can handle the most general class of graphs, which includes both connected/unconnected, directed/undirected graphs with colored/un-colored nodes and labeled/unlabeled links. Self-looped link is also allowed.

4. We have extended GBI to handle multi-inputs/outputs, directed/undirected graph with/without node and link labels and loop structure (including a self-loop). It is not capable of handling non-connected graph. The method was verified to work as expected using artificially generated data. The repeated pairwise chunking does not by any means ensure the optimal solutions. It only extracts frequently appearing patterns in an approximate manner. However, its time complexity is shown to be almost linear to the size of graph.

5. In order to make AGM more efficient, further improvement was made to the data structure and the algorithm, i.e., extension of code expression representing a graph, change of the definition of the canonical form and the improvement of the search method. This accelerated the execution speed by two order of magnitude. In fact, the past AGM needed much computation time to analyze the subgraph co-occurrence in the molecular substructures of chemical compounds having mutagenesis and carcinogenesis. With this improvement, it is now possible to solve this problem within a tractable time.

6. Extensive improvement was also made on GBI without loosing its merit of greedy approach. Two separate criteria were introduced one for generating chunks and the other for extracting chunks. Repeated chunking is based on frequency measure but a different measure such as class separability measure can now be used to select good set of chunks. Further, canonical labelling was introduced to identify whether two subgraphs that are generated by different chunking history are indeed isomorphic.

With this enhancement, both directed and undirected graphs are now uniformly treated. The most important improvement was to adopt a beam search to expand the search space, which is quite effective in reducing the omitted important patterns.

7. We applied GBI to a real world medical dataset of hepatitis B and C, and went through all the phases of data mining: data preprocessing, conversion to graphs, extraction of typical subgraphs, evaluation of medical expert, and repeated this cycle four times. During the course of analysis, we made an improvement such as biasing the chunking direction, the need that really came from actual practice.

8. We proposed a new method of building a classifier DT-GBI for a graph structured data using GBI recursively at each node of a decision tree and applied it to a preliminary study of hepatitis data analysis.

9. We extended the adjacency matrix elements which are basic graph representation in AGM to explicitly represent edge labels in a graph. By this extension, generic, efficient and complete mining of frequent subgraphs which include edges having various labels has been enabled.

10. AcGM has been developed which can mine frequent generic subgraphs and frequent connected subgraphs not limited to frequent induced subgraphs. This has been achieved by introducing biases to constrain join operation to generate candidate frequent subgraphs in AGM's search. Especially, the connected subgraph mining is very efficient, and highly practical result in application to Bioactive Compounds Analysis has been obtained.

11. B-AGM has been developed which can mine frequent sub-ordered trees, frequent sub-unordered trees, frequent subpathes and frequent subsequences not limited to frequent subgraphs. The application fields of AGM have been significantly extended by this development.

12. We extended AGM to do a complete search reflecting the 3 dimensional sub-graph structure taking into account the 3 dimensional coordinates of vertices in the graph.

13. The algorithms of the aforementioned AcGM and B-AGM have been further improved to enable very fast data mining of the structures. With this improvement, AcGM and B-AGM are now one of the fastest complete graph mining tools.

14. Moreover, AcGM was made to be a public software to return the benefit resulted in our research to the public society.

15. We proposed a standard of PMML (Predictive Model Markup Language) to represent graph structured data. PMML is a subset of XML. The current graph mining tools in public support a graph representation only dedicated to each tool.

This is the significant difficulty in sharing the graph data and their mined results. However, with our proposal, a powerful environment becomes available for flexibly combining and using many tools and system in graph mining.

16. We performed an extensive analysis of the hepatitis dataset which was provided by Chiba University Hospital using DT-GBI, and succeeded in predicting the level of fibrosis, type of hepatitis (B or C), and effectiveness of interferon therapy with a reasonably good accuracy using only the results of the safe and inexpensive blood inspection.

17. We proposed an algorithm that approximately solves the subgraph isomorphism problem.

This year, we proposed a graph mining method called Chunkingless Graph-Based Induction (Cl-GBI), which can solve two crucial problems that GBI has, i.e. 1) inability of finding overlapping patterns and 2) possibility of overlooking existing subgraphs due to inappropriate chunking order. In fact, the second problem is caused by the first one. We also developed a decision tree learner DT-ClGBI that employs Cl-GBI instead of GBI, and applied it to the analysis of the hepatitis dataset. On the other hand, the characteristics of the subgraph search in the aforementioned B-AGM have been theoretically analyzed, and its generic completeness has been proved. Moreover, a language to represent graph, GML(Graph Markup Language), based on the aforementioned PMML standard has been designed, and the set of open software tools for the graph representation, the data conversion and the AGM analysis by using was developed to return the benefit resulted in our research to the public society.

3. 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.

A collaborative research is currently underway 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.

4. Discovery of time dependent law equations from data

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

1. We have developed a theory of first principle discovery and implemented it to a working system that can discover multiple simultaneous equations under experimental setting. Notion of scales of the experimental data and an interesting property that is deduced by dimensional analysis are the basis of the method. These two together with simple mathematics can constrain the form of admissible relations among the variables.

2. We have extended the above approach to derive equations from observed data where no active experimentation is allowed. This extension expands the scope of the application areas of our approach to various practical domains. The manipulation of quantities is not possible, under the environment of passive observation, to obtain numeric data from which to extract the relations among quantities. We introduced a technique to emulate virtual experiments to identify the relations among quantities within a given set of observed data. The final system works for passively observed phenomena for which nothing is known about the equation formulae that are needed to describe them and no knowledge of dimensions of the variables involved is available. It can handle a system that is described by several equations and many variables. The simulation results indicate that the method is noise resistant.

3. We have developed a method that can enhance the reliability of the obtained

equations using two different sets of quantities for the same phenomenon and the information of scale-types of the quantities.

4. An approach to discover a complex law equation model consisting of simultaneous equations was developed when only the passive observation is available. This work investigated the mathematical properties of invariance, symmetry and lattice structure of a simultaneous equation, and established a principle to figure out the number of equations governing the observed data simultaneously and the configuration of quantities in the equations. Based on the principle, an algorithm to derive law based simultaneous equations from data is developed and implemented. Its high ability to discover the complex models for the data obtained from a process plant and a social phenomenon has been confirmed.

The above work is to discover law equations representing static relations holding among quantities associated with objects independent to time. In contrast, this year 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.

5. Derivation of association rules for data with numerical attributes

Basket Analysis is to derive frequently co-occurred symbolic features and the relations among them, i.e., association rules. However, its applicability is limited to some narrow field since most of practical data are mixtures of symbolic and numerical features. In this regard, the extension of Basket Analysis to make it applicable to the data containing numerical features is expected to highly widen the application area of data mining. We have worked on this issue in our following past work.

1. An approach to discretize numerical feature data into symbolic feature data was developed. The data are preprocessed by this approach and applied to Basket Analysis. This approach enables to apply Basket Analysis to the data containing numerical features under a certain rough discretization, i.e., approximation, of numerical data.

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

In this year, the aforementioned monotonic interval density measure has been

implemented into a tool program for quantitative association rule mining, and its performance has been tested in practical conditions. Moreover, a new classification approach based on the quantitative association rule mining has been developed, and its performance has been tested. The performance of these approaches demonstrated significant practicality on both efficiency and accuracy.

Publications

Original Papers

Adaptive Ripple Down Rules method based on minimum description length principle, T. Yoshida, T. Wada, H. Motoda and T. Washio: Intelligent Data Analysis, 8 (2004)239-265.

Generalization for Frequent Subgraph Mining, A. Inokuchi, T. Washio and H. Motoda: Transactions of Japanese Society for Artificial Intelligence, 19[5] (2004) 368-378.

Adaptive Ripple Down Rules Method based on Description Length, T. Yoshida, T. Wada, H. Motoda and T. Washio: Transactions of Japanese Society for Artificial Intelligence, 19[6] (2004) 460-471.

Density-Based Spam Detector, K. Yoshida, F. Adachi, T. Washio, H. Motoda, T. Homma, A. Hakashima, H. Fujikawa and K. Yamazaki: IEICE Trans. Inf. & Syst., E87-D[12] (2004) 2678-2688.

A selective sampling approach to active feature selection, H. Liu, H. Motoda and L. Yu: Artificial Intelligence, 159[1-2] (2004) 49-74.

Review Papers

The Voice of Practitioners in Data Mining: Data Mining Applications: Overview and Prospect, T. Washio: Journal of Japanese Society for Artificial Intelligence, 19[3] (2004) 373-375.

International Conferences

Compact Dual Ensembles for Active Learning, A. Mandvika, H. Liu and *H. Motoda, The 8th Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD-04), Sydney, Australia, May 26-28, 2004.

Preliminary Analysis of Interferon Therapy by Graph-Based Induction, *T. Yoshida, W. Geamsakul, A. Mogi, K. Ohara, H. Motoda, T. Washio, H. Yokoi and K. Takabayashi, The Third International Workshop on Active Mining (AM-2004), Kanazawa, Japan, Jun.1, 2004.

Application of DT-GBI to Promoter and Hepatitis Datasets, *H. Motoda, T. Yoshida, K. Ohara, W. Geamsakul, T. Washio, H. Yokoi and K. Takabayashi, Workshop on

Knowledge Discovery in BioMedicine, Auckland, New Zealand, Aug.10, 2004.

Constructing Compact Dual Ensembles for Efficient Active Learning, A. Mandvika, H. Liu and *H. Motoda, The 2004 Pacific Knowledge Acquisition Workshop, Auckland, New Zealand, Aug.9-10, 2004.

Density-based spam detector, *K. Yoshida, F. Adachi, T. Washio, H. Motoda, T. Homma, A. Nakashima, H. Fujikawa and K. Yamazaki, The 10th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD-2004), Seattle, USA, Aug.22-25, 2004.

Analysis of Hepatitis Dataset by Decision Tree Graph-Based Induction, *K. Ohara, T. Yoshida, W. Geamsakul, H. Motoda, T. Washio, H. Yokoi and K. Takabayashi, Discovery Challenge 2004, Workshop held in conjunction with the 8th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD-2004), Pisa, Italy, Sep.20, 2004.

Using a Hash-Based Method for Apriori-Based Graph Mining , *P. C. Nguyen, T. Washio, K. Ohara and H. Motoda, The 8th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD2004), Pisa, Italy, Sep.20-24, 2004.

Consumer Behavior Analysis by Graph Mining Technique, *K. Yada, H. Motoda, T. Washio and A. Miyawaki, The 8th International Conference on Knowledge-Based Intelligent Information and Engineering Systems, Wellington, New Zealand, Sep.22-24, 2004.

Constructive Inductive Learning based on Meta-Attributes, *K. Ohara, Y. Onishi, N. Babaguchi and H. Motoda, The 7th International Conference on Discovery Science, Padova, Italy, Oct.2-5, 2004.

Analysis of Hepatitis Dataset by Using Cl-GBI, A. *Mogi, P. C. Nguyen, K. Ohara, H. Motoda and T. Washio, Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ and IEICE-SIGAI on Active Mining, Hanoi, Vietnam, Dec.4-7, 2004.

Cl-GBI: A Novel Strategy to Extract Typical Patterns from Graph Data, *P. C. Nguyen, K. Ohara, H. Motoda and T. Washio, Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ and IEICE-SIGAI on Active Mining, Hanoi, Vietnam, Dec.4-7, 2004.

Knowledge Discovery from Consumer Behavior in an Alcohol Market by Using Graph Mining Technique, *M. Kuroda, K. Yada, H. Motoda and T. Washio, Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ and IEICE-SIGAI on Active Mining, Hanoi, Vietnam, Dec.4-7, 2004.

Extension of Basket Analysis and Quantitative Association Rule Mining, *T. Washio, A. Fujimoto and H. Motoda, Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI,

ICS-IPSJ and IEICE-SIGAI on Active Mining, Hanoi, Vietnam, Dec.4-7, 2004.

Scientific Discovery of Dynamic Hidden States and Differential Law Equations, *F. Adachi, T. Washio and H. Motoda, Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ and IEICE-SIGAI on Active Mining, Hanoi, Vietnam, Dec.4-7, 2004.

Contributions to International Conferences and Journals

H. Motoda	Intelligent Data Analysis: An International Journal(Editorial Board)
H. Motoda	Advanced Engineering Informatics (Editorial Board)
H. Motoda	International Journal of Human-Computer Studies (Editorial Board)
H. Motoda	Knowledge and Information Systems: An International Journal (Editorial Board)
H. Motoda	Discovery Science Conference (Steering Committee, Chair)
H. Motoda	Algorithmic Learning Theory Conference (Steering Committee)
H. Motoda	Pacific-Asia Conference on Knowledge Discovery & Data Mining (Steering Committee, Chair)
H. Motoda	Pacific Rim International Conference on Artificial Intelligence (Steering Committee)
H. Motoda	The 8th International Conference on Discovery Science (Conference Chair)
H. Motoda	The 9th Pacific-Asia Conference on Knowledge Discovery & Data Mining (Conference Chair)
H. Motoda	The 15th International Conference on Inductive Logic Programming (Program Committee)
H. Motoda	The 5th IEEE International Conference on Data Mining (Program Committee)
H. Motoda	The 11th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (Program Committee)
H. Motoda	The 10th International Conference on Rough Sets, Fuzzy Sets, Data Mining, and Granular Computing (Program Committee)
H. Motoda	The 16th European Conference on Machine Learning ECML (Program Committee)
H. Motoda	The 9th European Conference on Principles and Practice of Knowledge Discovery in Databases PKDD (Program Committee)
H. Motoda	The 22nd International Conference on Machine Learning (Program Committee)
H. Motoda	The Symposium on Abstraction, Reformulation and Approximation (Program Committee)
H. Motoda	The 9th Pacific-Asia Conference on Knowledge Discovery & Data Mining (Program Committee)
H. Motoda	International Workshop on Feature Selection for Data Mining Interfacing Machine Learning with Statistics (Program Committee)
T. Washio	Special Issue on Mining Graphs, Trees and Sequences (MGTS), Journal of Fundamental Informatica (Editorial Board)

T. Washio	The 2004 Pacific Rim Knowledge Acquisition Workshop (PKAW2004) (Program Committee)
T. Washio	Second International Workshop on Mining Graphs, Trees and Sequences (MGTS-2004) (Program Committee, Chair)
T. Washio	3rd Workshop on Multi-Relational Data Mining(MRDM04) (Program Committee)
T. Washio	The Fourth Asia-Pacific Conference on Web Intelligence (WI-2004) (Program Committee)
T. Washio	Joint Workshop of Vietnamese Society of AI, SIGKBS-JSAI, ICS-IPSJ and IEICE-SIGAI on Active Mining (Program Committee)

Publications in Domestic Meetings

Japanese Society for Artificial Intelligence	7 papers
The Behaviormetric Society of Japan	1 paper
The Pharmaceutical Society of Japan	1 paper

Academic Degrees

Master Degree of Engineering

A. Fujimoto	Development of Numerical Basket Analysis Approach

Sponsorship

Grant-in-Aid for Scientific Research on Priority Area (1)

H. Motoda	Implementation of Active Mining in the Era of Information Flood	¥11,400,000
H. Motoda	Active Mining from Structured Data	¥13,400,000

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

H. Motoda	Constructive Induction of Useful Attributes from Complex Structured Data	¥6,700,000
T. Washio	Development of Data Mining Method for 3-dimentional Graph Structured Data and Its Application to Identification System of Bioactive Molecules	¥6,700,000

Grant-in-Aid for Exploratory Research

T. Washio	Development of Unified Information Retrieval Method based on Feature Extraction from Various Data Format	¥900,000

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

K. Ohara	Development of Domain Adaptive Data Mining System using Personalization Techniques	¥1,600,000

Grant-in-Aid for JSPS Special Research Fellows

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

Division of Biological Sciences

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. The mechanism of energy coupling in ATP synthesis/hydrolysis
2. The mechanism and regulation of formations of cytoplasmic single membrane (endomembrane) organelles with varying acidic pH
3. The molecular structures and the molecular mechanisms of xenobiotic extruding pumps functioning as a host-defense mechanism in cellular level
4. Comprehensive studies on bacterial xenobiotic exporter genes and the regulation of the expression by two-component signal transduction systems
5. Physiological roles of efflux transporters in signal transduction and mammalian development
6. The mechanisms of biogenesis of the topa quinone cofactor in copper amine oxidase and other novel “built-in” cofactors in quinohemoproteins
7. Identification of novel protein kinase C-interacting proteins and elucidation of their roles in signal transduction
8. Development of a new method of the gene delivery system using hepatitis B virus surface antigen particles

Achievements

- Membrane dynamics during osteoclast differentiation
- Secretory-granules specific proton pump and its role in insulin secretion
- Highly efficient assemble of complex gene targeting construct by *in vitro* transposition reaction and *in vivo* homologous recombination
- Determination of the crystal structure of bacterial major multidrug exporter AcrB
- Site-directed mutagenesis studies based on the crystal structure of AcrB
- Indole-sensing mechanism on the up-regulation of drug exporter genes in *E. coli*
- Analysis of regulation network on bacterial multidrug exporters
- Analysis of ABCA5 knock-out mice, a novel ABCA subfamily transporter
- Studies on the sphingosine-1-phosphate export mechanism from platelet
- Identification of novel mammalian RND-type transporters
- Over-expression of secretory phospholipase D by recombinant *Streptomyces lividans*
- Identification of a tissue-non-specific homologue of axonal fasciculation and elongation protein zeta-1
- ENH1 scaffolds PKD1 and PKCε at Z-discs, forming a signaling complex that participates in the development of cardiac hypertrophy
- Chemical rescue of a site-specific mutant of bacterial copper amine oxidase for generation of the topa quinone cofactor
- Development of novel bio-nanoparticles for human tissue-specific delivery of genes and drugs
- Pore-spanning giant vesicles on microfabricated silicon substrates

Department of Structural Molecular Biology

Professor:	Katsuyuki TANIZAWA
Associate Professor:	Shun'ichi KURODA
Research Associate:	Kenji TATEMATSU
Post Doctoral Fellows:	Andrés D. MATURANA, Kenji SUZUKI, Tadanori YAMADA, Tomoko YAMASAKI, Junko UEDA, Joo-Hee JUNG
Research Assistants:	Mana IDEI, Setsuko NAGAO, Masumi MAEKAWA, Yoko MATSUSHITA
Graduate Students:	Miki IWATA, Kazutoshi ONO, Nobuo YOSHIMOTO, Takeshi MURAKAWA, Nobuyuki BOKUI, Junko IKUTA, Ken MIURA (~2004.7), Masami ISHIDA, Takeshi KASUYA, Minobu TANI
Support Staff:	Mayumi MURATA

Outlines

The primary research of this department continues to focus on the biochemical and molecular biological studies on various functional proteins, with particular emphasis on the amino acid-metabolizing enzymes. The active-site structures and catalytic functions of amino acid residues in several interesting enzymes are being investigated by means of affinity labeling, site-directed mutagenesis, various spectroscopies, and X-ray crystallography. One of the recent conspicuous findings is the copper ion-dependent, post-translational modification mechanism for the biogenesis of the topa quinone cofactor in copper amine oxidase. In addition, this department started to investigate the intracellular mechanisms involving protein kinase C family, which play important roles in the cell proliferation, differentiation, oncogenesis, and apoptosis by cross talking with other molecules. Recently, we have succeeded to identify several protein kinase C-interacting proteins and characterized them as regulatory proteins for the protein kinase activities and/or their subcellular localization and also as effectors of kinase signaling. In addition, we have developed hollow bio-nanoparticles displaying various biorecognition molecules, which are expected to be an ideal vector for the tissue- and cell type-specific gene and drug delivery system.

Current Research Programs

1. Chemical Rescue of a Site-specific Mutant of Bacterial Copper Amine Oxidase for Generation of the Topa Quinone Cofactor.

The topa quinone (TPQ) cofactor of copper amine oxidase is produced by posttranslational modification of a specific tyrosine residue through the copper-dependent, self-catalytic process. We have site-specifically mutated three histidine residues (His431, His433, and His592) involved in binding of the copper ion in the recombinant phenylethylamine oxidase from *Arthrobacter globiformis*. The mutant enzymes, in which each His was replaced by Ala, were purified in the Cu/TPQ-free, precursor form and analyzed for their Cu-binding and TPQ-generating activities by

UV–visible absorption, resonance Raman, and electron paramagnetic resonance spectroscopies. Among the three His-to-Ala mutants, only H592A was found to show a weak activity to form TPQ upon aerobic incubation with Cu^{2+} ions. Also for H592A, exogenous imidazole rescued binding of copper and markedly promoted the TPQ formation. Accommodation of a free imidazole molecule within the cavity created in the active site of H592A was suggested by X-ray crystallography. Although the TPQ cofactor in H592A mutant was readily reduced with substrate, its catalytic activity was very low even in the presence of imidazole. Combined with the crystal structures of the mutant enzymes, these results demonstrate the importance of the three copper-binding histidine residues for both TPQ biogenesis and catalytic activity, fine-tuning the position of the essential metal.

2. Over-expression of Secretory Phospholipase D by Recombinant *Streptomyces lividans*.

The structural gene for phospholipase D (PLD) of an actinomycete, *Streptoverticillium cinnamoneum*, together with its promoter region was introduced into *Streptomyces lividans* using a shuttle vector pUC702 for *Escherichia coli* and *S. lividans*. The simultaneous feeding of carbon and nitrogen sources was effective for the efficient secretion of PLD, and the amount of secreted PLD reached a maximum level (about 5.5×10^4 U/l, 118 mg/l) after about 60 h. In contrast to the original producer, *Stv. cinnamoneum*, this heterologous expression system is markedly efficient for the production of the secretory PLD.

3. ENH1 Scaffolds PKD1 and PKCε at Z-discs, Forming a Signaling Complex That Participates in the Development of Cardiac Hypertrophy.

Cardiac hypertrophy is triggered in response to mechanical stress and various neurohumoral factors, such as α-adrenergic agents, angiotensin II, and endothelin I. Several signaling pathways are involved in the generation of the hypertrophic response, and their specific outcome requires the assembly of precisely localized signaling complexes. Here, we investigate the patho-physiological role and intracellular localization of protein kinase D1 (PKD1) in the context of cardiac hypertrophy. In neonatal rat cardiomyocytes, stimulations with neurohumoral factors induced the translocation of active PKD1 to the Z-discs, whereas those with a cytokine leukemia inhibitory factor did not. PKCε-dependent activation of PKD1 was sufficient to induce the atrial natriuretic factor expression, sarcomeric reorganization, and cell size increase. A PDZ-3LIM protein ENH1 is necessary for bundling of the two kinases at the Z-discs; interference of its message completely suppressed the Z-disc formation. Thus, the ENH1/PKCε/PKD1 complex could play a central role in cardiac hypertrophy.

4. Development of Novel Bio-Nanoparticles for Human Tissue-Specific Delivery of Genes and Drugs.

Gene therapy is recognized as one of the most promising cures for cancer. Many attempts using virus vectors have been made for delivering genes to various cancer cells in human. While these gene therapies have shown noticeable efficacy, it has turned out that nonspecific introduction of genes into undesired cells and organs causes deleterious side effects. More importantly, the virus vector-derived DNA may induce unexpected

effects on human. Hepatitis B virus (HBV) is a human liver-specific DNA virus, whose genome harbors three overlapping envelope (env) genes in a single open reading frame, encoding S, M (pre-S2 + S), and L (pre-S1 + pre-S2 + S) proteins. In the last decade, the recombinant HBV env S and/or proteins were produced in yeast cells as particles and used as the immunogen for the new generation HB vaccines that were proven to be safely applicable to human. Recently, the pre-S1 peptide of L protein was also shown to possess the specific receptor for human liver cells, which is crucial for the infectivity of HBV. We previously succeeded overproduction of the HBV env L particles in yeast cells (up to 42% of the total soluble protein). In the present studies, we have shown that the delivery of a gene or a drug by the L particles is efficient and specific to human hepatocytes in cell culture. In the mouse xenograft model bearing human hepatocellular carcinoma cell line, intravenous injection of L particles containing the gene for green fluorescence protein (GFP) or a fluorescent dye results in the induction of fluorescence only in the human liver-derived cells but in neither other human cells nor mouse normal tissues. When the human clotting factor IX gene was transferred into the xenograft model by L particles, the therapeutic level of factor IX was found in plasma for at least 1 month (Yamada *et al.*, Nature Biotechnology **21**, 885-890, 2003). Unlike viral vectors, the L particle system is free from viral genomes, highly specific to human hepatocytes, safely and efficiently produced in yeast cells, and applicable for drug delivery system as well as gene delivery. In addition, we succeeded in re-targeting of L particles to non-liver cells. These advantages indicate that the L particle would be a promising and novel platform for cell- and tissue-specific gene and drug delivery system as mentioned recently by others (Lancet **362,** 48, 2003).

5. Pore-spanning Giant Vesicles on Microfabricated Silicon Substrates.

We report on a pore-spanning behavior of giant vesicles on a topographically patterned but chemically uniform surface. Micrometer-sized pores with sharp edges were formed by the combination of photolithography and anisotropic wet etching of silicon substrates. Each of giant vesicles spreads on the microfabricated substrates to form a pore-spanning vesicle membrane which is not in contact with the bottoms of the micropores. The tendency of giant vesicles to form the suspended membrane over the micropores is discussed in terms of the balance between adhesion and bending energies of a vesicle membrane at such a sharp edge of micropores.

Publications

Original Papers

Identification of a Tissue-non-specific Homologue of Axonal Fasciculation and Elongation Protein Zeta-1 (FEZ1), T. Fujita, J. Ikuta, J. Hamada, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda: *Biochem. Biophys. Res. Commun.*, 313 (2004) 738–744.

Enhanced Long-term Potentiation In Vivo in Dentate Gyrus of NELL2-Deficient Mice, S. Matsuyama, K. Aihara, N. Nishino, S. Takeda, K. Tanizawa, S. Kuroda, and M. Horie: *NeuroReport*, 15 (2004) 417–420.

Chemical Rescue of a Site-specific Mutant of Bacterial Copper Amine Oxidase for Generation of the Topa Quinone Cofactor, H. Matsunami, T. Okajima, S. Hirota, H. Yamaguchi, H. Hori, S. Kuroda, and K. Tanizawa: *Biochemistry*, 43 (2004) 2178–2187.

Expression of Fasciculation and Elongation Protein Zeta-1 (FEZ1) in the Developing Rat Brain, A. Honda, K. Miyoshi, K. Baba, M. Taniguchi, Y. Koyama, S. Kuroda, T. Katayama, and M. Tohyama: *Brain Res. Mol. Brain Res.*, 122 (2004) 89–92.

Over-Expression System for Secretory Phospholipase D by *Streptomyces lividans*, C. Ogino, M. Kanemasu, Y. Hayashi, N. Shimizu, A. Kondo, S. Tokuyama, Y. Tahara, S. Kuroda, K. Tanizawa, and H. Fukuda: *Appl. Microbiol. Biotechnol.*, 64 (2004) 823–828.

Review Papers

Molecular Function of Axonal Guidance-related Proteins, UNC-76/FEZ1/FEZ2, T. Fujita, J. Ikuta, A. Maturana, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda: *Recent Res. Devel. Biophys. Biochem.*, 4 (2004) 313–320.

Novel Tissue and Cell Type-Specific Gene Delivery System Using Surface Engineered Hepatitis B Virus Nanoprotein Particles, T. Yamada, A. Kondo, M. Ueda, M. Seno, K. Tanizawa, and S. Kuroda: *Current Drug Targets: Infectious Disorders*, 4 (2004) 163–167.

A New Clinical Technique Developed by Hollow Bio-Nanoparticles (in Japanese), S. Kuroda, T. Yamada, M. Seno, A. Kondo, M. Ueda, and K. Tanizawa: Chemical Industry, 55 (2004) 936–942.

Pinpoint Drug Delivery System Using Hollow Bio-Nanoparticles (in Japanese), T. Yamada, M. Seno, A. Kondo, M. Ueda, K. Tanizawa, and S. Kuroda: Kobunshi Ronbunshu, 61 (2004) 606–612.

Patents

"Sensing Tool and Sensing Method Using Hollow Nanoparticle" K. Tanizawa, S. Kuroda, K. Jung, H. Akiyama, and H. Nobumasa: JP2004-104702.

"Screening Method for Receptor-binding Compounds" A. Kondo, S. Kuroda, A. Ueda, J. Ishii, H. Fukuda, K. Tatematsu, and T. Yamasaki: JP2004-96184.

International Conferences

ENH1 Scaffolds PKD1 and PKCε at Z-Discs, Forming a Signaling Complex that Participates in the Cardiac Hypertrophy (Poster), *M. Iwata, A. Maturana, T. Fujita, K. Tatematsu, T. Okajima, J. Van Lint, K. Tanizawa, and S. Kuroda, 12th International Conference on Second Messengers and Phosphoproteins, Montreal, Canada, August 3–7, 2004.

Interaction of a RING-IBR Protein RBCK1 with Its Splicing Variant RBCK2 (Poster), *N.Yoshimoto, K. Tatematsu, T. Koyanagi, K. Tanizawa, and S. Kuroda, FASEB

Conference: Transcriptional Regulation During Cell Growth, Differentiation and Development, Saxtons River, Vermont, U.S.A., August 14–19, 2004.

Development of Novel Bio-Nanoparticles for Human Tissue-Specific Delivery of Genes and Drugs (Invited), *K. Tanizawa, T. Yamada, A. Kondo, H. Tada, M. Seno, M. Ueda, and S. Kuroda, 17th FAOBMB Symposium / 2nd IUBMB Special Meeting / 7th A-IMBN Conference "Genomics and Health in the 21st Century", The Imperial Queen's Park Hotel, Bangkok, Thailand, November 22–26, 2004.

High Throughput Screening System for Agonist of Human G Protein-coupled Receptor on Yeast Cell Surface (Oral), *K. Tatematsu, T. Yamazaki, J. Ishii, K. Tanizawa, A. Kondo, and S. Kuroda, 3rd Japan-Korea Workshop on Molecular Display, Kobe University, Kobe, Hyogo, July 22, 2004.

Mechanism of α-Proton Abstraction in the Catalytic Intermediate of Bacterial Copper Amine Oxidase (Oral), *T. Okajima and K. Tanizawa, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN 2004), Suita, Osaka, December 6–7, 2004.

Structure-function Studies on a Neuronal Axon Guidance Related Protein FEZ1 and its Homologue FEZ2 (Poster), *J. Ikuta, T. Fujita, A. Maturana, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, March 9–10, 2005.

Interaction of a RING-IBR Protein RBCK1 with Its Splice Variant RBCK2 (Poster), *N. Yoshimoto, K. Tatematsu, T. Koyanagi, T. Okajima, K. Tanizawa, and S. Kuroda, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, March 9–10, 2005.

Molecular Analysis of Hepatitis B Virus (HBV) Infection Using the L Envelope Protein Fused to Green Fluorescent Protein (GFP) (Poster), *T. Kasuya, A. Uyeda, T. Yamada, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, March 9–10, 2005.

Mechanism of α-Proton Abstraction in the Catalytic Intermediate of Bacterial Copper Amine Oxidase (Poster), *T. Murakawa, T. Okajima, M. Uchida, Y. Yamamoto, H. Hayashi, K. Tatematsu, S. Kuroda, and K. Tanizawa, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, March 9–10, 2005.

Involvement of a Hypothetical [Fe-S]-binding Protein in the Biogenesis of Quinohemoprotein Amine Dehydrogenase (Poster), K. Ono, M. Tani, T. Okajima, and *K. Tanizawa, 4th European-Japanese Bioorganic Conference (EJBC-4), Hotel Limani, Ushimado, Setouchi, Okayama, March 15–19, 2005.

Spectrophotometric, Kinetic, and Structural Characterization of Catalytic Intermediates of Copper/TPQ-dependent Amine Oxidase (Invited), T. Murakawa, Y.-C. Chiu, Y. Yamamoto, H. Hayashi, T. Okajima, and *K. Tanizawa, 4th European-Japanese Bioorganic Conference (EJBC-4), Hotel Limani, Ushimado, Setouchi, Okayama, March 15–19, 2005.

Publications in Domestic Meetings

Japanese Biochemical Society	2 papers
Japanese Society for Molecular Biology	4 papers
The Society for Biotechnology, Japan	1 paper
The Society of Chemical Engineers, Japan	1 paper
The Biophysical Society of Japan	1 paper
Divisional Meeting on Colloid and Interface Chemistry, the Chemical Society of Japan	1 paper
Bimonthly Meeting of Vitamin B Committee	1 paper

Academic Degrees

Doctor Degree of Science

M. Iwata	Molecular and Cell Biological Studies on the ENH1-PKCε-PKD1 Complex Involved in the Cardiac Hypertrophic Signaling Cascade

Sponsorship

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

S. Kuroda	Development of New Pinpoint Gene Delivery System Using Nanoparticles Fused with Bio-recognition Molecule.	¥6,000,000

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

S. Kuroda	Analysis of Signal Transduction Mechanism Involving Two NELL Proteins for the Differentiation of Neural Crest-Derived Cells.	¥6,500,000

Grant-in-Aid for Scientific Research for Young Scientist

T. Yamada	Establishment of Method of Gene Therapy and Drug Delivery System Using Bio-nanoparticles	¥1,200,000
A. D. Maturana	Role of Molecular Complex Containing PDZ-3LIM Protein ENH1 in Cardiac Hypertrophy Signaling Cascade	¥1,200,000
K. Suzuki	Stabilization of Lipid Bilayer and Purification of	¥1,100,000

		Membrane Protein Using Surface Microarchitecture	
N. Yoshimoto		Development of Targeted Removal System for Intracellular Disease-related Proteins Using Bio-missile Molecule	¥900,000

Grant-in-Aid for Scientific Research (21st Century COE)

M. Iwata		Molecular Mechanism of Cardiac Hypertrophy Controlled by PKD1 and a PDZ-LIM Protein ENH1 and Development of Treatment Method Using a PKC Regulatory Protein ENH2	¥500,000
J. Ikuta		Structure-Function Studies on Axonal Guidance-Related Protein FEZ1 and Its Homologue FEZ2 in Neuronal Cells	¥500,000
T. Murakawa		Mechanism of Proton Tunneling in Enzyme Catalyzed Reaction Mechanism	¥500,000

Health and Labour Sciences Research Grants

S. Kuroda		Development of Bio-Nanocarriers for Pinpoint Drug Delivery System and Its Application for Cancer Therapy	¥5,000,000

Cooperative Research

K. Tatematsu	Bio-Leaders, Ltd.	Production and Development of New Live Bacterial Vaccines	¥369,000

Entrusted Research

K. Tanizawa	Agriculture, Forestry, and Fisheries Research Council	*De Novo* Design, and Analysis of Structure and Function of Quinone-Containing Built-in Enzymes	¥3,047,000
K. Tanizawa	Japan Society for the Promotion of Science	Survey and Research on the Academic Trends in Biological Sciences –Post-Genomic Era–	¥2,000,000
K. Tanizawa	Mitsubishi Electric Company, Ltd. (NEDO)	Analysis of Intracellular Signal Networks for Industrial Application of Genomics	¥4,712,000
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	¥10,000,000
S. Kuroda	Ministry of Education, Culture, Sports, Science, and	Protein 3000 Project	¥3,000,000

	Technology		
S. Kuroda	Osaka Science and Technology Center (Ministry of Economy, Trade and Technology)	Development of Proteome-based High Throughput Screening System Using Combinatorial Biochemistry.	¥1,785,000
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.	¥40,000,000

Other Research Funds

K. Tanizawa	Vitamin B Committee	Research on Built-in Cofactors	¥350,000
S. Kuroda	Suzuken Memorial Foundation	Development of New Treatment Method for Viral Hepatitis Using Hollow Bio-Nanoparticles That Can Deliver Drugs and Genes Specifically to Liver in High Efficiency	¥1,000,000
S. Kuroda	Mochida Memorial Foundation for Medical and Pharmaceutical Research	Development of Treatment Method for Viral Diseases Using Hollow Bio-Nanoparticles Targeting Infected Cells and Tissues	¥1,000,000
K. Tatematsu	The Inamori Foundation	Development of Targeted Removal System “Bio-missile” for Intracellular Disease-related Proteins Using Ubiquitin System	¥1,000,000
T. Fujita	Mochida Memorial Foundation for Medical and Pharmaceutical Research	Molecular Mechanism of Gene Expression and Signal Transduction during Hormone Secretion by Neurosecretory Cells	¥500,000

Department of Single Molecule Biophysics

Associate Professor:	Yoh WADA
Research Associate:	Ge-Hong SUN-WADA
Graduate Students:	Hiroyuki HOSOKAWA, Shigeru KAGATA
Under Graduate Students:	Eviryanti AGUNG
Researchers:	Minako AOYAMA, Chikako YAZAWA

Outlines

Mammalian endomembrane organelles including Golgi apparatus, lysosomes, endosomes, and secretory vesicles have luminal acidic pH established by vacuolar type H^+-ATPase. The Vacuolar-type proton-translocating ATPases (V-ATPases), multimeric proton pumps, are involved in a wide variety of physiological processes. We examined V-ATPase localization and function in highly differentiated mammalian cells to find multiple isoforms of mouse Vo subunit *a* (*a*1, *a*2, *a*3 and *a*4), components of membrane embedded region of the enzyme. V-ATPase with distinct *a* isoform is localized to specific subcellular compartments: *a*1 to secretory vesicles, *a*2 to Golgi, and *a*3 to late endosome (LE) and lysosome.The V-ATPase is also localized to the plasma membrane of highly differentiated cells such as osteoclasts and kidney epithelial cells. We have been interested in regulation of V-ATPase localization in highly differentiated mammalian cells.

Current Research Projects

1. Diversity of Subunit Structure of Vacuole type H^+ ATPase

The vacuolar ATPase (V-ATPase) is located to the endomembrane compartments along with secretory and vacuolar systems, and acidifies lumen of organelles by transporting protons across the membranes. It is also localized to the plasma membrane of differentiated cells including osteoclast or renal and bladder epithelia cells and acidifies the extracellular space. We have identified four subunit *a* isoforms (*a*1, *a*2, *a*3, and *a*4) of V-ATPase in mouse. *a*1 is predominantly localized to secretory vesicles, and *a*2 is associated with Golgi, whereas *a*3 is a late endosomal/lysosomal resident. *a*4 is specifically expressed in renal intercalated cells and localized to the plasma membranes. As well as the Vo, the membrane peripheral V1 sector also exhibits structural divergence. V-ATPase with an *E*1 isoform is expressed specifically in the acrosomal membrane of sperm with the *a*2 isoform, whereas the ubiquitously expressed *E*2 is the component in other tissues. Brain expresses a unique *G*2 isoforms as well as a ubiquitously expressed isoform *G*1. *C*2, *d*2 and *G*3 isoforms were expressed in a tissue-specific manner, in contrast to the ubiquitously expressed *C*1, *d*1 and *G*1 isoforms. *C*2 was expressed predominantly in lung and kidney, and *d*2 and *G*3 specifically in kidney. Thus, the divergent physiological functions of V-ATPase in various acidic compartments are established, in part, by utilizing distinctive subunit isoforms.

2. Simple Strategies to Create Complex Mammalian Gene Targeting Constructs

Construction of targeting vectors for ES-cell mediated gene modifications requires

highly elaborated DNA works and time-consuming processes. Especially, the creation of a conditional KO construct demands a variety set of functional elements including multiple *lox* P or FRT sites, as well as the positive and negative selection markers at the specific positions along a substantially long continuous DNA fragment to be replaced with the genuine genomic sequences. It turned out to be very difficult to create such targeting vectors by conventional DNA manipulation relied upon DNA ligase and restriction enzymes. Recently, *in vivo* modifications by the use of homologous recombination in *E. coli* has been developed in several laboratories and this novel methodology has been proven to be an efficient strategy. We developed a couple of plasmids that facilitate the *in vivo* DNA manipulations: pBSDTA-II provides a backbone vector with a multiple rare restriction sites and the negative selection marker for ES-cells, and pMODloxZeo series has the *lox* P sequences as well as Zeocin resistance gene. In addition, we designed a cassette plasmid whose *lox* P-FRT-Kan/G418-*lox* P-FRT segments could be transposed into large DNA fragments. By using the series of plasmids, we are able to create complex targeting vectors in short period.

Publications

Original Paper

Regulatory Elements directing Gut-Specific Expression of *GATA6* Gene during Mouse Early Development, G.-H. Sun-Wada, Y. Kamei, Y. Wada, and M. Futai: *J. Biochem.* 135, (2004) 165-169.

Review Papers

Diverse and Essential Roles of Mammalian Vacuolar-Type Proton Pump ATPase: Toward the Physiological Understanding of Inside Acidic Compartments, G. -H. Sun-Wada, Y. Wada and M. Futai: *Biochim Biophys Acta*. 1658 (2004) 106-114.

Proton Pumping ATPases and Diverse Inside-Acidic Compartments, M. Futai, Y. Wada and G. -H. Sun-Wada: Yakugaku Zasshi. 124 (2004) 243-260.

Books

Proton Translocating ATPase: Unique Enzyme Coupling Catalysis and Proton Translocation by Mechanical Rotation, M. Futai, G. -H. Sun-Wada, and Y. Wada, in ATPase Handbook, eds. M. Futai, J. H. Kaplan, J., and Y. Wada, *STM Books, Wiley VCH*, (2004) 235-260.

Vacuolar-Type Proton ATPases:Subunit Isoforms and Tissue-Specific Functions, G. -H. Sun-Wada, Y. Wada, and M. Futai, in ATPase Handbook, eds. M. Futai, J. H. Kaplan, and Y. Wada, *STM Books, Wiley VCH*, (2004) 379-394.

International Conferences

Subcellular Localization of V-ATPase Subunit Isoforms (invited). *Y. Wada, Experimental Biology 2004, Washington DC, U.S.A., April 16-22, 2004.

Vacuolar-Type Proton Pump ATPases (V-ATPases) and Inside Acidic

Organelles/Compartments: Rotational Mechanism and Diverse Physiology (invited), *M. Futai, G-H Sun-Wada, and Y. Wada, Herbsttagung der Gesellschaft fur Biochemie und Molekular Biologie, Munnster, Germany, Sept.19-22, 2004.

Vacuolar-Type Proton ATPase in Osteoclasts: Its Unique Composition, Expression and Localization (invited). *Y. Wada, 1st Meeting of Bone Biology Forum, Shizuoka, Oct. 22-23, 2004.

Multiple Isoforms of Mammalian V-ATPase: Their Specific Subcellular Localization and Function (poster), *Y. Wada, G-H. Sun-Wada, and M. Futai, 17th FAOBMB symposium, Bangkok, Thailand, Nov.22-27, 2004

Simple Strategy to Create Complex Mammalian Targeting Constracts (poster), *G.-H. Sun-Wada, M. Aoyama, M. Futai, and Y. Wada, Sanken International Symposium of Scientific and Industrial Nanotechnology -2004, Osaka, Dec. 6-7, 2004

Vacuolar-Type Proton ATPases, Their Unique Roles in Highly Differentiated Cells (poster), *Y. Wada, G-H Sun-Wada, and M. Futai, Sanken International Symposium of Scientific and Industrial Nanotechnology -2004, Osaka, Dec. 6-7, 2004

Publications in Domestic Meetings

Japanese Biochemical Society	2 papers
Japan Society for Cell Biology	1 paper
Japanese Bioenergetics Group	1 paper

Academic Degrees

Master Degree of Engineering

Hiroyuki Hosokawa	Mechanical Rotation of FoF1-ATP Synthase

Master Degree of Science

Shigeru Kagata	Heterologous Expression and Characterization of Mammalian rab7 Protein in Yeast

Sponsorship

Grants-in-Aid for Scientific Research on Priority Areas

Y. Wada	Membrane Dynamics during Mammalian Development	¥23,800,000
G.-H. Sun-Wada	Mechanism of Biological Nanomotors	¥1,000,000

Grant-in-Aid for Scientific Research

G.-H Sun-Wada	Genetic Diseases and V-ATPase	¥6,890,000

Grant-in-Aid for Exploratory Scientific Research

Y. Wada	Highly Efficient Gene Manipulation by Homologous Recombination in *E. coli.*	¥1,500,000

Entrusted Research

Y. Wada	Japan Science and Technology Corporation (CREST) Function and Biogenesis of Acidic Organelles	¥5,830,000

Department of Cell Membrane Biology

Professor:	Akihito YAMAGUCHI
Associate professor:	Satoshi MURAKAMI
Research Associate:	Takahiro HIRATA
Post Doctoral Fellows:	Takashi MATSUMOTO, Tsuyoshi NISHI, Syoko NISHI
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Research Students:	Yasuko SENDA, Yu HISANO
Support Staff:	Mari NISHIDA, Chiemi TAKENAKA, Reiko SATO, Aiko YONEMITSU

Outlines

Xenobiotic extruding pumps have recently been known to be widely distributed in living organisms from mammalian to bacteria as a host-defense mechanism in cellular level. These pumps not only confer multidrug resistance of cancer cells and pathogenic bacteria but also cause hereditary diseases through the mutation. The purposes of our laboratory are to elucidate the molecular structures and the molecular mechanisms of these xenobiotic exporters and the roles of these exporters in cell functions. In addition, the exporters having xenobiotic exporter-like molecular structures are identified in brain and platelets in order to elucidate the possible roles of exporters in intercellular signal transduction.

We previously reported the high-resolution crystalline structure of the xenobiotic exporter AcrB, that is a trimer having jellyfish-like shape. The structure well explains TolC-docking, dual entrance model and possible proton penetrating pathways. 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. This structural information enable us to be in outstanding position to elucidate the molecular mechanism of transport process combining with molecular biological information such as mutation studies, which is now on-going.

Now we are studying on three main projects: 1. Crystallographic and protein engineering analysis of bacterial xenobiotic exporters. 2. Studies on the regulatory networks of xenobiotic exporter gene expression. 3. Identification of novel exporters that mediates secretion of signal transducing molecules in mammalian cells.

Current Research Programs

1. Crystallographic and protein engineering analysis of xenobiotic exporters.

We have succeeded in determining the first crystalline structure of bacterial multidrug efflux transporter AcrB published in *Nature* **407**, 971-977 (2002). We are

trying to solve the structure of co-crystals of AcrB and its substrates. We are also performing the mutagenesis studies based on the crystal structure.
In 2004, we revealed the importance of phenylalanine cluster region of AcrB on the substrate recognition by mutation studies. In addition, we identified the TolC-docking residues in AcrB by disulfide cross-linking.

2. Studies on the regulatory networks of xenobiotic exporters in *E. coli*.

We previously constructed the set of *E. coli* 37 putative drug exporter gene library. Among them, 20 genes actually encode drug exporters. Although *E. coli* has intrinsic 20 drug exporter genes, most of them are hardly expressed under the normal growth conditions. However, the signals that induce the expression of these genes are unknown. We found that indole and N-acetylglucosamine induces some drug exporter genes via both two component systems and two-component system-independent pathway. Indole acts as an intercellular signal transducer that depends on the cell growth stage.

3. Identification of novel exporters that mediates secretion of signal transducing molecules in mammalian cells using cultured cells and knockout mice.

We constructed the knockout mice of a novel ABCA-type gene, ABCA5, which is mainly expressed in brain and testis. The knockout mice die at about 10-12 weeks after birth by dilated cardiomyopathy. ABCA5 protein is located in the lysosome and the knockout mice revealed the lysosomal disease-like symptoms. We are now studying the biochemical characterization of the ABCA5 protein using specific monoclonal antibodies. In addition, we found that sphingosine-1-phosphate is exported from platelet probably by unknown efflux transporters. We are now making an effort to identify the transporter.

Publications

Original Papers

Effects of Efflux Transporter Genes on Susceptibility of *Escherichia coli* to Tigecycline (GAR-936), T. Hirata, A. Saito, K. Nishino, N. Tamura, A. Yamaguchi: Antimicrob. Agents Chemother., 48, (2004) 2179-2184.

Membrane Protein Crystallization Using Laser Irradiation, H. Adachi, S. Murakami, A. Niino, H. Matsumura, K. Takano, T. Inoue, Y. Mori, A. Yamaguchi and T. Sasaki: Japanese Journal of Applied Physics, 43, (2004) L1376-L1378.

SOSHO Project (Crystal Design Project)~Development of Novel Growth Methods for Protein Crystals~, H. Adachi, H. Kitano, S. Murakami, K. Takano, H. Matsumura, T. Inoue, Y. Mori and T. Sasaki: The Journal of Structural Biology, 10, (2004) 1-18.

Role of Histone-Like Protein H-NS in Multidrug Resistance of *Escherichia coli*, K. Nishino and A. Yamaguchi: J. Bacteriol., 186 (2004) 1423-1429.

Extramembrane Central Pore of Multidrug Exporter AcrB in *Escherichia coli* Plays an Important Role in Drug Transport, S. Murakami, N. Tamura, A. Saito, T. Hirata and A.

Yamaguchi: J. Biol. Chem., 279 (2004) 3743-3748.

Review papers
The Sophisticated Proton Pump, V-type ATPase, K. Yokoyama and T. Nishi: Tanpakushitsu Kakusan Koso, 49 (2004) 2035-2043

Structure and Function of Multi-drug Efflux Transporters, S. Murakami and A. Yamaguchi: Bioscience and Industry, 62 (2004) 11-16.

Patents
Crystallization method for macromolecule and crystal growing device, H. Kitano and H. Adachi, Tokugan 2004-261541

Protein crystallization device with novel temperature controller, H. Adachi, T. Sasaki, Y. Mori, K. Takano, T. Inoue, H. Matsumura and S. Murakami, Tokugan 2004-011704

International Conferences
Structure and Mechanism of a Multidrug Exporter (Invited), *S. Murakami and A. Yamaguchi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, Japan, March 9-10, 2005.

Miniaturized Quorum-Sensing Assay of *Pseudomonas aeruginosa* LasR-LasI in *Escherichia coli* system and the Evaluation of 3-oxo-C_{12}-Homoserine Lactone Analogues (Poster), *T. Hirata, A. Kobayashi, H. Hirakawa, M. Horikawa, M. Ishiguro and A. Yamaguchi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, Japan, March 9-10, 2005.

Analysis of the Mechanism of Proton Translocation through the Integral Vo Domain of the Vacuolar (H^+)-ATPases (Poster), *S. Kawasaki-Nishi, T. Nishi and A. Yamaguchi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, Japan, March 9-10, 2005.

Indole Sensing Mechanisms that Control Growth phase-dependent Expression of Xenobiotic Exporter Genes (Poster), *H. Hirakawa, A. Kobayashi, T. Hirata, H. Nitta, N. Kato and A. Yamaguchi, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium 2005, Oku-Biwako Makino Prince Hotel, Shiga, Japan, March 9-10, 2005.

Structure and Mechanism of Multidrug Efflux Transport Nano-machine (Invited), * S. Murakami and A. Yamaguchi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004), ISIR, Osaka Univ., Osaka, Japan, Dec. 6-7, 2004.

Direct Interaction of Multidrug Efflux Transporter AcrB and Outer membrane Channel TolC Detected by Site-directed Disulfide Cross-linking (Poster), *N. Tamura, S. Murakami and A. Yamaguchi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004), ISIR, Osaka Univ., Osaka, Japan Dec. 6-7, 2004.

Studies on the Substrate-recognition Site of Multidrug Efflux Transporter AcrB using AcrB/AcrD Chimera (Poster), *N. Kobayashi, N. Tamura, S. Murakami and A. Yamaguchi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004), ISIR, Osaka Univ., Osaka, Japan Dec. 6-7, 2004.

N-acetylglucosamine as an Inducer for the Expression of Bacterial Multidrug Exporter Genes (Poster), *Y. Inazumi, H. Hirakawa, T. Hirata and A. Yamaguchi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004), ISIR, Osaka Univ., Osaka, Japan Dec. 6-7, 2004.

Indole Signaling Induces the Expression of Xenobiotic Efflux Nano-machine via Two-component System-dependent and Independent Pathways (Poster), * H. Hirakawa, T. Hirata and A. Yamaguchi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004), ISIR, Osaka Univ., Osaka, Japan Dec. 6-7, 2004.

X-ray Crystallographic Analysis of Multi-drug Efflux Transporter (Invited), *S. Murakami, R. Nakashima, T. Matsumoto, E. Yamashita and A. Yamaguchi, The 8th International Conference on Biology and Synchrotron Radiation (BSR2004), the Egret Himeji , Hyogo, Japan, Sep. 7-11, 2004.

Structure, Function and Regulation of Bacterial Xenobiotic Exporters (Invited), A. Yamaguchi, Gordon Research Conferences (Bacterial Cell Surfaces), Colby-Sawyer College New London, NH, June 27-July 2, 2004.

Structure of Bacterial Multidrug Efflux Transporter AcrB (Invited), *S. Murakami, R. Nakashima, T. Matsumoto, E. Yamashita and A. Yamaguchi, The Sixth Conference of the Asian Crystallographic Association, Hong Kong University of Science and Technology, Hong Kong, China, June 27-30, 2004.

Up-Regulation of a Drug Exporter Gene, *mdtEF*, by N-acetyl-D-glucosamine in *Escherichia coli*. (Poster), Y. Inazumi, H. Hirakawa, K. Nishino, *T. Hirata and A. Yamaguchi, American Society for Microbiology 104 general Meeting, Ernest N. Morial Convention Center, New Orleans, LA, United States, May 24-27, 2004.

Regulation of Drug Exporter Genes by Intercellular Signal Molecules in *Escherichia coli*. (Poster), *H. Hirakawa, Y. Inazumi, T. Hirata and A. Yamaguchi, American Society for Microbiology 104 general Meeting, Ernest N. Morial Convention Center, New Orleans, LA, United States, May 24-27, 2004.

Crystal Structure of Bacterial Efflux Protein AcrB (Invited), S. Murakami, *R. Nakashima, E. Yamashita and A. Yamaguchi, International Workshop on Structural Chemical Biology of Membrane Protein Complex Functions. Center for Advanced Science and Technology, Hyogo, Japan, April 19-20, 2004.

Publications in Domestic Meetings

Japanese Society for Bacteriology	3 papers
Creation of Novel Nano-material / system synthesized by Self-organization for Medical Use (CREST)	1 paper
RIKEN Structural Biology Symposium	1 paper
The Japanese Biochemical Society	9 papers
Membrane-Drug Interaction Symposium	6 papers
Spring-8 Symposium	1 paper
The Crystallographic Society of Japan	1 paper
Sakigake Live 2004	6 papers
21st Century COE program, Student Seminar	4 papers
The Molecular Biology Society of Japan	4 papers
The Biophysical Society of Japan	1 paper
Japanese Bioenergetics Group	3 papers
The Pharmaceutical Society of Japan	3 papers

Academic Degrees

Doctor Degree of Pharmaceutical Sciences

N. Tamura	Analysis of the structure and function of *E. coli* xenobiotic exporters by the protein-engineering approach.

Master Degree of Pharmaceutical Sciences

F. Ishibashi	Functional analysis of *E. coli* xenobiotic exporter, AcrB by the site directed mutagenesis into transmembrane domains.
Y. Inazumi	Investigation of compounds that induce MdtEF, a multidrug exporter of *E. coli*, and analysis of the induction mechanism.
N. Kobayashi	Studies on the substrate-recognition site of *E. coli* multidrug efflux transporter AcrB using AcrB/AcrD chimera.
S. Hashimoto	Identification and analysis of novel RND-type membrane transporters in mice.

Bachelor Degree of Pharmaceutical Sciences

Y. Senda	Studies on the transcriptional regulation mechanism by two-component signal transduction system, EvgSA in *E. coli*.
Y. Hisano	Topology determination of MFS type xenobiotic exporter, EmrB, which cooperates with outer membrane channel TolC

Sponsorship

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

A. Yamaguchi	Studies on the Nano-structure and Transport Mechanism of Antiport-type Efflux Transporter for Organic Compounds.	¥28,900,000

Grant-in-Aid for Scientific Research on the Foundation Area (S)

A. Yamaguchi	Post-genome Analysis of Bacterial Xenobiotic Exporter and Studies on the Novel Resistance Mechanism.	¥26,000,000

Grant-in-Aid for 21st Century COE program

A. Yamaguchi	Towards Creating New Industries Based on Inter-Nanoscience.	¥10,000,000

Grant-in-Aid for JSPS Research Fellows

N. Tamura	Principles for Topology Formation of Polytopic Membrane Proteins.	¥1,000,000
N. Kobayashi	Structure and Functional Analysis of the first ABC-type Drug-Exporter of Gram-negative Bacteria, MacB.	¥900,000
H. Hirakawa	Studies on the Transcriptional Networks of Xenobiotic Transporters Regulated by the Sense-and-Response System for Environmental Changes in Bacteria.	¥1,000,000

Cooperative Research

S. Murakami	Rigaku Co. Ltd.		¥100,000
S. Nishi	Uehara Memorial Foundation,	Investigation of the Role of V-ATPases in Neuronal Cells	¥2,000,000

Entrusted Research

A. Yamaguchi	Japan Science and Technology Agency (CREST), entrusted	Investigation of the Structure and Function for Xenobiotics Transporters and Clarification of Multidrug Resistance Mechanism.	¥6,500,000
S. Murakami	Japan Science and Technology Agency (Sakigake 21), entrusted	Structural Analysis of Drug Recognition Mechanism in Multidrug Efflux Transporter for Drug Resistance.	¥1,300,000
T. Hirata	National Agriculture and Bio-oriented Research Organization, entrusted	Molecular Mechanism and Regulation of Acquisition of Drug Resistance in *Escherichia coli.*	¥3,000,000
T. Nishi	Japan Science and Technology Agency	Novel Intracellular Network System Involved with Tissue-	¥1,000,000

	(Sakigake 21), entrusted	specific Isoform.	
S. Murakami	Ministry of Education, Culture, Sports, Science and Technology, Protein 3000 Project, entrusted	Research programs at Universities (Brain and Nervous System)	¥1,600,000

(Other Allocations)

A. Yamaguchi	COE fund	Atomic Scale Processing for the Creation of Highly Harmonised Functional Materials	¥850,000

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.	¥62,500,000
S. Murakami	Japan Science and Technology Agency (Sakigake 21)	Structural Analysis of Drug Recognition Mechanism in Multidrug Efflux Transporter for Drug Resistance.	¥15,450,000
T. Nishi	Japan Science and Technology Agency (Sakigake 21)	Novel intracellular network system involved with tissue-specific isoform.	¥8,840,000
S. Murakami	New Energy and Industrial Technology Development Organization (NEDO)	Development of crystallization and processing system for membrane protein using femt-second laser.	¥3,000,000

Division of Quantum Beam Science & Technology

Outline

The quantum beam is the general term for all kinds of radiation beams producing quantum mechanical effects on materials. It includes photon beams and charged particle beams such as lasers, X-rays, synchrotron radiation, γ-rays and free electron lasers, electrons, positrons, muons and ions, as well as neutron beams. Quantum beam science has developed from radiation science and its research fields are classified into two groups. One of them is study on production, control and measurement of new high-brightness and high quality quantum beams, which are remarkably developing recently. The other is study on processes induced by quantum beams in materials, as well as on applications to materials science based on accurate understanding of these phenomena induced by a quantum beam.

The division of Quantum Beam Science and Technology is composed of the department of Accelerator Science and the department of Beam Materials Science. In the department of Accelerator Science, studies are conducted on accelerators, which are main apparatuses for producing quantum beams, and on production, control and measurement of quantum beams using accelerators. In the department of Beam Materials Science, basic studies are conducted to investigate phenomena induced by quantum beams and to apply them to materials science; that is, production and application of new materials such as functional materials and materials working under extreme conditions. Both departments closely work together with different points of view; generation of new quantum beams and applications of them to materials science. This division also cooperates with the Radiation Laboratory, attached to the Institute, in order to promote advanced studies conducted at a university 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

- Remodeling of the L-band linac in progress to improve stability and reproducibility of operation drastically.
- Measurement of angular distributions of Self-Amplified Spontaneous Emission (SASE) for the fundamental peak and higher harmonic peaks due to non-linear harmonic generation.
- Development of a new type of wiggler with strong focusing force, called the edge focusing wiggler, for SASE and FEL
- Study on stability of the L-band linac with the autoregressive model
- Improvement of performance of the Siam Photon Source in Thailand and design study of the first undulator for it.

- First comprehensive and quantitative studies on charge carriers and reactive intermediates of conjugated polymer molecules by pulse radiaolysis technique.
- Drastic improvements in the S/N ratio of the subpico-, pico-, and nano-second pulse radiolysis system.
- Success in analysis of reaction mechanisms of high sensitive resists for nanoelectronics.
- Formation of size-controlled nano-wires along particle trajectories in polymeric materials.
- Pulse radiolysis studies on biological systems including DNA, active oxygen, and NO
- Application of slow positron beams to polymer science and technology as the probes for nano-sized space in the materials.

Department of Accelerator Science

Professor:	Goro ISOYAMA
Associate Professor:	Ryukou KATO
Research Associates:	Toshiji IKEDA, Shigeru KASHIWAGI
Graduate Students:	Tetsuya IGO, Chikara OKAMOTO, Takanori NODA, Kenji KOBAYASHI, Shuto UMEZONO
Research Student:	Takanori KANEMITSU

Outlines

Particle accelerators are widely used from basic science to industrial applications. In this department, we conduct research on accelerators and quantum beams such as a free electron laser (FEL). Although accelerators are artificial things, fundamental aspects of physics such as non-linearity and the collective effect become apparent when extreme performance is pursued. Because new kinds of quantum beams extend the world we can see with, they are expected to be used in a large variety of fields extending from basic research to applications. To put it concretely, we conduct researches on production of a highly brilliant electron beam with a linear accelerator and related beam dynamics, development of an infrared FEL for user experiments and SASE (Self-Amplified Spontaneous Emission) in the infrared region. In addition to these, we collaborate with the National Synchrotron Research Center (NSRC) in Thailand for development of a synchrotron radiation source.

Current Research Programs

1. Remodeling of the L-band linac

We began to remodel the L-band linac extensively in the fiscal year 2002. We had been making a trial run of the linac in real earnest since October 2004 after the completion of the remodeling. The most serious problem left till 2004 was nice and random intensity fluctuations observed in the RF power output from the klystron. In order to identify a source of the problem, we examined all the transmission system for the RF power including the klystron, but we could not find it. At the begging of the fiscal year 2004, a new timing system including an RF mater oscillator was ready and we replaced the old system with the new one. It turned out that the fluctuations of the RF power had disappeared. Thus, the source of the problem was found to be the old mater oscillator and the problem was solved. We replaced the old phase shifter in the RF transmission line for the buncher, which had had a spark problem, with a new one. We continued improving the computer control system of the linac for new functions and higher performance, so that we have established the base for a ordinary user to be able to operate the linac, including start-up and shutdown. Although a few objectives remain unrealized, stability of the electron beam and reproducibility of operation are remarkably improved compared with those before the remodeling. The commissioning of the L-band linac has been completed and user experiments have begun with it.

2. Basic Study on SASE in the Far-Infrared Region

SASE (Self-Amplified Spontaneous Emission) is a process that spontaneous light emitted by high-energy electrons in a wiggler is amplified exponentially to high-power coherent light with an FEL amplifier. Because no mirrors are necessary for the optical resonator, it is expected to be a promising candidate for realizing X-ray lasers. We are conducting basic study on SASE in the infrared region using the existing FEL system and a high-intensity single-bunch beam accelerated with the L-band linac. Our SASE operates in the exponential regime, where the light power grows exponentially as the electron beam moves along the wiggler. In this exponential regime, the SASE power is very sensitive to fluctuations of the electron beam. The SASE power, on the other hand, intrinsically fluctuates, because the number of coherent photons generated in an electron bunch is limited. With the renewed L-band linac, we have begun study to separate contributions of the electron beam and SASE itself in the measured intensity fluctuations of SASE using the auto-regressive model. It was found that fluctuations of the electron beam contribute significantly to the measured intensity fluctuations of SASE in previous experiments using the L-band linac before remodeling.

3. Development of a High Performance Wiggler for SASE

We are developing a new type of wiggler to be used for Self-Amplified Spontaneous Emission (SASE), which squeezes the electron beam small so that gain of SASE is enhanced, in collaboration with the insertion device group of the High Energy Accelerator Organization. It is a Halbach type wiggler with an edge angle for focusing and named the edge-focus wiggler. We have made a model wiggler with 5 periods and evaluated its performance. The magnetic field was measured at some magnet gaps and the field gradient was calculated with the measured magnetic field. Peak values and distributions of the magnetic field agree quite well with those calculated with a three-dimensional magnetic-field program and thus we have demonstrated the idea of the edge-focusing wiggler. The calculated field gradient varies sinusoidally twice as many as the magnetic field, but in addition to the major component, the measured field gradient shows a component varying with the magnetic field and the relative deviation reaches almost +/-10 %. The measured field gradient integrated along the bream axis, however, agrees well with the calculated one. This peculiar feature shows up equally in every wiggler period and consequently it should be due to some systematic origin, but up to now the cause is unknown.

4. Development of the Synchrotron Radiation Source

We are conducting study to develop and improve the accelerator system for the synchrotron radiation source, called the Siam Photon Source, in collaboration with the National Synchrotron Research Center in Thailand. All the coils of 16 quadrupole magnets for the storage ring, which came from SORTEC, were found defective probably due to an inappropriate manufacturing process, so that we had decided to replace all the 64 coils with new ones. A quadrupole magnet was removed from the storage ring, and coils were changed, and then the magnet was installed again. This process was repeated 16 times until all the coils were changed and finally the quadrupole magnets were precisely aligned in the storage ring. After completing this work, we succeeded in operating the storage ring again without any problems. We measured the betatron functions and the dispersion function of the storage ring, and

confirmed that the symmetry of these functions was recovered again. As a result, the maximum beam current and the beam lifetime as well as the injection efficiency were considerably improved. The maximum beam current stored in the storage ring has exceeded 200 mA and the beam lifetime is longer than 7 hours at 100 mA. With this we have achieved the goal of our study at the beginning for the installation, commissioning, and improvement of the accelerator system for the synchrotron radiation source.

Publications

Original Papers

Development of the Edge-Focusing Wiggler for SASE, S. Kashiwagi, A. Mihara, R. Kato, G. Isoyama, S. Yamamoto and K. Tsuchiya: Nucl. Instr. Meth. A528 (2004) 203-207.

Stability Analysis of the RF Linac Based on an AR Model, R. Kato, S. Isaka, H. Sakaki, S. Kashiwagi and G. Isoyama: Nucl. Instr. Meth. A528 (2004) 244-248.

Beam Test of Multi-Bunch Energy Compensation System in the Accelerator Test Facility at KEK, S. Kashiwagi, H. Hayano, K. Kubo, T. Korhonen, S. Nakamura, T. Naito, K. Oide, S. Takeda, N. Terunuma, J. Urakawa: Jpn. J. Appl. Phys. 43 (2004) 5617-5622.

Bunch Length Monitor Using Two-Frequency Analysis for RF Gun System, Ryunosuke Kuroda, Shigeru Kashiwagi, Kazuyuki Sakaue, Masakazu Washio, Hitoshi Hayano and Junji Urakawa: Jpn. J. Appl. Phys. 43 (2004) 7747-7752.

Review Papers

X-Ray Generation using the Inverse Compton Scattering, R. Kuroda, S. Kashiwagi, M. Washio: Japanese Society of Radiation Chemistry 77 (2004) 41-45 (in Japanese).

Books

New Synchrotron Radiation Sources, M. Watanabe and G. Isoyama, In X-Ray Spectrometry: Recent Technological Advances, K. Tsuji, J. Injuk, and R.Van Grieken (editors), John Wiley & Sons, Ltd, (2004) 29-47.

International Conferences

The Recent Progress of Siam Photon Laboratory, (Invited) *R. Apiwatwaja, P. Songsiriritthigul, W. Pairsuwan, T. Ishii, G. Isoyama, The 3rd Asian Particle Accelerator Conference, March 22-26, 2004, Gyeongju, Korea, WEM-104.

Beam Stability Improvement of the Siam Photon Source, (Poster) *R. Apiwatwaja, S. Rugmai, S. Rujirawat, N. Sa-nguansak, G. G. Hoyes, W. Pairsuwan, T. Ishii, G. Isoyama, The 3rd Asian Particle Accelerator Conference3, March 22-26, 2004, Gyeongju, Korea, THP-16017.

Upgrade of the L-band Linac at ISIR, Osaka University for Higher Operational Stability, (Oral) *G. Isoyama, Y. Honda, S. Kashiwagi, R. Kato, T. Kozawa, S. Seki, S. Suemine,

S. Tagawa, T. Yamamoto, Y. Yoshida, The 3rd Asian Particle Accelerator Conference3, March 22-26, 2004, Gyeongju, Korea, TUM-204.

Femto-second Bunch Length Measurement using the RF Deflector, (Poster) *S. Kashiwagi, K. Kobayashi, R. Kato, G. Isoyama, A. Saeki, Y. Matsui, J. Yang, N. Kudo, M. Washio, H. Hayano, M. Kuriki, The 9th European Particle Accelerator Conference, July 2004, Lucerne, Switzerland, pp.2691-2693.

Present Status of Photo-cathode RF Gun System and its Applications at Waseda University, (Poster) *R. Kuroda, D. Ueyama, M. Kawaguchi, N. Kudo, T. Kuribayasi, T. Saito, K. Sakaue, S. Minamiguchi, R. Moriyama, Y. Hama, K. Hidume, H. Hirama, M. Washio, S. Kashiwagi, J. Urakawa, H. Hayano, X.J. Wang, The 9th European Particle Accelerator Conference , July 2004, Lucerne, Switzerland, pp.2685-2687.

Beam Diagnostics for a Photocathode RF-gun System, (Poster) *K. Sakaue, R. Kuroda, N. Kudo, M. Washio, S. Kashiwagi, J. Urakawa, H. Hayano, The 9th European Particle Accelerator Conference, July 2004, Lucerne, Switzerland, pp.2688-2690.

Analysis of Intensity Fluctuations of SASE using the AR Model, (Poster) *R. Kato, S. Kashiwagi, S. Isaka, C. Okamoto, T. Yamamoto, S. Suemine, G. Isoyama, H. Sakaki, The 26th International Free Electron Laser Conference and 10th FEL Users Workshop, August 29 - September 3, 2004, Trieste, Italy, pp.167-170 (MOPOS30).

First Model of the Edge-Focusing Wiggler for SASE, (Poster) *S. Kashiwagi, K. Kobayashi, T. Noda, R. Kato, G. Isoyama, S. Yamamoto, K. Tsuchiya, The 26th International Free Electron Laser Conference and 10th FEL Users Workshop, August 29 - September 3, 2004, Trieste, Italy, pp.458-461 (TUPOS25).

Upgrade of the L-Band Linac at ISIR, Osaka University for a Far-Infrared FEL, (Poster) *R. Kato, G. Isoyama, S. Kashiwagi, S. Suemine, T. Yamamoto, The 26th International Free Electron Laser Conference and 10th FEL Users Workshop, August 29 - September 3, 2004, Trieste, Italy, pp.462-465 (TUPOS26).

Development of Compact Soft X-ray Source Based on Laser Undulator, (Poster) *R. Kuroda, D. Ueyama, T. Saito, S. Minamiguchi, K. Hidume, M. Washio, S. Kashiwagi, J. Urakawa, H. Hayano, The 26th International Free Electron Laser Conference and 10th FEL Users Workshop, August 29 - September 3, 2004, Trieste, Italy, pp.466-469 (TUPOS27).

Soft X-ray Imaging in a Water Window Region using High Activation Energy Positive Photoresist, (Poster) *R. Kuroda, D. Ueyama, K. Hidume, T. Oka, Y. Hama, M. Washio, S. Kashiwagi, K. Ushida, H. Hayano and J. Urakawa, The 6th International Symposium on Ionizing Radiation and Polymers, September 25-30, 2004, Houffalize, Belgium.

Development of Picosecond Pulse Radiolysis System at Waseda University, (Poster) *M. Kawaguchi, K. Ushida, S. Kashiwagi, R. Kudora, T. Kuribayashi, M. Kobayashi, Y. Hama and M. Washio, The 6th International Symposium on Ionizing Radiation and

Polymers, September 25-30, 2004, Houffalize, Belgium.

Present Status of High Quality Beam Facility at Waseda University, (Poster) *M. Washio, H. Kawai, Y. Hama, N. Kudo, M. Kobayashi, T. Kuribayashi, M. Kawaguchi, R. Kuroda, K. Maeda, F. Nagasawa, D. Ueyama, K. Hizume, X. J. Wang, H. Hayano, J. Urakawa and S. Kashiwagi, The 7th Biennial Trombay Symposium on Radiation & Photochemistry, January 7-12, 2004, Mumbai, India.

Operational Stability of the L-band Linac at ISIR, Osaka University, (Poster) *R. Kato, S. Kashiwagi, T. Yamamoto, S. Suemine, G. Isoyama, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, December 6-7, 2004, Osaka, Japan, p.92 (P003).

Development of Edge-Focusing Wiggler for X-ray SASE, (Poster) *Shigeru Kashiwagi, Kenji Kobayashi, Takanori Noda, Ryukou Kato, Goro Isoyama, Shigeru Yamamoto, Kimichika Tsuchiya, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, December 6-7, 2004, Osaka, Japan, p.96 (P007).

Publications in Domestic Meetings

The 1st Particle Accelerator Society of Japan, August 4-8, 2004, Nihon University, Funabashi, Japan	10 papers
The 3rdth Scientific Meeting of the Japanese Society of Radiation Safety Management, December 1-3, 2004, Hokkaido University, Sapporo, Japan	1 papers
The 17th Annual Meeting of the Japanese Society of Synchrotron Radiation Research and Joint Symposium of the Synchrotron Radiation Facilities, January 7-9, 2005, Tosu, Japan	2 papers
The 47th Debate Meeting of the Japanese Society of Radiation Chemistry, October 9-11, 2004, Hokkaido University, Sapporo, Japan	2 papers
The 60th Annual Meeting of the Physical Society of Japan, March 24-27, 2005, Tokyo University of Science, Noda, Japan	2 papers

Academic Degrees

Master Degree of Science

T. Noda	Research and Development of the Strong Focusing Undulator for SASE.

Master Degree of Engineering

C. Okamoto	Measurement of the SASE intensity in the Far-Infrared Region and Analysis of Intensity fluctuations using the Auto Regressive Model.

Sponsorship

Grant-in Aid for Scientific Research on Exploratory Research

G. Isoyama	Development of a Novel Method for Reducing the Electron Beam Emittance of the Synchrotron Light Source.	¥900,000

Department of Beam Materials Science

Professor:	Seiichi TAGAWA
Associate Professor:	Yukio YAMAMOTO
Research Associates:	Kazuo KOBAYASHI, Akinori SAEKI
Graduate Students:	Atsuro NAKANO, Satoshi TSUKUDA, Hiroki YAMAMOTO, Yoshiko KOIZUMI, Yusuke DOI, Ryuhei YAMAGAMI, Takumi SHIGAKI
Under Graduate Students:	Hidekazu SUGAWARA
Post Doctoral Fellow:	Yoshitake TERASHIMA, Anjali ACHARYA
Support Staff:	Minori KITO (until July 31, 2004) Kaoru KOJIMA (from August 1, 2004)

Outlines

Main subjects of the present department are utilization of quantum beams for molecular science, research on mechanisms of phenomena induced by quantum beams, and analysis of microscopic structure of materials. Quantum beams mean both beams such as photons and beams inducing interactions with materials in the microscopic level of quantum mechanics. The beams cause completely different physico-chemical reactions in condensed matters from conventional chemical reactions. Features of beams are highly developed for electrons, ions, positrons, as well as photons (synchrotron radiation, γ-rays, and lasers).

Current Research Programs

1. Analysis of Primary Process in Interactions between Beams and Molecular Materials

Physico-chemical reactions, which occur within nano- and pico- second region, are considered to dominate followed reactions and products in molecular materials. The direct observation of reactive intermediates is carried out to elucidate the mechanisms and to control the reaction by using next measurement techniques in the program.

2. Research on 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 3 psec approaching to shorter time region. Excited state dynamics have been already 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, X rays, and laser beams to design newly developed lithography technique in the present program.

5. Radiation-Induced Reactions in Aromatics

Aromatics have high radiation resistance. The characteristic has been used in electron beam lithography. Especially, the radiation–induced reaction of aromatics is important to improve and understand the resist materials. Primary process of irradiated aromatics from nano- to picosecond time scale is investigated by electron beam pulse radiolysis.

6. Ionizing Radiation Induced Damage in DNA

Ionizing radiation induces a variety of damage in both direct and indirect effect. In living cells, ~40-50% of the lesions induced in DNA by low LET radiation arise from direct effects. However, most mechanistic studies have focused on the indirect effects of radiation by which DNA damage is induced by diffusible water radicals. Much less is known about the mechanisms of the direct effects of radiation. To elucidate the direct-type mechanism and related quantitative characteristics caused by direct ionization of DNA, the yields of γ-radiation-induced single- and double-strand breaks as well as formation of 8-oxy-dG have been measured. The strand break yields from direct-type damage are comparable to the yields from indirect-type damage. The yield of direct-type strand breaks is substantially (G = 0.35), and that of the formation of 8-oxy-dG is even higher (G = 0.42).

We measured dynamics of charge transport processes by using time-resolved microwave conductivity (TRMC). A novel DNA-lipid complex, which was prepared by mixing DNA with cationic amphiphilic lipids, was confirmed to form double strands even in organic solvents, and was employed as a sample. On photolysis of anthraquinone-bound the DNA-lipid complex, the TRMC signals from charge carriers in dioxane solutions and transient absorption are measured and discussed on the basis of comparison among the kinetic traces.

Publications

Original Papers

Thermally Dehydration of a Poly(vinyl alcohol) Film Promoted by Diphenyliodonium Trifluoromethanesulfonate: Absorption Spectra and elemental Analysis Results, Y. Yamamoto, and S. Tagawa: Bull. Chem. Soc. Jpn. 77 (2004) 591.

Delocalization of Positive and Negative Charge Carriers on Oligo- and Poly-fluorenes Studied by Low-Temperature Matrix Isolation Technique, Y. Koizumi, S. Seki, A. Acharya, A. Saeki, and S. Tagawa: Chem. Lett. 33 (2004) 1290.

Formation of benzene trimer radical cation in γ-irradiated low temperature 2-methylpentane matrices: M. Todo, K. Okamoto, S. Seki, S. Tagawa: Chem. Phys. Lett.399 (2004) 378

Dynamics of Positive Charge Carriers on Si Chains of Polysilanes, S. Seki, Y. Koizumi, T. Kawaguchi, H. Habara, S. Tagawa: J. Am. Chem. Soc. 126 (2004) 3521.

Activation of SoxR-dependent Transcription in Pseudomonas Aeruginosa, K. Kobayashi and S. Tagawa: J. Biochem. 136 (2004) 607.

Polarized Coloration of Stretched Poly(vinyl alcohol) Films by Heat Treatment. Y. Yamamoto and S. Tagawa: J. Mater. Sci. 39 (2004) 653.

157 nm-Induced Resist Outgassing Studied by Films Thickness Loss and in-situ Quadrupole Mass Spectrometer, Y. Matsui, S. Seki, S. Tagawa, S. Kishimura, and M. Sasago: J. Photopolym. Sci. Technol. 17 (2004) 671.

Adjacent Effect on Positive Charge Transfer from Radical Cation of n-Dodecane to Scavenger Studied by Picosecond Pulse Radiolysis, Statistical Model, and Monte Carlo Simulation. A. Saeki, T. Kozawa, Y. Yoshida, and S. Tagawa: J. Phys. Chem. A 108 (2004) 1475.

Fabrication of Nanowires Using High-Energy Ion Beams. S. Tsukuda, S. Seki, M. Sugimoto, A. Idesaki, S. Tanaka, A. Oshima, and S. Tagawa: J. Phys .Chem. B 108 (2004) 3407.

Dependence of Acid Generation Efficiency on the Protection Ratio of Hydroxyl Groups in Chemically Amplified Electron Beam, X-ray and EUV Resists. H. Yamamoto, T. Kozawa, A. Nakano, K.Okamoto, S. Tagawa, T. Ando, M. Sato, and H. Komano: J. Vac. Sci. Technol. B 22 (2004) 3522.

Modelling and Simulation of Chemically Amplified Electron Beam, X-ray and EUV Resist Processes, T. Kozawa, A. Saeki and S. Tagawa: J. Vac. Sci. Technol. B 22 (2004) 3489.

Pulse Radiolysis Study on Proton and Charge Transfer Reactions in Solid Poly(methyl methacrylate), A. Nakano, K. Okamoto, T. Kozawa and S. Tagawa: Jpn. J. Appl. Phys. 43 (2004) 4363

Effects of Ester Groups on Proton Generation and Diffusion in Polymethacrylate Matrices. A. Nakano, K. Okamoto, T. Kozawa and S. Tagawa: Jpn. J. Appl. Phys. 43 (2004) 3981.

Proton Dynamics in Chemically Amplified Electron Beam Resists, H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, Y. Yamamoto, T. Ando, M. Sato, H. Komano and S. Tagawa: Jpn. J. Appl. Phys. 43 (2004) L849.

Polymer Screening Method for Chemically Amplified Electron Beam and X-Ray Resists. H. Yamamoto, A. Nakano, K. Okamoto, T. Kozawa and S. Tagawa: Jpn. J.

Appl. Phys. 43 (2004) 3971.

Precise Control of Nanowire Formation Based on Polysilane for Photoelectronic Device Application, S. Tsukuda, S. Seki, A. Saeki, T. Kozawa, S. Tagawa, M. Sugimoto, A. Idesaki, S. Tanaka: Jpn. J. Appl. Phys. 43 (2004) 3810.

Study of Interfaces in Polymer Bilayers by Slow Positron Beam, Y. Terashima, S. Seki, K. Miyamoto, M. Tashiro, Y. Honda, S. Tagawa: Mater. Sci. Forum 445 (2004) 349.

Inhomogeneous Distribution of Crosslinks in Ion Tracks in Polystylene and Polysilanes, S. Seki, S. Tsukuda, K. Maeda, Y. Matsui, A. Saeki, and S. Tagawa: Phys. Rev. B 70 (2004) 144203

Radiolytically prepared poly(vinyl alcohol) hydrogel containing α-cyclodextrin, Y. Yamamoto, S. Tagawa: Radiat. Phys. Chem.69 (2004) 347.

Formation of Defect Structures in Au-Polysilane Interfaces Probed by Low Energy Positron Beams, Y. Terashima, S. Seki, M. Tashiro, Y. Honda, S. Tanaka: Solid State Commun. 132 (2004) 641.

Review Papers
Radiation Damage of DNA-Model for Direct Ionization of DNA-, K. Kobayashi, S. Tagawa, Housyasenkagaku 77 (2004) 25-35.

International Conferences
Transient Spectroscopy of Radical Cations of a Variety of Substituted Polysilanes, *S. Seki, T. Koizumi, T. Kawaguchi, H. Habara, and S. Tagawa: 37th Silicon Symposium, Philadelphia, USA, May 20-22, 2004.

Cross-Linked Silicon Based Polymer Nanowire Formation by High Energy Charged Particles, S. Tsukuda, S. Seki, S. Tagawa, and M. Sugimoto: 37th Silicon Symposium, Philadelphia, USA, May 20-22, 2004.

The Dependence of Acid Generation Efficiency on the Protection Ratio of Hydroxy Groups in Chemically Amplified Electron Beam, X-ray and EUV Resists, *H. Yamamoto, A. Nakano, K. Okamoto, T. Kozawa, S. Tagawa, T. Ando, M. Sato, and H. Komano: 48th EIPBN, Sandiego, USA, June 1-4, 2004.

Radiolysis Studies of Benzene: Pico-and Subpicosecond Pulse Radiolysis and γ-Radiolysis at Low Tempaerature, *K. Okamoto, M. Todo, A. Saeki, T. Kozawa, S. Seki, Y. Yoshida, and S. Tagawa: 2004 Gordon Research Conference, Colby College, ME, USA, June 20-25, 2004.

Delocalization of Positive and Negative Charge Carriers on Oligo- and Poly-Fluorenes Studied by Low Temperature Matrix Isolation Technique, *Y. Koizumi, S. Seki, Anjali Acharya, A. Saeki, and S. Tagawa: 2004 Gordon Research Conference, Colby College,

ME, USA, June 20-25, 2004.

Charge and Energy Transfer In the Presence of High Concentrated Additives, A. Saeki, S. Seki, T. Kozawa, S. Tagawa, 2004 Gordon Research Conference, Colby College, ME, USA, June 20-25, 2004.

Dynamics of Positive Charge Carriers on Si Chains of Polysilanes, *S. Seki, Y. Koizumi, T. Kawaguchi, H. Habara, and S. Tagawa: 2004 Gordon Research Conference, Colby College, ME, USA, June 20-25, 2004.

Nanostructure Fabrication Processes in the Combination of Radiation Chemistry and Nanotechnology (Invited), S. Tagawa*: 2004 Gordon Research Conference, Colby College, ME, USA, June 20-25, 2004.

Present Status of Linac Facility at Osaka University, A. Saeki, International Symposium on Ultrafast Accelerators for Pulse Radiolysis, New York, USA, June 25-28, 2004.

Beam Application to Nanotechnology Based On Subpicosecond Pulse Radiolysis, S. Tagawa, International Symposium on Ultrafast Accelerators for Pulse Radiolysis, New York, USA, June 25-28, 2004.

Dependence of Acid Yield on Acid Generator in Chemically Amplified Resist for Post-optical Lithography, *A. Nakano, K. Okamoto, Y. Yamamoto, T. Kozawa, S. Tagawa, T. Kai, and H. Nemoto, Microprocess and Nanotechnology Conference2004, Osaka, Japan, October 26-29, 2004.

Potential Cause of Inhomogeneous Acid Distribution, *H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato and H. Komano, Microprocess and Nanotechnology Conference2004, Osaka, Japan, October 26-29, 2004.

Formation of Nanowires Based on π-Conjugated Polymers by High-Energy ion Beam Irradiation, S. Tsukuda, S. Seki, M. Sugimoto, S. Tagawa, Microprocess and Nanotechnology Conference2004, Osaka, Japan, October 26-29, 2004.

Conductivity Measurement of Nano-Structures by Microwave Technique (Poster), *A. Saeki, Y. Ohno, S. Seki, K. Matsumoto, and S. Tagawa: JapanNano 2005, February 21-22, 2005.

Deprotonation Mechanism of Poly(4-hydroxystyrene) and its Derivative (Poster), *A. Nakano, K. Okamoto,Y.Yamamoto, T. Kozawa, T. Kai, H. Nemoto, T. Shimokawa, S. Tagawa: SPIE30th, San Jose, CA, USA, February 27-March 4, 2005.

Basic Aspects of Acid Generation Processes in Chemically Amplified Resists for Electron-Beam Lithography, T. Kozawa and S. Tagawa: SPIE30th, San Jose, CA, USA, February 27-March 4, 2005.

Outgassed Species from Various Triphenylsulfonium Salts during 157 nm, Y. Matsui, S. Seki, S. Tagawa, S. Irie, T. Itani: 4th International Symposium on 157 nm Lithography, Tokyo, Japan, Aug. 25-28, 2003.

Transport Properties of Charge Carries in Single-Walled Carbon Nanotubes by Flash-Photolysis Time-Resolved Microwave Conductivity Technique, Y. Ohno, K. Maehashi, K. Inoue, K. Matsumoto, A. Saeki, S. Seki, S. Tagawa: Proc. ICPS-, 27, 2004

Outgassing Characteristics of Acetal Resists for 157 nm Lithography Investigated by Time-Resolved Measurement, Y. Matsui, S. Seki, S. Matsui, S. Tagawa, S. Irie, T. Itani: Proc. SPIE 5376 (2004) 178.

Contributions to International Conferences and Journals

S. Tagawa	13th Microprocess and Nanotechnology Conference (Organizing Committee)
S. Tagawa	International Nuclear Conference '02 (Organizing Committee)

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	14 papers
Chemical Society of Japan	2 papers
Atomic Energy Society of Japan	1 paper
The Japan Society of Applied Physics:	3 papers
Society of Polymer Science, Japan	1 paper
The Japanese Biochemical Society	1 paper

Academic Degrees

Master Degree of Engineering

Y. Koizumi	Delocalization of Positive and Negative Charge Carriers on Oligo-and Poly-fluorene Backbones
H. Yamamoto	Study on Reaction Mechanism of Chemically Amplified Resists for Nanolithography

Sponsorship

Grant-in-Aid for Scientific Research on Priority Areas

K. Kobayashi	Structure-Function of the Sensor Protein for Short-Lived Intermediates	¥5,900,000

Grant-in-Aid for Scientific Research

S. Tagawa	Femtosecond Pulse Radiolysis Study on Radiation-Induced Reactions in Nanoscopic Region	¥7,200,000
A. Saeki	Charge carrier mobility in isolated polymer chain and	¥1,300,000

	functionalization of electric property of polymer studied by electron accelerator	
Anjali ACHARYA	Electronic Conductivity of Charge Carriers on Isolated Biomedical Conjugated Polymer chains	¥1,100,000
Y. Terashima	Microstructural Characterization for Polymer Films by Slow Positron Beams	¥ 900,000

Entrusted Research

S. Tagawa,	Advanced Semiconductor Engineering and Technology	Mechanisms of Polymer Etching Processes by Ultra Low Energy Ion Beams	¥5,250,000
S. Tagawa	Advanced Semiconductor Engineering and Technology	Reaction Mechanism in Chemically Amplified Resist Materials	¥1,575,000
S. Tagawa,	Semiconductor Leading Edge Technology Inc.	Outgassing Characters from F2 Laser Resist Materials	¥4,000,000

Cooperative Research

S. Tagawa,	Japan Atomic Energy Research Institute	Ion Beam Pulse Radiolysis in Condensed Matter
S. Tagawa,	Japan Atomic Energy Research Institute	Nanostructure Formation along Charged Particle Trajectory

Activity of Facilities

Nanoscience and Nanotechnology Center

Director Professor: Hiroshi IWASAKI
Support Staff: Manami HASE

Outlines

Nanoscience and Nanotechnology Center was founded in April 2002 for developing Bottom-up Nanotechnology, Top-down Nanotechnology, and their Industrial Application. This center consists of four divisions, (1) Nanomaterial and Nanodevices, (2) Beam Science for Nanotechnology, (3) Nanoscience and Nanotechnology for Industrial Applications and (4) Nanocharacterization (newly established on April 1st, 2004) together with four laboratories (Radiation Laboratory, Electron Microscope Laboratory, Electronic Processing Laboratory and Open Laboratory) and Nanotechnology Process Foundry.

Division of Nanomaterials and Nanodevices

Outlines

The main purpose of this department is to construct function harmonized nano-materials which can mimic flexible data processing like human body.

By using typical "Bottom-up Nanotechnology" of artificial lattice technique, we combine metal, inorganic and (bio)organic materials at an atomic/molecular level to new nano-materials.

The object of this department is to research molecular-scale devices based on the function of single molecule. We are developing new techniques for the measurement of physical and chemical properties of single or several molecules.

Design and syntheses of supramolecules such as artificial DNA, proteins, photosynthetic molecules, and nanoparticles having more efficient and selective functions than those of single molecules have been investigated towards constructions of organized supramolecular systems such as artificial living cells and nanodevices exhibiting multifunctions, complex properties, and conjugated functions.

Proteins and their complex with other biomolecules are regarded as nano bio devices. The research of our group is focused on structural and functional studies on such devices. We are also interested in developing highly sensitive biosensors and nano machines.

Achievements

- Construction of functional nano-materials, which can mimic flexible data processing like human body.
- Investigation of relationship with structure and material properties at nano-scale.
- Control of nano-sacle interface among organic, inorganic, and metal materials.
- Development of bottom up nano technology system.
- Creation of super-five senses sensor and brain type memory.
- Programmed self-assembly and self-organization for molecular device.
- Selective nano-fabrication by chemical surface modifications.
- Electronic properties of single molecule connected to metals or semiconductors.
- Novel techniques on scanning probe microscopy and scanning electron microscopy for molecular devices.
- Molecular design of DNA wires by synthesis and assembly of molecule-conjugated DNA.
- Synthesis and assembly of photochemical probe molecules for bioimaging.
- Photochemical control of functionalized artificial proteins.
- Preparation of nanoparticles by self-assembly.
- Preparation of molecular devices by synthesis and assembly of functionalized polymers.
- Structural and functional studies of nano bio devices.
- Development of ultra-sensitive biosensors.
- Characterization of nano machines acting as a drug efflux transporter.

Department of Artificial Nanomaterials for Bio-Information Systems

Professor: Hitoshi TABATA
Research Associate: Hiromasa SAEKI
Associate Professor: Michael HERRMANN
Research Associate: Hiroaki MATSUI
Graduate Students: Atsuhiro DOI, Eriko MIZUNO
Under Graduate Students: Yuichi KITAGAWA, Koji TSURUTA, Kazuya TAMEKUNI
Supporting Staff: Megumi IKEDA

Outlines

In our group, we are studying about frontier materials such as strongly collated compounds and/or artificial super lattices formed by a laser MBE technique, which enables us to control the crystal structure with atomic scale accuracy.
Oxide electrics have been studied, for example, low dimensional physics in oxide magnetic materials, fluctuation in spin glass or relaxor ferroelectrics, multi ferrotronics in ferromagnetic-ferroelectrics, spintronics in wide band gap semiconductors and photo induced magnetic materials.
Furthermore, the research about bio sensor/memory devices, which are constructed by self organizing system such as DNA and bio, related molecules are discussed. Observation in the nano-scale region is also performed by scanning probe microscopy.
A new method based on THz-spectroscopy is also constructing for direct detecting of hydrogen bond of base pairs in DNA double helix and/or that of protein-DNA molecules.

Current Research Programs

Development of Spintronics with Widegap Oxide Semiconductor(ZnO)

Recently, the semiconductor with spin is widely focused from the viewpoint of advance technology and basic science. This work aims at two targets, one is the clarification of basic properties for Cobalt-doped ZnO, the other is the control of magnetic conduction by using heterostructure. It is quite important to evaluate the magneto-optic effect in specifying the origin of ferromagnetism. According to comparison between measurement at 20K and calculation of high energy XMCD spectra at CoL2,3 edge, we can say that doped Co ions occupied Zn site tetrahedraly with the valence of 2+ (collaborated with Fujimori laboratory of Tokyo University) . XMCD spectra insist that the ferromagnetism comes from Co^{2+} ions with tetrahedral site, and we can neglect the possibility of other ferromagnetic impurity like Co metal cluster. According to the MCD spectra in visible and ultraviolet region, the peak of which origin is d-d* transition of Co^{2+} about 1.8eV was seen, and a strong peak can be observed at the band edge of ZnO (about 3.4eV). These peaks show the magnetic field response and it suggests that the origin of ferromagnetism is intrinsic. And, we report fabrication of Mg-rich strained $Mg_{0.37}Zn_{0.67}O$/ZnO multi-quantum wells (MQWs) structure. Nanostructures utilized MQWs in the areas of semiconductor materials are

promising for producing a great deal of research interest regarding physical coupling between magnetic and electronic properties. From the results of high-resolution x-ray diffraction and AFM, the appearance of pronounced Pedellösung fringes arising from interference between coherent x-ray waves reflected with sample structure and surface roughness below 1 nm were a suggestion of the high crystalline quality. Furthermore, it is suggested that the sift of exciton emission to high photon energy due to quantum effect and the enhancement of hole mobility at low temperatures confine two dimensionally electrons into ZnO wells. High Mg-component $Mg_{0.37}Zn_{0.67}O$ barrier layers on Zn-terminated ZnO (0001) substrates are effective for applications of Tunneling magneto-resistance (TMR) devices and studies of low-dimensional properties coupled of spin and electron.

Expansion Relaxor Ferroelectric Materials into Ferroelectric and Ferromagnetic (Multiferroic) Materials

Relaxor phenomenon in ferroelectrics is characterized mainly by frequency dispersion and broad peaks in the dielectric susceptibility versus temperature variation. Recently, this property is of great interest in the field of dielectric materials due to interesting of the fundamental and applied point. In our work, we have studied the dielectric properties of relaxor in $Ba(Zr_xTi_{1-x})O_3$ replaced Ti^{4+} by Zr^{4+} for $BaTiO_3$. In this year, to research the relaxor phenomenon related to the substitution of homovalence atom, we presented a comparative material $Ba(Hf_xTi_{1-x})O_3$ replaced Ti^{4+} by Hf^{4+} for $BaTiO_3$. $Ba(Hf_xTi_{1-x})O_3$ ceramics show that the Hf substitution affects the dielectric susceptibility versus temperature variation as well as $Ba(Zr_xTi_{1-x})O_3$. It is important for relaxor phenomenon to replacement of homovalence atom for $BaTiO_3$.

Next, multiferroics, relaxor ferroelectric materials added magnetic property, are expected to use in new electric device and memory storage. $PbFe_{0.5}(Ta_xNb_{1-x})_{0.5}O_3$ is reported to exhibit relaxor behavior in the literature. In this work, as environmentally friendly lead free oxide, we suggest $Ba(Fe,Ta)_{0.5}O_3$-$Ba(Fe,Nb)_{0.5}O_3$. Magnetic property of $Ba(Fe,Ti)_{0.5}O_3$ films show that saturation magnetization has relationship with crystallinity of thin films. As FWHM of XRD pattern increase, magnetization decrease. This seems to be cased that Fe ions occupy perovskite B-site randomly, weakferromagentic is supposed to be related spin canting. On the other, relaxor-like behavior is observed in dielectric measurement. This result is seemed clue for material searching.

Photoinduced Magnetization in Spinel and Garnet Ferrite Thin Films

The creation of a photon-mode type optical memory using electron transition by photoexcitation can be expected for faster and greater volume information processing. With this in mind, the material whose magnetic properties can be directly controlled by light has been sought in various material systems. The purpose of this study is to create a material that shows a high temperature cluster glass and a melt of cluster glass phase by light irradiation which results in the large photoinduced magnetization (PIM). The research results of this year are as follows. Thin film of $Ni_{0.7}Zn_{0.3}Fe_{1.7}Ti_{0.3}O_4$ was formed on the Al_2O_3(0001) substrate using a pulsed laser deposition technique. The film shows the melt of cluster glass state by light irradiation below the spin-freezing temperature (230 K). This PIM was found to strongly depend on the Ti content in the

films. The spectroscopic measurements revealed that the photoinduced charge transfer between Ti^{4+} and Fe^{2+} ions are responsible for this PIM. The change in the valence state of Fe ions by the charge transfer is considered to influence the local magnetic anisotropy in the film, resulting in the melt of cluster glass state. Furthermore, we focused on the garnet type ferrite system. In the $Y_3(Fe, Al)_5O_{12}$ films formed on $Y_3Al_5O_{12}$ (111) substrates, the high spin-freezing temperature (400K) was achieved by controlling the various conditions during film deposition such as compositions and O_2 pressures. The enhancement of PIM was found in Si-dopied $Y_3(Al, Fe)_5O_{12}$ films. The results of M-H measurements with and without light irradiation suggest that one axial magnetic anisotropy is induced by photoinduced rearrangement of Fe^{2+} ions. Thus, the cluster glass phenomena at high temperature and photoinduced magnetization in spinel and garnet ferrite thin films have been investigated. These results are strongly expected to be utilized for the development of novel magneto-optical devices.

Direct Detection of DNA Using ISFET Based on PNA

Molecular recognition based on hybridization process is important in biotechnology. In recent research and development of bioassays, discrimination systems of double strands nucleic acids from single stranded ones with high efficiency and specificity are coming to crucial key technology. So we focused on a direct detection system for DNA hybridization that combines device function with molecular recognition of heterogeneous hybridization. Peptide nucleic acid (PNA) is a structural deoxyribonucleic acid (DNA) analogue with a neutral N-(2-aminothyl)-glycine based psedopeptide backbone. Compared to DNA duplex, PNA has a higher thermal stability of duplexes, a highly discrimination of mismatch DNA and binding independent of salt concentration. Direct DNA detection has been demonstrated using Ion-Sensitive Field-Effect Transistors (IS-FETs) based on PNA. IS-FETs ,which is consisting of Ta_2O_5 gate insulator, is purchased from BAS Inc. PNA was immobilized on the Ta_2O_5 gate surface using aminosilnae via glutaraldehyde as a bifunctional crosslinker. After PNA immobilization, the Schiff base was reduced by mild hydride donors, cyanoborohydride(BH_3CN^-) and we monitored the difference between the signal output from the PNA-immobilized IS-FET before and after DNA hybridization with measurements of I-V characteristics. Variations in surface charge density on a gate region of an IS-FET were monitored as shifts in threshold voltage after DNA hybridization. Large positive shifts in threshold voltage, as high as 170 mV, were observed during ID-VG measurements. The changes in threshold voltage observed for neutral PNA-immobilized IS-FETs were more than 5 times greater than those for negative-charged DNA-immobilized IS-FETs. Thus, this approach demonstrates that the PNA-modified IS-FET-based biosensor works more effectively as a signal transducer of genetic information.

(This work has been supported by CREST(Core Research and Evolutional Science and Technology) of JST(Japan Science and Technology Agency) and collaborated with Prof. Kawai group.)

DNA Nano-patterning

Recently DNA properties have been investigated to realize new functional bio-devices. However, there are few reports on DNA nano-patterning to make bio-nanodevices. Therefore, we have attempted DNA nano-patterning by using a

nanoimprint method. On a glass substrate coated with poly-L-lysine, which is known as a material for DNA immobilization by UV radiation, about 100 μl of a 1 μg/μl salmon's milt-DNA solution was applied and was dried at 60 ˚C for an hour, and was irradiated by UV for 2 min. The substrate was imprinted at 100 ˚C and 6 MPa for 5 min with a mold of $Si0_2$ on Si substrate. We confirmed the DNA nano pattern to observe the substrate by fluorescence microscopy after the DNA was dyed by YO-PRO-1 iodide). DNA consisted of line at about 700 nm as line width, and the very fine lines correspond to convex patterns of the mold surface. The imprint would make the poly-L-lysine reform by exposing it under high pressure and high temperature. In this matter, these novel DNA nano-patterning processes would be available for the DNA nano-device by using self-organization.
(These studies were supported by CREST/JST with Prof. T. Kawai.)

Electrical Measurement of Nano-structured Molecules by Top-contacted Geometry Electrode

We are now studying the electrical transport phenomenon of materials in nanoscale. We have measured the nano-structured materials such as TPPS nanorods and DNA network by nanogap electrodes. The fabrication technique of nanogap electrode without wet processes is based on the technique developed by the Dr. Mizutani and Dr. Naitoh group in AIST and Matsumoto group in Kawai laboratory.

This technique enables us to fabricate nanogap electrode without photo- or EB lithography. The gap length between electrodes is confirmed to be about 100 nm with reproducibility. As the top-contacted geometry type electrode is fabricated by this technique. It is possible to measure the electrical conductivity of materials without structural deformation due to the electrodes.

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Polar and Non-polar Growth in ZnO Homoepitaxy,(Poster) *H. Matsui and H. Tabata, The 3rd International Workshop on ZnO and Related Materials, Sendai, Japan, Oct. 5-8, 2004

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Contributions to International Conferences and Journals

H. Tabata	International Conference on Solid State Devices and Materials 2004 (SSDM2004)（Publishing Committee）
H. Tabata	International Conference on Solid State Devices and Materials 2005 (SSDM2005) (Steering Committee)

H. Tabata	International Conference on Solid State Devices and Materials 2005 (SSDM2005)（Publishing Committee）
H. Tabata	12th International Conference on Solid Films and Surfaces (ICSFS-12) (Program Committee)
H. Tabata	The 5th Korea-Japan Conference on Ferroelectricity （Publishing Committee）
H. Tabata	11th International Workshop on Oxide Electronics (International Committee)
H. Tabata	SPIE International Symposium “Smart Materials, Nano-, and Micro-Smart Systems”(Program Committee)

Publications in Domestic Meetings

The Japan Society of Applied Physics	19 papers
The Physical Society of Japan	2 papers
Others	2 papers

Sponsorship

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

H. Tabata	Room Temperature Spintronics by Ultimate Control of Interface and Crystal Growth	¥2,400,000

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

H. Tabata	Symmetry Broken Ferroelectric Relaxors Formed by Artificial Superlattices and Brain Mimetic Memories	¥9,100,000

Other Research Fund

H. Tabata	Special Coordination Funds for Promoting Science and Technology	Spin-Electronics Formed with Oxide Semiconductors	¥23,954,000
H. Tabata	Consortium R&D Projects for Regional Revitalization	Development of LIPS Method and its Application to the Future Model Touch Panel	¥1,186,500
H. Tabata	Sumitomo Seika Chemicals Co., Ltd.	Research for Visible Light Sensitive Photo Catalysis	¥2,100,000
H. Tabata	Kawasaki Heavy Industries, Ltd.	Research of Functional Materials	¥500,000

Department of Single-Molecular Integrated Devices

Professor: Tomoji KAWAI
Associate Professor: Takuya MATSUMOTO
Research Associate: Masateru TANIGUCHI
Researcher: Akihiko TAKAGI

Outlines

The object of this department is to research molecular-scale devices based on the function of single molecule. We are developing new techniques for the measurement of physical and chemical properties of single or several molecules.

Current Research Programs and Achievements

Kinetic and Thermodynamic Control by Chemical Bond Rearrangement on Surfaces

The (2×1)-reconstructed Si(001) surface, where the surface lattice structure undergoes a reconstruction in which adjacent silicon dimers pair together and form dimers through a σ bond and a π bond, is intriguing in that the chemistry at the surface is frequently analogous to that in organic chemistry owing to its covalent nature. Alkenes, for example, are known to bind to silicon dimers on the Si(001) surface to produce four-member ring analogs in a similar way to [2+2] cycloaddition reactions in organic synthesis. The mechanisms of cycloadditions on the surface have also been argued in terms of orbital symmetry in a similar fashion to organic chemistry. We have found evidence that the driving force that determines the product distribution for acetone adsorbed on the Si(001) surface can be changed from kinetic (producing a four-member-ring species; see scheme) to thermodynamic (producing the dissociation species) upon raising the surface temperature. This means that it is possible to control the product distribution on the Si(001) surface by changing the determinant factor from kinetic to thermodynamic control, which is a result of reversible binding of the surface species. These results suggest approaches for future applications to increase the degree of selectivity in the attachment of organic molecules to the Si(001) surface.

A Novel Fabrication Technique of Nano-Gap Electrodes

We have developed a fabrication method for nanogap electrodes without employing photo- or electron-beam lithography to measure the electrical characteristics of nanostructured molecules. This angle-controlled shadow-masking method enables us to construct nanogap electrodes without a wet process after the molecules are positioned on the substrate. The proposed method makes it possible to measure electrical characteristics without structurally deforming or denaturing the molecules due either to the step edge of an electrode or to the organic solvents used in the wet process. The results demonstrate that a gap length between the electrodes of less than 100 nm can be fabricated reproducibly. We have measured the electrical characteristerivative

molecules (TPPS: 5,10,15,20-tetraphenyl-21H,23H-porphyics of lambda DNA (λ-DNA) networks and molecular nanorods made of porphyrin-drine tetrasulfonic acid) in which J-aggregates are formed inside. Experimental findings reveal that the electrical conductivity of λ-DNA decreased under a vacuum condition, whereas that of TPPS nanorods decreased under oxygen and nitrogen gas-purged conditions.

DNA-Template Assembly of Au Nanoparticles Via Step-by-Step Binding Reaction.

DNA is a key material in the fabrication of nanostructures by the 'bottom-up' process, which incorporates highly selective chemical recognition and self-assembly. In particular, DNA-templated assembly of nanoparticles has been studied intensively in the hope of building nanoscale circuits where nanoparticles might play roles such as conductive , quantum dots, anchor sites for molecules, and so on. We demonstrated DNA-template assembly of gold-nanoparticles AuNP via step-by-step binding reaction. The control of hydrophilicity for mica surface makes it possible to preserve the structure of AuNP-binded DNA network with resistance to Au-thiolate reaction in ethanol solvent. This method realizes the formation of a continuous AuNP array with uniform height and small width.

Electrical Properties of Programmed Molecular Wire

Although terms such as molecular electronics or molecular device are becoming popular, there is still a lack of organic linkage between nanotechnologyies such as a micro fabrication processing and molecular design and synthesis. For the development of molecular electronics, it is of course important to advance the measurement technology for the electric properties of molecules. But the design and synthesis of a new molecule is more essential to obtain a molecule-specific device operation that cannot be realized in silicon devices. We synthesized a molecular wire composed of three parts, each of which has a different design feature. The insulated molecular wire is prepared and cross-linked between nanogap electrodes whose spacing is 20 nm. The electric measurements and molecular calculations of the molecular wire indicate that the hopping mechanism plays a dominant role in the electric conduction.

Ambipolar organic field-effect transistor

Organic filed-effect transistor based on copper-phthalocyanine and cyanoethylpullulan gate insulator shows ambipolar operation using gate insulator hysteresis, which appears at less than 1 millihertz. The gate insulator has spontaneous polarization of 1.6 microcoulomb per square centimeters and the coercive electric field of 50 kilovolt per centimeter. The field-effect mobilities of hole and electron are 4.1 x 10^{-3} and 3.5 x 10^{-6} square centimeters per volt per second, respectively. Ambipolar transistor represents a step toward inverter circuits to serve as driver elements of paper display and electronic paper.

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Time-Resolved Force Detection using Dynamic-Mode Scanning Force Microscopy, *T. Matsumoto and T. Kawai, 8th Int. Conference on Nanometer Scale Science and Technology, Venice, Italy, June. 28-July.2, 2004

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Three Distinct Conformations of Porphyrin Wheels Adsorbed on Cu (100) Observed by Scanning Tunneling Microscopy, *A. Takagi, N. Aratani, T. Matsumoto, A. Osuka and T. Kawai, 8th Int. Conference on Nanometer Scale Science and Technology, Venice, Italy, June. 28-July.2, 2004

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Scanning Force Microscopic Observations of Escherichia Coli Ribosomes, *T. Matsuura, K. Kobayashi, H. Tanaka, T. Matsumoto and T. Kawai, 8th Int. Conference on Nanometer Scale Science and Technology, Venice, Italy, June. 28-July.2, 2004

One-Dimensional Assembly and Local Surface Potential Mapping of Au Nanoparticles on a DNA Network (Invited), *F. Yamada, Y. Otsuka, A. Takagi, T. Matsumoto, H.Tanaka and T. Kawai, 8th Int. Conference on Nanometer Scale Science and Technology, Venice, Italy, June. 28-July.2, 2004

Tunneling Conduction Through Cytochrome c Molecule, *M. Kataoka, T. Matsumoto and T. Kawai, 8th Int. Conference on Nanometer Scale Science and Technology, Venice, Italy, June. 28-July.2, 2004

Fabrication Method of Nano-Gap Electrodes Without Wet Process and Electrical Measurement of Nano Structured Molecules, *Y. Otsuka, Y. Naitoh, T. Matsumoto, W. Mizutani, H. Tabata and T. Kawai, 8th Int. Conference on Nanometer Scale Science and Technology, Venice, Italy, June. 28-July.2, 2004

Electronic Properties of Biomolecular System: Toward the Realization of Bottom-Up Molecular Scale Electronics (Invited), *T. Matsumoto and T. Kawai, International Seminar on Organic-Molecular Materials, Shizuoka, Japan, August. 8-9, 2004

Measurements of Contactless Microwave Conductivity and Infrared Absorption in Poly(dG)-Poly(dC) and Poly(dA)-Poly(dT) DNA Molecules, *H. Matsui, T. Yanagimachi, K. Abe, T. Suzuki, M. Taniguchi, S. Tanaka, T. Kawai, Hasanudin, N. Kuroda and N. Toyota, The 5th International Conference on Biological Physics, Gothenburg, Sweden, August. 23-27, 2004

Surface Potential Images of Molecular Systems on Insulating Substrates by Frequency-Mode Scanning Force Microscopy, *T. Matsumoto, F. Yamada, A. Takagi and T. Kawai, Seventh International Conference on Non-Contact Atomic Force Microscopy , Seattle, Washington U.S.A., September. 12-15, 2004

Adsorption of DNA Molecule and DNA Patterning on Si Substrate, *S. Tanaka, M. Taniguchi and T. Kawai, Scanning Probe Microscopy in Life Sciences, University Medicine Berlin, Berlin, Germany, October.13, 2004

Characteristics of Electrochemical Transistor, *M. Taniguchi and T. Kawai, Organic Materials for Electronics and Photonics, Okinawa, Japan, November.3-6, 2004

Conductance Measurement of a DNA Network in Nano-Scale by Point Contact Current Imaging Atomic Force Microscopy, *H. Tanaka, A. Terawaki, Y. Otsuka, H. Y. Lee, T. Matsumoto and T. Kawai, Material Material Research Society Fall Meeting, Boston, USA , Nov.30-Dec.3, 2004

Scanning Probe Microscopy Methods for Biomolecular Electronics (Invited), *T. Matsumoto and T. Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004(SISSIN-2004):Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

Investigation of Enzymatic Activity for Lipid Biulayers Patterning by Surface Plasmon Resonance and Atomic Force Microscopy, *S. E. Lee, H. S. Jung, F. Yamada, T. Matsumoto, H.Y. Lee and T. Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004(SISSIN-2004):Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing ,Osaka, Japan, December. 6-7, 2004

Fabrication of Gold Electrode by Nanotransfer Printing,*K. Ojima, K. Nakamatsu, T. Kanno, T. Matsumoto, S. Matsui and T. Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004(SISSIN-2004):Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

Surface Potential Measurement of the DNA and Au Nanoparticls on Insulating Substrate, *F. Yamada, A. Takagi, T. Kusaka, T. Matsumoto, H. Tanaka and T. Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004(SISSIN-2004):Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

Adsorption of Ribosomes Onto Solid Surfaces from Solution, *T. Matsuura, H. Tanaka, T. Matsumoto and T. Kawai, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004(SISSIN-2004):Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

Incorporation of Molecules into the DNA Duplexes, *K. Adachi, M. Taniguchi and T. Kawai, Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

Reevaluation of the Mobility in a Field-Effect Transistor Based on Polymeric Insulating Layer, *E. Mizuno, M. Taniguchi and T. Kawai, Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

Fabrication and Properties of Electrochemical Transistors, *M. Taniguchi and T. Kawai, Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing, Osaka, Japan, December. 6-7, 2004

A Simple Fabrication Method of Nanogap Electrodes for Top-Contacted Geometry:Application to Porphyrin Nanorods and a DNA Network, *Y. Otsuka, Y. Naitoh, T. Matsumoto, W. Mizutani, H. Tabata and T. Kawai, The 12th International Colloquium on Scanning Probe Microscopy, Atagawa (Sizuoka),Japan, December. 9-11, 2004

Surface Potential Measurement of the DNA-Au Nanoparticle Complex on Insulating Substrate, *F. Yamada, A. Takagi, T. Kusaka, T. Matsumoto, H. Tanaka and T. Kawai, The 12th International Colloquium on Scanning Probe Microscopy, ,Atagawa (Sizuoka),Japan, December. 9-11, 2004

Conductivity Measurement Through Cytochrome c Molecules, *M. Kataoka, T. Matsumoto and T. Kawai, The 12th International Colloquium on Scanning Probe Microscopy, Atagawa (Sizuoka),Japan, December. 9-11, 2004

Direct Printing of Gold Electrode for Molecular-Scale Devices, *K. Ojima, K. Nakamatsu, T. Kanno, T. Matsumoto, S. Matsui and T. Kawai, The 12th International Colloquium on Scanning Probe Microscopy, Atagawa (Sizuoka),Japan, December. 9-11, 2004

Contributions to International Conferences and Journals

T. Matsumoto	International Symposium on Surface Science and Nanotechnology
T. Matsumoto	The 13th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques (STM'05)/ The 13th International Colloquium on Scanning Probe Microscopy (ICSPM13)

Publications in Domestic Meetings

The Japan Society of Applied Physics	17 papers
The Surface Science Society of Japan	5 papers
The Chemical Society of Japan	2 papers
Others	9 papers

Sponsorship

Grant-in-Aid for Scientific Research (B)

T. Matsumoto	Stroboscopic Scanning Probe Microscopy and Time-Resolved Molecular-Scale Imaging of Photoexcited Carriers	¥6,100,000

Exploratory Research

T. Matsumoto	Imaging of Transient Photoexcited Carreir Formation by Time-Resolved Force Measurement	¥2,200,000

Grant-in-Aid for Young Scientists (B)

M. Taniguchi	Synthesis of Programmed Molecular Wires and Electrical Measurements of Them Using Nano-Gap Electrodes	¥1,900,000

Entrusted research

T. Matsumoto	Japan Science and Technology Corporation	Mesoscopic Devices of Huge Porphyrin Arrays	¥1,300,000

Other Research Funds

T. Matsumoto	Japan Science and Technology Corporation	Mesoscopic Devices of Huge Porphyrin Arrays	¥11,300,000
M. Taniguchi	Shin-Etsu Chemical Co., Ltd	Development of FET	¥2,000,000
M. Taniguchi	Kansai Research Foundation from Technology Promotion	Development of high-mobility FET Based or Polymers Using Inkjet Process	¥1,000,000

Department of Supramolecular Chemistry

Professor: Hiroaki SASAI
Research Associates: Masayuki ENDO, Shinobu TAKIZAWA

Outlines

Towards the construction of organized supramolecular systems with multifunctionality, the design and syntheses of supramolecules such as spherical nanoparticles, artificial DNA, proteins, photosynthetic molecules, and metal-bridged polymers having more efficient and selective functions than those of single molecules have been investigated.

Current Research Programs

1. 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-*i*-Pr)$_4$ generates a chiral metal-bridged polymer which catalyzed Michael reaction and carbonyl-ene reaction respectively with high enantioselectivities.

2. Spherical Nanoparticles as Asymmetric Catalysts

Taking advantage of the facile adsorption of thiols to the surface of gold cluster, the disulfide bearing (*R*)-BINOL moieties at each terminal position has been successfully introduced on monolayer-protected metal cluster (MPC). Treatment of the metal cluster with Ti(O-*i*-Pr)$_4$ afforded an insoluble Ti-BINOLate complex with high catalyst activity in the asymmetric alkylation of aldehyde with dialkylzinc. As an alternate approach, dendrimer-like catalyst was synthesized by immobilization of (*R*)-BINOL derivative on the polymer obtained by micellar polymerization system. The polymer-supported Ti-BINOLate complex generated with this polymer also exhibited high catalytic activity. Further applications of functional particles to new asymmetric reactions are in progress.

3. Construction of DNA Nanostructures for Nanofabrication

To construct the DNA nano-scale architectures for integration of functionalities, DNA supramolecular structures and nanostructures by association of multiple double helix DNA strands have been developed. DNA-porphyrin conjugates as a chemical connector for assembling four duplexes were designed, synthesized, and characterized. Integration of multiple porphyrins into multiple DNA bundled structures was achieved in vertical way by programming the DNA sequences. DNA array structures were also constructed by arranging the DNA tiles and the DNA-porphyrin connectors. DNA-tube structures with length of 20 μm were constructed and analyzed by AFM. Photofunctional groups, nanoparticles, and proteins can be integrated into these DNA nano-scale scaffolds in a

programmable way.

4. Photochemically Controllable Enzymes for Cancer Therapy.
The strategy for developing photochemically controllable enzymes by regulating protein-protein interaction and peptide bond cleavage has been investigated by introducing photoremovable, photoisomerizable, and photodegradable molecules. Dimer interface of an endonuclease *Bam*HI was site-selectively photofunctionalized for suppressing the enzymatic activity. With photoactivation of the molecules, the enzyme recovered the activity, and the level of the activity was regulated by adjusting the photoirradiation time. Photochemical activation of an apoptosis-related caspase-3 was also examined. A photodegradable 2-nitrophenylglycine was incorporated into the specific position on the peptide chain. While the enzyme perfectly lost the activity without photoirradiation, the activity was clearly expressed with short-time irradiation. The photofunctionalized enzymes can be introduced into a cell by attaching a protein-transduction domain and would be used for induction of apoptosis by selective photoirradiation.

Publications

Original Papers

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Development of Novel Chiral Spiro Ligand Bearing Oxazolines, T. Kato, K. Marubayashi, S. Takizawa, and H. Sasai : Tetrahedron: Asymmetry, 15 [23] (2004) 3693-3697.

Enantioselective Aldol-type Reaction Using Diketene, T. Kawase, S. Takizawa, D. Jayaprakash, and H. Sasai : Synth. Commun., 34 [24] (2004) 4487-4492.

Spiro Bis(isoxazole) as a New Chiral Ligand, K. Wakita, M. A. Arai, T. Kato, T. Shinohara, and H. Sasai : Heterocycles, 62 [1] (2004) 831-838.

Design and Synthesis of Photochemically Controllable Caspase-3, M. Endo, K. Nakayama, Y. Kaida, and T. Majima : Angew. Chem. Int. Ed., 43 [42] (2004) 5643-5645.

Photochemical Regulation of the Activity of an Endonuclease BamHI Using an Azobenzene Moiety Incorporated Site-selectively into the Dimer Interface, K. Nakayama, M. Endo, and T. Majima : Chem. Commun., [21] (2004) 2386-2387.

Effects of Benzyl-ether Type Dendrons as Hole-harvesting and Shielding for the Neutralization of Stilbene Core Radical Cations with Chloride Ion During Two-photon

Ionization of Stilbene Dendrimers Having the Stilbene Core and Benzyl-ether Type Dendrons, M. Hara, S. Samori, X. Cai, S. Tojo, T. Arai, A. Momotake, J. Hayakawa, M. Uda, K. Kawai, M. Endo, M. Fujitsuka, and T. Majima : J. Am. Chem. Soc., 126 [43] (2004) 14217-14223.

Transient Phenomena of Polyphenyls in the Higher Triplet Excited States, X. Cai, M. Sakamoto, M. Hara, S. Tojo, K. Kawai, M. Endo, M. Fujitsuka, and T. Majima : J. Phys. Chem. A, 108 [43] (2004) 9361-9364.

Photocatalytic Oxidation Reactivity of Holes in the Sulfur- and Carbon-doped TiO_2 Powders Studied by Time-Resolved Diffuse Reflectance Spectroscopy, T. Tachikawa, S. Tojo, M. Fujitsuka, K. Kawai, M. Endo, T. Ohno, K. Nishijima, Z. Miyamoto, and T. Majima : J. Phys. Chem. B, 108 [50] (2004) 19299-19306.

Design and Synthesis of Photochemically Controllable Restriction Endonuclease BamHI by Manipulating the Salt-Bridge Network in the Dimer Interface, M.Endo, K. Nakayama, and T. Majima : J. Org. Chem., 69 [13] (2004) 4292-4298.

Structural Arrangement of two DNA Double Helices Using Cross-linked Oligonucleotide Connectors, M. Endo and T. Majima : Chem. Commun., [11] (2004) 1308-1309.

Rate Constant of Bimolecular Triplet Energy Transfer from Chrysene in the Higher Triplet Excited States, X. Cai, M. Sakamoto, M. Hara, S. Tojo, K. Kawai, M. Endo, M. Fujitsuka, and T. Majima : J. Phys. Chem. A, 108 [] (2004) 7147-7150.

Unnatural Base Pairs Mediate the Site-specific Incorporation of an Unnatural Hydrophobic Component into RNA Transcripts, M. Endo, T. Mitsui, T. Okuni, M. Kimoto, I. Hirao, and S. Yokoyama : Bioorg. Med. Chem. Lett., 14 [10] (2004) 2593-2596.

Site-specific Incorporation of a Photo-crosslinking Component into RNA by T7 Transcription Mediated by Unnatural Base Pairs, M. Kimoto, M. Endo, T. Mitsui, T. Okuni, I. Hirao, and S. Yokoyama : Chem. Biol., 11 [1] (2004) 47-55.

Stepwise Photocleavage of Two C-O Bonds of 1,8-Bis[(4-benzoylphenoxy)-methyl]naphthalene with Three-Step Excitation Using Three-Color, Three-Laser Flash Photolysis, X. Cai, M. Sakamoto, M. Hara, S. Tojo, A. Ouchi, K. Kawai, M. Endo, M. Fujitsuka, and T. Majima : J. Am. Chem. Soc., 126 [24] (2004) 7432-7433.

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Review Papers

Asymmetric Ligands Bearing Spiro Skeleton and their Applications to Enantioselective

Catalysis (In Japanese): S. Takizawa, D. Jayaprakash, M. L. Patil, C. Muthiah, and H. Sasai : Materials Integration, 17 [5] (2004) 3-6.

Development of Novel Immobilization Methods for Multifunctional Asymmetric Catalysts (In Japanese), S. Takizawa and H. Sasai : Seisan to Gijyutsu, 56 [4] (2004) 43-45.

Trend in the Development of Novel Chiral Ionic Liquids (In Japanese) : M. L. Patil, S. Takizawa, and H. Sasai : Chemical Industry, 55 [11] (2004) 877-880.

Development of the First Spiro Bis(isoxazoline) Ligands (SPRIXs) and Their Applications to Catalytic Enantioselective Reactions (In Japanese): M. A. Arai, T. Shinohara, T. Arai, and H. Sasai : J. Synth. Org. Chem. 62 [1] (2004) 59-69.

DNA Nanotechnology. DNA Nanostructures Assembled from DNA Super molecules (In Japanese): M. Endo and T. Majima : Kagaku (Kyoto, Japan), 59 [10] (2004) 70-71.

Book

Lanthanide Complexes in Asymmetric Two-center Catalysis, M. Shibasaki, H. Sasai, and M. Yoshikawa, In *Transition Metals for Organic Synthesis*, Vol. 1, M. Beller, and C. Bolm, Eds., Wiley-VCH, (2004) 363-378.

Patents

Preparation of Quaternary Ammonium Salts Having a Spiro Chirality and Its Application to Asymmetric Reactions, A. Shimomoto, K. Yonezawa, S. Takizawa, and H. Sasai, JP2004261766, (2004).

Preparation of Novel Spiro Compounds, M. L. Patil, C. V. L. Rao, S. Takizawa, and H. Sasai, JP2004259127, (2004).

Preparation of Optically Active Spiro Bis(isoxazoline) Derivatives and Their Metal Complexes as Asymmetric Catalysts, H. Sasai, K. Wakita, T. Kato, M. A. Arai, JP2004263647, (2004).

Preparation of Chiral Phase Transfer Catalysts with a Spiro Skeleton and Their Application to Asymmetric Reactions, K. Yonezawa, A. Shimomoto, S. Takizawa, and H. Sasai, JP2004258567, (2004).

Preparation of Optically Active Spiro Bis(isoxazole) Derivatives and Their Metal Complexes as Asymmetric Catalysts, H. Sasai, K. Wakita, T. Kato, M. A. Arai, JP2004262328 (2004).

Preparation of Optically Active Binuclear Vanadium Complexes and Optically Active Binaphthols Using Them as Catalysts, H. Sasai and S. Takizawa, JP2005075774, (2005).

Preparation of Optically Active Binaphthols and Their Metal Complexes as Catalysts, H. Sasai and S. Takizawa, JP2005075770, (2005).

Formation of Solid Polymer Electrolytes for Batteries, H. Sasai, S. Takizawa, and S. Abe, JP2005050778, (2005)

Preparation of Asymmetric Catalysts, M. Shibasaki, H. Sasai, and Y. Tahara, JP2004168628, (2004).

Preparation of Asymmetric Catalysts, M. Shibasaki, H. Sasai, and Y. Tahara, JP2004300332, (2004).

International Conferences

Design and Synthesis of Novel Spiro-type Ligands (Poster), *T. Tsujihara, K. Wakita, T. Kato, A. Shimomoto, M. L. Patil, C. V. L. Rao, T. Shinohara, M. A. Arai, S. Takizawa, and H. Sasai, 17th French-Japanese Symposium on Medicinal and Fine Chemistry (FJS-2004), Miyagi, Japan, May 17-20, 2004.

Dual Activation in a Homolytic Coupling Reaction Promoted by an Enantioselective Dinuclear Vanadium(IV) Catalyst (Poster), H. Somei, Y. Asano, *T. Yoshida, S. Takizawa, H. Yamataka, and H. Sasai, 17th French-Japanese Symposium on Medicinal and Fine Chemistry (FJS-2004), Miyagi, Japan, May 17-20, 2004.

The aza-Morita-Baylis-Hillman Reaction Catalyzed by Chiral Phosphine-Binol as an Organocatalyst, *K. Matsui, S. Takizawa, and H. Sasai, 16th International Symposium on Chirality (ISCD 16), New York, USA, July 11-14, 2004.

Development of Novel Chiral Spiro-type Ligands, *H. Sasai, K. Wakita, T. Kato, Y. Honda, M. A. Arai, T. Shinohara, C. Muthiah, T. Tsujihara, and S. Takizawa, The 36th International Conference on Coordination Chemistry (ICCC-36), Mérida Yucatán, México, July 18-23, 2004.

Dual Activation in a Homolytic Coupling Reaction Promoted by an Enantioselective Dinuclear Vanadium(IV) Catalyst (Poster), H. Somei, Y. Asano, *T. Yoshida, S. Takizawa, H. Yamataka, and H. Sasai, 15th International Conference on Organic Synthesis (ICOS-15), Aichi, Japan, Aug. 2-6, 2004.

The aza-Morita-Baylis-Hillman (aza-MBH) Reaction Promoted by Chiral Phosphine-BINOL as an Organocatalyst (Poster), *K. Matsui, S. Takizawa, and H. Sasai, 15th International Conference on Organic Synthesis (ICOS-15), Aichi, Japan, Aug. 2-6, 2004.

Novel Bifunctional Asymmetric Organocatalysts for aza-Morita-Baylis-Hillman (aza-MBH) Reaction, *K. Matsui, S. Takizawa, and H. Sasai, The 7th IUPAC International Conference on Heteroatom Chemistry (ICHAC-7), Shanghai, China, Aug. 20-25, 2004.

Catalytic Enantioselective Direct Henry Reaction, S. Takizawa, K. Murai, K. Wataguchi, T. Hara, and *H. Sasai, Rare Earths ’04 in Nara, Nara, Japan, Nov. 7-12, 2004.

Novel Bifunctional Organocatalysts for Enantioselective aza-Morita-Baylis-Hillman (aza-MBH) Reaction (Poster), *K. Matsui, S. Takizawa, and H. Sasai, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Development and Application of Novel Immobilization Method for Multicomponent Asymmetric Catalysts (Poster), S. Takizawa, K. Marubayashi, *N. Inoue, and H. Sasai, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Dual Activation in a Homolytic Coupling Reaction Promoted by an Enantioselective Dinuclear Vanadium Catalyst (Poster), T. Yoshida, *T. Katayama, H. Somei, Y. Asano, S. Takizawa, and H. Sasai, THE INTERNATIONAL SYMPOSIUM ON DYNAMIC COMPLEX (ISDC-2005), Nagoya, Japan, Jan. 9-10, 2005.

Development of Novel Spiro-type Ligands, T. Tsujihara, P. Koranne, M. Chinnasamy, K. Wakita, J. Yogo, S. Takizawa, and *H. Sasai, THE INTERNATIONAL SYMPOSIUM ON DYNAMIC COMPLEX (ISDC-2005), Nagoya, Japan, Jan. 9-10, 2005.

Development and Application of a Novel Method for the Immobilization of Multicomponent Asymmetric Catalysts (Poster), *K. Marubayashi, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Development of Artificial Enzymes with Relevance to Bioluminescence (Poster), *T. Kawase, D. Jayaprakash, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Design and Synthesis of Novel Chiral Spiro Ligands and Ionic Liquids (Poster), *C. V. L. Rao, M. L. Patil, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Study of Novel Chiral Ligands Bearing Spiro Skeleton and their Applications to Asymmetric Cyclizations (Poster), *C. V. L. Rao, M. L. Patil, S. Takizawa, and H. Sasai, 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" Third International Symposium 2005, Shiga, Japan, Mar. 9-10, 2005.

Development of Novel Chiral Spiro-type Ligands (Poster), *T. Tsujihara, P. Koranne, K. Wakita, M. Chinnasamy, J. Yogo, S. Takizawa, and H. Sasai, 229th ACS National Meeting, San Diego, CA, USA, Mar. 13-17, 2005.

DNA Supramolecular Chemistry, M. Endo and T. Majima, 11th Symposium of

Intelligent Electrophotonic Materials and Molecular Electronics (SIEMME'11), XiQiao Hotel, iangbin West Road No.1, Kunming City, unnan, Kunming, China, Nov. 5-8, 2004.

Photochemical Control of the Protein Activity by Manipulating the Dimer Interface, M. Endo, K. Nakayama, and T. Majima, 2004 Korea-Japan Symposium on Frontier Photoscience "Photochemsitry and Nanotechnology", Samsung Fire & Marine Insurance HRD Center, Daejeon, Korea, Nov. 20-23, 2004.

Construction of Supramolecular Structures using DNA-porphyrin Conjugates, M. Endo, T. Shiroyama, M. Fujitsuka, and T. Majima, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Photochemical Regulation of Caspase-3 Activity, M. Endo, K. Nakayama, Y. Kaida, and T. Majima, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN-2004)-Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, Dec. 6-7, 2004.

Publications in Domestic Meetings

National Meeting of Chemical Society of Japan	13 papers
Symposium on Progress in Organic Reactions and Syntheses	1 paper
Congress of Organic Chemistry	5 papers
Symposium on Organic Synthesis	1 paper
Symposium on Organometallic Chemistry	1 paper
Congress of Heterocyclic Chemistry	1 paper
Perspective in Nano-supramolecule as Catalysts	2 papers
Symposium of Organic Synthesis for Young Scientists	2 papers
Symposium on Basic Organic Chemistry	2 papers
Symposium on Photochemistry	3 papers

Sponsorship

Grant-in-Aid for Scientific Research (2)

H. Sasai	Development of Artificial Enzyme with Synergistic Multi-cooperation in Active Sites	¥2,000,000

Grant-in-Aid for JSPS Fellows

H. Sasai	Novel Asymmetric Catalytic Synthesis	¥400,000

Japan Science and Technology Corporation

S. Takizawa	Preparation of Functionalized Nanoparticles by Self-assembly	¥17,100,000

Grant-in-Aid for Scientific Research

M. Endo	Development of Photochemically Controllable Enzymes for Cancer Therapy	¥3,500,000

Department of Nanobiology

Professor: Katsuyuki TANIZAWA
Associate Professor: Toshihide OKAJIMA
Research Associate: Ryousuke NAKASHIMA

Outlines

Proteins and those complexed with other biomolecules are regarded as nano bio devices. The research of our group is focused on structural and functional studies of the nano bio devices, as well as their applications in the interdisciplinary field. We are also interested in the development of highly sensitive biosensors and construction of nano machines.

Current Research Programs

Mutational and Crystallographic Investigation of the Role of Aspartate 298 in the Catalysis of Bacterial Copper Amine Oxidase.

Copper amine oxidase from *Arthrobacter globiformis* (AGAO) contains a Cu^{2+} ion and an auto-catalytically generated quinone cofactor, topa quinone (TPQ), which mediates electron transfer from amine substrate to molecular oxygen. The overall catalytic reaction can be divided into the initial reductive and the following oxidative half-reactions. In the former half-reaction, a substrate amine reacts with the C5 carbonyl group of the oxidized TPQ, forming the substrate Schiff base (SSB), which is further converted to the product Schiff base (PSB). During this step, an invariant acidic residue serves as a catalytic base to abstract the α-proton of substrate from SSB. To elucidate the role of Asp298, the putative catalytic base in AGAO, in the reductive half-reaction, the mutant enzyme in which Asp298 is substituted by Ala (D298A) was analyzed for its structural and spectral properties. Kinetic experiments for the TPQ biogenesis indicated that the rate is only about two times slower than that of the wild-type enzyme. However, the catalytic efficiency of D298A decreased by about 10^5-fold, consistent with the essentiality of Asp298. Global analysis of UV-visible spectral changes observed upon addition of 2-phenylethylamine to D298A showed slow formation of SSB intermediate (k_{obs} = 4.2 s^{-1}) and further slower its breakdown (k_{obs} = 4.8 X 10^{-4} s^{-1}). To determine the structures of intermediates, the crystals of holo D298A were soaked with 2-phenylethylamine in different periods of time. X-ray diffraction analyses of these crystals soaked for 1 h and 7 days revealed the structures of the SSB and PSB intermediates formed in the active site, respectively, which were assigned based on single-crystal microscopy. In the SSB structure, the pro-S α-proton to be abstracted by the catalytic base is positioned perpendicularly on the plane formed by the Schiff base double bond and the aromatic ring of TPQ, consistent with the stereospecificity of α-proton abstraction, governed by the maximum overlap of σ and π electrons.

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. This structural information enable us to be in outstanding position to elucidate the molecular mechanism of transport process.

Publications

Original Papers

Molecular Function of Axonal Guidance-related Proteins, UNC-76/FEZ1/FEZ2, T. Fujita, J. Ikuta, A. Maturana, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda: Recent Res. Devel. Biophys. Biochem., 4 (2004) 313–320.

Enhanced Long-term Potentiation In Vivo in Dentate Gyrus of NELL2-Deficient Mice, S. Matsuyama, K. Aihara, N. Nishino, S. Takeda, K. Tanizawa, S. Kuroda, and M. Horie: NeuroReport, 15 (2004) 417-420.

Identification of a Tissue-non-specific Homologue of Axonal Fascination and Elongation Protein Zeta-1, T. Fujita, J. Ikuta, J. Hamada, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda: Biochem. Biophys. Res. Commun., 313 (2004) 748-754.

Chemical Rescue of a Site-specific Mutant of Bacterial Copper Amine Oxidase for Generation of the Topa Quinone Cofactor, H. Matsunami, T. Okajima, S. Hirota, H. Yamaguchi, H. Hori, S. Kuroda, and K. Tanizawa: Biochemistry, 43 (2004) 2178-2187.

Novel Tissue and Cell Type-Specific Gene Delivery System Using Surface Engineered Hepatitis B Virus Nanoprotein Particles, T. Yamada, A. Kondo, M. Ueda, M. Seno, K. Tanizawa, and S. Kuroda: Current Drug Targets: Infectious Disorders, 4 (2004) 163–167.

Over-Expression System for Secretory Phospholipase D by *Streptomyces lividans*, C. Ogino, M. Kanemasu, Y. Hayashi, N. Shimizu, A. Kondo, S. Tokuyama, Y. Tahara, S. Kuroda, K. Tanizawa, and H. Fukuda: Appl. Microbiol. Biotechnol., 64 (2004) 823–828.

Review Papers

Role of Copper Ion in Bacterial Copper Amine Oxidase: Spectroscopic and Crystallographic Studies of Metal-substituted Enzymes, T. Okajima: Annual Report of Osaka University, 2002-2003, Vol. 4, p54.

A New Clinical Technique Developed by Hollow Bio-Nanoparticles (in Japanese), S. Kuroda, T. Yamada, M. Seno, A. Kondo, M. Ueda, and K. Tanizawa: Chemical Industry, 55 (2004) 936–942.

Pinpoint Drug Delivery System Using Hollow Bio-Nanoparticles (in Japanese), T. Yamada, M. Seno, A. Kondo, M. Ueda, K. Tanizawa, and S. Kuroda: Kobunshi Ronbunshu, 61 (2004) 606–612.

International Conferences

Crystal Structure of Bacterial Multidrug Efflux Transporter AcrB, S. Murakami, R. Nakashima, E. Yamashita, A. Yamaguchi, International Workshop on Structural Chemical Biology of Membrane Protein Complex Functions, University of Hyogo, Kamigohri, Japan, April 19-20, 2004.

Crystal Structure of Bacterial Multidrug Efflux Transporter AcrB, S. Murakami, R. Nakashima, T. Matumoto, E. Yamashita, and A. Yamaguchi, The Sixth Conference of the Asian Crystallographic Association (AsCA'04), Symposium, "Macromolecular assemblies", Hong Kong, China, June 27-30, 2004.

Interaction of a RING-IBR Protein RBCK1 with Its Splicing Variant RBCK2 (Poster), N. Yoshimoto, K. Tatematsu, T. Koyanagi, K. Tanizawa, and S. Kuroda, FASEB Conference: Transcriptional Regulation During Cell Growth, Differentiation and Development, Saxtons River, Vermont, U.S.A., August 14-19, 2004.

X-ray Crystallographic Analysis of Multi-drug Efflux Transporter, S. Murakami, R. Nakashima, T. Matumoto, E. Yamashita, and A. Yamaguchi, The 8th International Conference on Biology and Synchrotron Radiation (BSR2004) Symposium, "Membrane Proteins", Hyougo, Japan, September, 7-11, 2004.

Development of Novel Bio–Nanoparticles for Human Tissue-Specific Delivery of Genes and Drugs (Invited), K. Tanizawa, T. Yamada, A. Kondo, H. Tada, M. Seno, M. Ueda, and S. Kuroda, 17th FAOBMB Symposium / 2nd IUBMB Special Meeting / 7th A-IMBN Conference “Genomics and Health in the 21st Century”, Bangkok, Thailand, November 22–26, 2004.

Mechanism of α-Proton Abstraction in the catalytic intermediate of bacterial copper amine oxidase (Oral), T. Okajima and K. Tanizawa, International Symposium on Scientific and Industrial Nanotechnology 2004 (SISSIN 2004), Suita, Osaka, Japan, December 6-7, 2004.

Improving Gene/Drug Delivery to Human Hepatocytes with Hepatitis B Virus Surface Antigen L particles (Poster), J. Jung, T. Yamada, K. Tanizawa, and S. Kuroda, Third 21st Century COE “Towards Creating New Industries Based on Inter-Nanoscience” International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

The ENH1-PKCε-PKD1 Complex and the PKC-regulating Protein ENH2: Novel Therapeutic Targets in Cardiac Hypertrophy (Poster), M. Iwata, A. Maturana, M. Ishida, K. Tatematsu, T.Okajima, K. Tanizawa, and S. Kuroda, Third 21st Century COE

"Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

Mechanism of α-Proton Abstraction in the Catalytic Intermediate of Bacterial Copper Amine Oxidase (Poster), T. Murakawa, T. Okajima1, M. Uchida, Y. Yamamoto, H. Hayashi, K. Tatematsu, S. Kuroda, and K. Tanizawa, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

Molecular Analysis of Hepatitis B virus (HBV) Infection Using the L Envelope Protein Fused to Green Fluorescent Protein (GFP) (Poster), T. Kasuya, A. Uyeda, T. Yamada, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

Structure-function Studies on a Neuronal Axon Guidance Related Protein FEZ1 and its Homologue FEZ2 (Poster), J. Ikuta, T. Fujita, A. Maturana, T. Okajima, K. Tatematsu, K. Tanizawa, and S. Kuroda, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

Interaction of a RING-IBR Protein RBCK1 with Its Splice Variant RBCK2 (Poster), N. Yoshimoto, K. Tatematsu, T. Koyanagi, T. Okajima, K. Tanizawa, and S. Kuroda, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

Retargeting of Hepatitis B Virus-derived Nanoparticles to Mouse Tissues and Tumor Cells by Using Combinatorial Biochemical Technique (Poster), A. Uyeda, M. Inoue, T. Yamada, K. Tanizawa, and S. Kuroda, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium, Makino, Shiga, Japan, March 9-10, 2005.

Spectrophotometric, Kinetic, and Structural Characterization of Catalytic Intermediates of Copper/TPQ-dependent Amine Oxidase (Invited), T. Murakawa, Y.-C. Chiu, Y. Yamamoto, H. Hayashi, T. Okajima, and K. Tanizawa, 4th European-Japanese Bioorganic Conference (EJBC-4), Hotel Limani, Ushimado, Setouchi, Okayama, March 15–19, 2005.

Publications in Domestic Meetings

Japanese Biochemical Society	1 paper
Spring8 symposium	1 paper
Divisional Meeting on Colloid and Interface Chemistry, the Chemical Society of Japan	1 paper
Japanese Society for Molecular Biology	5 papers
Japan Bioenergetics Group	1 paper
Bimonthly Meeting of Vitamin B Committee	1 paper

Sponsorship

Grants-in-Aid for Scientific Research

T. Okajima	Biogenesis of built-in cofactors	¥1,200,000

Entrusted Research

K. Tanizawa	Agriculture, Forestry, and Fisheries Research Council	*De Novo* Design, and Analysis of Structure and Function of Quinone-Containing Built-in Enzymes	¥3,047,000
K. Tanizawa	Japan Society for the Promotion of Science	Survey and Research on the Academic Trends in Biological Sciences –Post-Genomic Era–	¥2,000,000
K. Tanizawa	Mitsubishi Electric Company, Ltd. (NEDO)	Analysis of Intracellular Signal Networks for Industrial Application of Genomics	¥4,712,000
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	¥1,400,000

Other Research Funds

K. Tanizawa	Vitamin B Committee	Research on Built-in Cofactors	¥350,000

Department of Nanosystem Design

Guest Professor, Ryusuke NISHITANI (2004.4- 2004. 6)

Outlines

The local optical and electronic analysis of materials on a nanometer scale is an indispensable research for the development of nanometer electronics. The STM based spectroscopy enables us its analysis by combination of spectroscopic apparatus with STM technology. In this study, we have developed a system of STM-induced luminescence measurement, and carried out spectroscopic measurements of molecular luminescence on the metal surfaces.

Achievements

1. The STM-induced luminescence on a nanometer scale has been obtained in air by combining the STM in air and the spectrograph instruments.
2. The molecular luminescence of porphyrin film on a nanometer region has been observed in air for the first time. The spectra excited by tunneling electron injected from STM shows peaks which are nearly identical to photo luminescence peaks.
3. The enhancement of STM luminescence is observed for the porphyrin molecules on the substrates of noble metals, Au and Ag, but not on the Graphite and ITO.
4. The mechanism of molecular luminescence and its enhancement on noble metals can be explained in terms of the local plasmon induced luminescence and the plasmon enhanced molecular luminescence.
5. The molecular luminescence by STM can be analyzed by a model of the interaction of molecules with electromagnetic fields in a cavity, surrounded by the STM tip and the metal substrate, which is originated from the plasmon polarization created by tunneling electron from STM. The polarization of molecular luminescence should be resonated with the plasmon field to enhance the molecular luminescence resulted from plasmon field on noble metals.

Publication

STM-excited molecular fluorescence from porphyrin thin films, H. Liu, R. Nishitani, Y. Ie, T. Yoshinobu, Y. Aso, H. Iwasaki: Jpn. J. Appl. Phys., 2005, Vol.44 No.18 pp.L566 - L569.

Department of Nanosystem Design

Guest Associate Professor Takeyoshi SUNAGAWA (2004.4. - 2004.6.)

Outlines

For the electrodeless measurements of conductivity and charge carrier mobility in various kinds of material, an improvement of in-situ time-resolved microwave conductivity (TRMC) and transient optical spectroscopy (TOS) was performed. Based on his know-how about the design of microwave circuit and resonant cavity, sensitivity and signal-to-noise (S/N) ratio in the TRMC signals which are induced by photo or radiation exposure are intended to be realized. In addition, formation process and dynamics of charge carriers in luminous materials were investigated.

Achievements

In order to enhance the accuracy of TRMC experiments, characterizations of electric power and output for every component which comprises the microwave circuit were performed. As a result, it was found that appropriate type of microwave detector and its mount geometry can enhance the sensitivity and S/N ratio. For the separation of real and imaginary pars of dielectric absorption of microwave experimentally, basic data on overlap of microwave from main and reference arms were taken. He has devoted his efforts to a design of instrument which in aimed at the experiments at low temperature. The designed resonant cavity and the low temperature system are under construction. Measurement of charge carrier mobility in polymer-electron acceptor complex was carried out and the estimation of the mobility without using electrodes was achieved[1]. In addition, preliminary experiments of luminous materials was performed using the same measurement system, and signal was confirmed for the first time.

Publications

[1] A. Saeki, S. Seki, Y. Koizumi, T. Sunagawa, K. Ushida, and S. Tagawa, “Increase of Mobility of Photogenerated Positive Charge Carriers in Polythiophene” *J. Phys. Chem. B* (2005) in press.

Department of Nanosystem Design

Guest Professor　Ryo SHIMIZU (2004.7.1 - 2004.9.30)

Outlines

The department aims to develop the protocol for designing of nanoscale system on the materials.

Achievements

The method of structure-based drug design (SBDD) was developed for generating novel inhibitors specific clinically important enzymes.

The following lectures were given.

“Development of New Drugs using Structure-Based Drug Design Technique, Part I.” (Jun. 26, 2004)

“Development of New Drugs using Structure-Based Drug Design Technique, Part II.” (Aug. 11, 2004)

“Development of New Drugs using Structure-Based Drug Design Technique, Part III.” (Sep. 10, 2004)

Department of Nanosystem Design

Guest Associate Professor: Takanori ICHIKI (2004.7. - 2004.9.)

Outlines

For the realization of new functional bio-devices with DNA, fusion of top-down and bottom-up nanotechnology is considered to be most promising approach. We investigated the microfabrication of the silicon mold that is necessary in DNA patterning process using nanoimprint lithography.

Achievements

High-aspect-ratio molds for nanoimprint lithography have been achieved by dry etching of silicon substrates in fluorocarbon plasmas. A seminar about the fabrication of nano-gap electrodes and advanced bio-devices using advanced nano/microfabrication technologies for ULSI was held.

Publications

Original Papers

Non-Destructive On-Chip Cell Sorting System with Real-Time Microscopic Image Processing, K. Takahashi, A. Hattori, I. Suzuki, T. Ichiki and K. Yasuda : J. Nanobiotechnology, 2 (2004) 5-12.

Hydrophilic Patterning of Polymer Surfaces Using a Scanning Microplasma Jet Source, T. Ideno and T. Ichiki : J. Photopolymer Sci. and Technol., 17 (2004) 173-176.

Localized and Ultrahigh-Rate Etching of Silicon Wafers Using Atmospheric-Pressure Microplasma Jets, T. Ichiki, R. Taura, and Y. Horiike : J. Appl. Phys. 95 (2004) 35-39.

Review Papers

Application of Microplasmas, K. Terashima, T. Ito, H. Fujiwara, K. Katahira, A. Kono, J. Wang, M. Aramaki, T. Ichiki : J. Plasma Fusion Res., 80(10) (2004) 845-853.

Books

New Technology for Biochip and Application, T. Ichiki, CMC books, 2004.

Patents

Microplasma jet source, T. Ichiki, Pat. No. 3616088.

International Conference

Microdevice Technologies forBiomolecular and Cellular Manipulation,(Invited) *T. Ichiki, The 1st International Symposium on Molecule-Based Information Transmission and Reception (MB-ITR2005), Okazaki, Japan, Mar. 3-7, 2005

Microchip Techbnology for High-throughput Screening of Molecular Functions,

(Invited) *T. Ichiki, Fifth Int. Symp. on Biomimetic Materials Processing (BMMP-4), Nagoya, Japan, Jan. 26-28, 2005

Microplasma Processes for MEMS Applications,(Invited) *T. Ichiki, T. Ideno, H. M. L. Tan, and R. Taura, 25th Int. Symp. on Dry Process, Tokyo, Japan, Nov. 30-Dec. 1, 2004

Atmospheric-pressure Plasma Micro-jet and Its Applications to Plasma Processing and Micro Analytical Systems,(Invited) *T. Ichiki,, Gordon Research Conference, Plymouth, USA, Aug. 17, 2004

Plasma Technologies for Microfluidics for Novel Bioanalytical Systems,(Invited) *T. Ichiki, 51st Int. Symp. American Vacuum Society, Anaheim, USA, Nov. 16, 2004

Nano/Microfabrication Technologies for Nanobio-devices,(Invited) *T. Ichiki, The 4th Int. Symp. Advanced Fluid Information and The 1st Int. Symp. Transdisciplinary fluid Integration (AFI/TFI2004), Sendai, Japan, Nov. 11, 2004

Feasible Pattering of Functional Biomolecules by Self-assembled Beads Printing,(Invited) K. Takahashi, N. Ichikawa, *H. Fukuda and T. Ichiki, 2004 Int. Microprocesses and Nanotechnology Conference, Osaka, Japan, Oct. 26-29, 2004

Maskless Etching of Microstructures Using a Scanning Microplasma Etcher,(Poster) *T. Ideno and T. Ichiki, Proc. 7th Asia Pacific Conference on Plasma Science and Technology, Fukuoka, Japan, Jun. 29-Jul. 2, 2004

Microreactor Array Chips for High-throughput Function Analysis of Biomolecules Using Magnetic Beads,(Poster) *Y. Hosoi and T. Ichiki, Int. Conf. on Solid State Dev. and Mater.(SSDM 2004), Tokyo, Japan, Sep.16-18, 2004

Development and Characterization of 3D Scanning Microplasma Jet Etcher,(Poster) *Helen M. L. Tan, T. Ideno and T. Ichiki, 2nd Int. Workshop on Microplasmas, Oct. 6-8, 2004

Evaluation of Cell Electrophoretic Mobility Using Microcapillary Electrophoresis Chips, (Poster) *F. Omasu, Y. Nakano and T. Ichiki, Eighth International Conference on Miniaturized Chemical and Biochemical Analysis Systems (Micro Total Analysis Systems 2004), Malmö, Sweden, Sep. 26-30, 2004

Microfluidic Devices Integrated with Permalloy Micropatterns for Bead-based Assay, (Poster) *N. Ichikawa, Y. Katsuyama, Y. Nagasaki and T. Ichiki, Eighth International Conference on Miniaturized Chemical and Biochemical Analysis Systems (Micro Total Analysis Systems 2004), Malmö, Sweden, Sep. 26-30, 2004

Department of Nanosystem Design

Guest Professor　Ichiro YAMASHITA (2004.10. - 2004.12.)

Outlines

Synthesis of the magnetic ferritin based on the chemical reaction of Co and Pt and the measurement of their magnetic properties.

Measurement of the interaction between DNA and ferritin molecule on the solid substrate.

Achievements

CoPt cores were successfully synthesize in the apoferritin cavity.
It was experimentally observed that DNA molecules which were positioned on the solid surface interact somehow with ferritin molecules.
The magnetic properties of CoPt-ferritin was measured and it was shown that they have weak magnetic moment. The reason of this result is not clear at this moment.

Publications

Original Papers

A 7-nm Nanocolumn Structure Fabricated by Using a Ferritin Iron-core Mask and Low-energy Cl Neutral Beams, T. Kubota, T. Baba, S. Samukawa, H. Kawashima, Y. Uraoka, T. Fuyuki and I. Yamashita : Appl. Phys. Lett., 84[9] (2004) 1555-1557.

Bio-template Synthesis of Uniform CdSe Nanoparticles Using Cage-shaped, Apoferritin , I. Yamashita: Chemistry Letters, 9(2004) 1158-1159.

Review Papers

Fabrication of the Ultra Super LSI Using Bio-nanotechnology, M. Muraoka, K. Iwahori, I. Yamashita : Kagaku, 59 (2004) 38-39.

Books

Advanced Chemistry VI　The Nano-interface, Colloid, Nanotchonolg, Molecular Electronics, and Nano-analysis, M. Muraoka, K. Iwahori, I. Yamashita : MARUZEN Co., Ltd., 2004, 127-135.

The Synthesis, Adjustment and Control of Metal Nanoparticles and their Application, I. Yamashita : Technical Information Institute Co., Ltd., 2004, Total 408 pages

An Encyclopedia of Electronic Properties and Materials, M. Muraoka, K. Iwahori, I. Yamashita : Asakurashoten, 2004, in press

The Synthesis, Preparation and Control Method of Metal Nanoparticles and the Application; The Synthesis of Inorganic Material Nanoparticles and their Application for the Bio-Nano-Process, K.Iwahori, M. Muraoka, I. Yamashita :
Technical Information Institute Co., Ltd., 2004.

International Conference

Biological Pathway to Nanoelectronics Devices(Invited), *I. Yamashita, SPIE International Symposium, Smart Materials, Nano-, and Micro-Smart Systems, Miyagi, Japan, Apr. 10, 2004.

Nano Fabrication based on Self-assembly of Protein(Invited), *I.Yamashita, Asia-Pacific Conference of Transducers and Micro-Nano Technology, Hokkaido, Japan, Jul. 4, 2004.

Protin Supramolecules for Nano-Electronics Device Fabrication, *I. Yamashita, Viruses&Protein Cages as Materials Conference, Montana, USA, Aug. 1, 2004.

Fabrication of a 7-nm High-aspect Nanocolumn Structure by Low Energy Neutral Beam Etching on a Ferritin Iron-core Mask, *T. Baba, T. Kubota, Y. Uraoka, T. Fuyuki, I. Yamashita, S. Samukawa, AVS 51st International, Anaheim, USA, Nov. 14, 2004.

Nano Device Fabrication Based on Self-assembly of Protein(Invited), *I. Yamashita, SMBN2004, ISMM2004, Kagawa, Japan, Nov. 24, 2004.

Fabrication of 7-nm Nanocolumn Structure Using Ferritin Iron-Core Mask and Highly Anisoteopic Neutral Beam Etching, *T. Kubota, T. Baba, H. Kawashima, Y. Uraoka, T. Fuyuki, I. Yamashita, S. Samukawa, Tokyo, Japan, Nov. 30, 2004.

Biological Pathway to the Nanoelectronics Devices, AFI/TFI, *S. Yoshii, I. Yamashita, Miyagi, Japan, Apr. 10, 2004.

Biological Path to Nanoelectronics Devices(Invited), *I. Yamashita, Smart Materials, Nano-and Micro-Smart Systems, Austlaria, Dec. 12, 2004.

Fabrication of Nanometric Structure by Protein supramolecule(Invited),*I. Yamashita, Nanoarchitectonics Workshop NAMINA2005 , Ibaragi, Japan, Mar. 3, 2005.

The Effects of N-terminal Residues on the Self-assembly of L-chain Apoferritin, *K. Yoshizawa, K. Iwahori, Y. Mishima, I. Yamashita, Nanoarchitectonics Workshop , NAMINA2005, Ibaragi, Japan, Mar. 3, 2005.

Ferritin Cage as a Nanoscale Platform for Chemical Modification, *Y. Fukushige, M. Muraoka, I. Yamashita, Nanoarchitectonics Workshop NAMINA2005, Ibaragi, Japan, Mar. 3, 2005.

Synthesis of Hybrid Nanomaterials of Cage-shaped Protein with Synthetic Polymer, *M. Muraoka, N. Kishimoto, I. Yamashita, 229th ACS National Meeting, USA, Mar. 13, 2005

Biological Path for Nanofabrication of Size-and Shape-controlled Nanoparticle Synthesis (Invited), *I. Yamashita, 229th ACS National Meeting, USA, Mar. 13, 2005.

Cobalt Oxide Nanoparticle Synthesis Using Cage-shaped Protein Cavity, *R. Tsukamoto, K. Iwahori, M. Muraoka, I. Yamasita, 229th ACS National Meeting, USA, Mar. 13, 2005.

Fabrication of Semiconductor Nano-particles in the Protein Cage of Apoferritin, *K. Iwahori, K. Yoshizawa, I. Yamashita, 229th ACS National Meeting, USA, Mar. 13, 2005.

The Bio-Nano-Process:Making Semiconductor Devices Using Protein Supramolecules, (Invited), *I. Yamashita, MRS Spring Meeting, USA, Mar. 28, 2005.

Department of Nanosystem Design

Guest Associate Professor: Koji Furukawa (2004. 9.-2004.12.)

Outlines

Antibody can be regarded as an excellent nanobio tool derived from living organisms because of its ability to recognize antigens specifically in dissociation constant less than nanomolar order. The research of this group is focused on elucidating how such high affinity antibody is evolved through the affinity maturation system governed by dynamics of antibody repertoire.

Current Research Programs

Dynamics of an immune response.

Dynamic shaping of the antibody repertoire is essential for effective immunity. A novel approach was established for clarifying how the antibody repertoire is shaped over time for development of a specific immune response. Over 500 immunoglobulin G1 clones harboring VH186.2 were obtained from the spleen, bone marrow, and microdissected individual germinal centers of (4-hydroxy-3-nitrophenyl) acetyl-immunized C57BL/6 mice at various time points postimmunization. Statistical analyses provided an index for defining clonal diversity and cluster analyses gave a three-dimensional landscape with which clone distance was visualized with the expression level of antibodies. This landscape approach facilitated understanding of the dynamics shaping the actual antibody repertoire, in which pre-existing naturally occurring population persisted and provided a significant impact upon the repertoire.

Publications

Original Papers

A Landscape for the Dynamics of an Immune Response, A. Furukawa, K. Furukawa, and T. Azuma: Biochem. Biophys. Res. Commun. 319 (2004) 469-478.

BASH-Deficient Mice: Limited Primary Repertoire and Antibody Formation, But Sufficient Affinity Maturation and Memory B Cell Generation, M. Yamamoto, T. Nojima, K. Hayashi, R. Goitsuka, K. Furukawa, T. Azuma, and D. Kitamura: in Anti-NP Response, Int. Immunol. 16 (2004) 1161-1171.

Department of Nanosystem Design

Guest Professor: Katsuhiko TAKAGI (2005.1. – 2005.3.)

Outlines

Composite films of a meso-(tetramethylpyridinium)porphyrin (TMPyP) hybrid incorporated in mesoporous silica (MPS) cast on a methyl viologen (MV^{2+})/titania nanosheet hybrid were synthesized and a light induced charge separation between the two could be observed. These composite thin films were able to initiate a one-electron reduction of the MV^{2+} ions accompanied by the simultaneous decomposition of the TMPyP organic dye within the mesoporous silica channels.

Achievements

The laminated hybrid-composites consecutively stacked with TMPyP/MPS and MV^{2+}/MPS were synthesized. It could be seen that UV light irradiation of the laminated composite films of a nanostructured hybrid of TMPyP and MV^{2+} which were separately adsorbed within MPS and TN was able to induce the simultaneous decomposition of TMPyP and the formation of $MV^{\bullet+}$. The photocatalytic one-electron reduction of MV^{2+} during the 355-nm laser flash photolysis of composite thin films was also investigated using transient absorption spectroscopy. A broad transient absorption band at 500-700 nm, which is assigned to $MV^{\bullet+}$, was observed after the laser flash. The decomposition of the TMPyP accommodated in the mesoporous silica is observed to proceed simultaneously with the reduction of MV^{2+} incorporated in the TN interlayers, resulting in the photoinduced long-lived charge separation between the TN and MPS.

Department of Nanosystem Design

Guest Associate Professor : Minoru YAMAJI (2005.1. - 2005.3.)

Outlines

Upon photoirradiation of chemical compounds, a variety of photochemical reactions proceed via the excited states. Photochemical properties of chemical intermediates produced upon photolysis were paid attention while those in the further excited states, especially higher excited triplet states, have been done less attention. Furthermore, photochemical behaviors of radical cations and anions in the excited states have not been studied precisely. The aims of the present research are to reveal the photochemical properties of highly excited triplet molecules, and chemical dynamics of cationic and anionic radicals in the excited state.

Achievements

By using two-color two-laser photolysis techniques, bond dissociation in higher excited triplet states was found for some photostable molecules. These findings demonstrate possibilities for photodecomposition of photostable chemical compounds.

1) ω-Bond cleavage of some carbonyl compounds having C-O and C-Si bonds which are stable to one-photon excitation was found in the higher excited triplet states. This work has been published in *Chem. Phys. Lett.*.

"Homolytic cleavage of C-Si bond of *p*-trimethylsilylmethylacetophenone upon stepwise two-photon excitation using two-color two-laser flash photolysis"
X. Cai, M. Sakamoto, M. Hara, S. Inomata, M. Yamaji, S. Tojo, K. Kawai, M. Endo, M. Fujitsuka, and T. Majima
Chem. Phys. Lett. **2005**, *407*, 402-406.

2) An efficient α-cleavage of some carbonyl compounds having C-O bonding at α-position in the highly excited triplet states was shown.
3) Occurrence of β-bond fission in aromatic compounds having aromatic moieties linked with a C-O bond was found in the higher excited triplet states, and the quantum yields for dissociation were shown to be correlated with the C-O bonding energy. From the results, the energy level of the reactive higher triplet state was estimated.

Division of Beam Science for Nanotechnology

Outlines

The division of beam science for nanotechnology is composed of five research departments: beam science for nanofabrication, quantum beams for nanotechnology, beam processing for nanotechnology, advanced nanofabrication, and ultra-fast spectroscopy of nanostructures.

Quantum beam science is one of the most important fields for nanoscience and nanotechnology. The researches are performing by using ultra-short electron beam, slow positron beam, ion beam, electron lithography and so on. The studies such as time-space reaction analysis with ultra-short electron beam, nano-structure analysis with slow positron beam and nano beam-process, are expected for ultimate nanofabrication and a new nano quantum beam science.

Achievements

- Development of laser photocathode RF linear accelerator
- Generation of femtosecond electron beam
- Femtosecond pulse radiolysis based on equivalent velocity spectroscopy
- Double-decker electron accelerator and attosecond pulse radiolysis
- Primary Process of Quantum Beam-Induced Nanofabrication
- Analysis of spur reactions for nanofabrication
- Improvement of L-band linear accelerator for nanoscience
- Generation of intense slow-positron beam
- Study of annihilation process of positrons in polymeric materials using AMOC
- Study of primary radiation reactions in resists using positron annihilation technique
- Single-particle induced chemical reactions and nanotechnology
- Study of physical properties of single molecular by using quantum beam
- Study of nano-process with quantum beam
- Modeling of nano-process in resist

Department of Beam Science for Nanofabrication

Professor:	Yoichi YOSHIDA
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Outline

Elucidation of ultrafast reactions in nano-space of the materials is very important for the development of ultimate fabrication process with quantum beam for the next nanotechnology. A technique of femtosecond pulse radiolysis based a femtosecond electron beam and a femtosecond laser light is a powerful tool for the studies of quantum-beam-induced reactions in a femtosecond time region and in nano-space. It is also expected for the development of quantum-beam fabrication process for nanotechnology.

For the development of femtosecond pulse radiolysis, we have firstly succeeded to generate a 98-femtosecond electron pulse in a photo-cathode RF gun based electron accelerator (linac) by a technique of rotating the bunch in longitudinal beam phase-space at electron charge of 0.17 nC and beam energy of 31 MeV. A new pulse radiolysis based an equivalent velocity spectroscopy has been developed by using the produced femtosecond electron pulse and a femtosecond laser light.

The photo-cathode RF gun linac was also used successfully to generate double-decker electron beams. The double-decker electron beams are expected for the studies of quantum-beam-induced reactions on femtosecond/attosecond time scale in the next ultimate fabrication. It is also expected for the researches in femtosecond and attosecond science.

Current Research Programs

1. Observation of 98-femtosecond Single Electron Bunch by Rotating Longitudinal Bunch Phase Space in Magnetic Field

Recently, a femtosecond pulse radiolysis system with time resolution of <100fs is developed in Osaka University. In order to achieve such time resolution, a laser-driven photocathode RF gun based linear accelerator (linac) was constructed to produce a low-emittance femtosecond electron beam, such as <3 mm-mrad and < 100 fs. The photocathode RF linear accelerator is also produced a synchronized electron pulse with laser pulse. The time jitter between the electron pulse and the analyzing laser light is improved in the pulse radiolysis experiment.

The femtosecond electron bunch generation system was consisted of a photocathode rf gun, a booster linear accelerator and a magnetic bunch compressor. A 1.6-cell S-band (2856 MHz) rf gun was used to generate a low-emittance picosecond electron bunch. A single solenoid magnet was mounted at the exit of the rf gun to compensate the emittance growth due to space charge effect. The rf gun was driven by an all solid-state

LD-pumped Nd:YLF picosecond laser. The laser consisted of a laser oscillator, a regenerative amplifier, and a frequency converter. The oscillator was mode-locked with a frequency of 79.3 MHz, the 36^{th} sub-harmonic of the 2856 MHz accelerating rf, by adjusting the cavity length of the oscillator with a semiconductor saturable absorber mirror. The time jitter between the oscillator output and the reference 79.3 MHz rf signal was measured to within a root-mean-square (rms) value of 0.3 ps using a phase detector technique. The electron beam produced by the RF gun was accelerated with a 2 m single S-band travelling-wave linac downstream of the solenoid magnet. The peak rf inputs of the rf gun and the linac were 10 MW and 25 MW, respectively, which was produced by a 35 MW Klystron. The stability of the rf power was 0.1% peak-to-peak. The repetition rate of the operation was 10 Hz in the experiment.

The magnetic bunch compressor was constructed with two 45^{o}-bending magnets and four quadrupole magnets for the rotation of the bunch in the longitudinal phase space distribution. All magnets were carefully arranged with the minimum lattice error to reduce the linear and nonlinear aberrations. To compensate high-order momentum compactions during pulse bunch compression, the energy modulation of the bunch in the longitudinal phase space distribution, before the bunch compression, was optimized by rephrasing the linac with a high-power rf phase shifter installed in a 25 MW rf line, as shown in Fig. 1. The dispersion function of the bunch in the compressor was controlled carefully by adjusting the magnetic fields of four quadrupole magnets.

Finally, the compressed bunch length was observed by measuring Cherenkov radiation emitted from the electrons of the bunch in air at the exit of the compressor with a femtosecond streak camera. The optical measurement system to guide the Cherenkov radiation to the streak camera, as shown in Fig. 1, consisted of a thin Al mirror and two convex lenses. Its optical pass length was 2 m. An optical band pass filter, which is centered at 450 nm and has a half width of 12.5 nm, was used to reduce the radiation pulse broadening due to optical dispersion. A slit width of 15 μm in the streak camera was used to avoid the pulse broadening due to space charge effect in the camera. The time resolution of the streak camera was 183 fs in FWHM and 78 fs in rms. Finally, the rms bunch length was obtained to be 98 fs at bunch charge of 0.17 nC by fitting the bunch shape to a Gaussian distribution. The effect of space charge on the bunch compression was investigated with different electron charge. The beam transverse emittance was also measured. The electron pulse has being used for the study of ultrafast electron-induced reactions on femtosecond scale in nanospace.

2. Equivalent Velocity Spectroscopy for Improvement of Time Resolution on Electron Beam Pulse Radiolysis System

The pulse radiolysis is a powerful method for ultrafast reaction/phenomena studies. A femtosecond pulse radiolysis system is developed in ISIR by using the photocathode RF gun linac. The time resolution of the pulse radiolysis is decided on pulse length of both the electron beam and analyzing light, time jitter between the electron beam and the analyzing light, and degradation of time resolution due to the velocity difference between light and electron in sample. The 98 fs electron pulse was used as a pump source. An 80 fs Ti: Sapphire laser pulse was used as an analyzing light. The timing jitter between electron beam and laser light is corrected by a femtosecond streak camera. To avoid degradation of time resolution due to the velocity difference between light and electron in sample, a technique of equivalent velocity spectroscopy was constructed in

the new femtosecond pulse radiolysis to improve the time resolution into femtosecond time region.

The concept of the equivalent velocity spectroscopy was based on a 98-femtosecond electron pulse and an 80-femtsecond laser light. The electron beam and the laser light were injected with an angle of θ in sample. The angle (θ) was adjusted as $\theta = \arccos(1/n)$, where n is the refractive index of sample. Furthermore, the shape of electron beam pulse is rotated to overlap on the light pulse. Therefore, the degradation of time resolution due to the velocity difference between light and electron in sample can be avoided in the system. As a performance test, the time spectrum of optical absorption of the hydrated electron in water was measured at wavelength on 800nm. As the results measured with and without the electron pulse rotation, the rise time of absorption of the hydrated electron in water measured by the equivalent velocity spectroscopy is 1.4 ps faster than the case of ordinary slanted incident. This result indicates that the time resolution of the pulse radiolysis was improved in the equivalent velocity spectroscopy. In the next step, the equivalent velocity spectroscopy will be used for the experiments in femtosecond/attosecond time region.

3. Double-decker Electron Accelerator and Attosecond Science

An attosecond pulse radiolysis is considered for the future time-space reaction analysis into attosecond time region. To achieve the attosecond time resolution, an attosecond electron beam and an attosecond analysis light, which should be synchronized with each other without time jitter, are required. In order to obtain such beams, a double-decker electron accelerator system based on the photocathode RF gun linac was designed. In the system, two electron pulses with different time and different positions are generated from the photocathode by the irradiation of two laser lights produced from a mode-locked laser, and are compressed into attosecond after acceleration. The former of the electron pulses is used to produce an analysis light by coherent radiation, while the latter is used as an irradiation pulse. The analysis laser light is not used in the system, resulting in a low time jitter between the electron pulse and the analysis laser. A time resolution of femtosecond/attosecond can be expected in the system.

In order to generate double-decker electron pulses, we developed an double pulse laser injection system at the exit of the Nd:YLF laser as shown in Fig.4(a). The picosecond laser beam of Nd:YLF laser was divided into two by a beam splitter. The time interval of the two pulse should be the integral multiple of 350ps, because the RF gun is operated by 2856MHz (1period=350ps) RF. The time delay was adjusted to 1.4 ns in the experiment.

By using the laser injection system, we successfully measured the double-decker electron beams. Fig.4(b) shows the double beam profiles at the exit of the RF gun, the linac, the pulse compressor. The beam transverse normalized emittance of 3~4mm-mrad was observed for both beams at an electron charge of 0.5nC/pulse. The beam energy was 31MeV. Finally, the electron pulses was compressed down to be 380fs(rms). In next step, the double-decker electron beams are utilized for studies of ultrafast reactions by means of pulse radiolysis.

4. Spur Reactions and Nanofabrication

The spatial resolution of the nanofabrication is limited with bulk reactions which

occur after the spur reactions in material. The reaction mechanism of the spur and bulk reactions were studied by using the time-space reaction analysis based on a Monte Carlo simulation. As an example, the electron thermalization processes in n-hexane and CCl_4 were investigated. The electron thermalization distance distributions were simulated and compared with a spur model based on diffusions of a thermalized electron and a positive ion (geminate ion pair, generated by the ionization) in irradiated non-polar liquid under the Coulomb attracting potential. Comparing the electron thermalization distance distributions in n-hexane and CCl_4, where the electron thermalization distance distribution in CCl_4 was obtained with dissociative electron attachment, we found that the electron thermalization distance in CCl_4 (2.5 nm) is obtained to be shorter than that in n-hexane (6.6 nm), resulting in a small spur size. It is due to the reactions of the electron before its thermalization. The result indicates that the reduction of the spur size should be important in the next nanofabrication.

Publications

International Conferences

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Generation of a Femtosecond Electron Photocathode Linac for Nanoscience and Nanotechnology, J. Yang, T. Kozawa, Y. Yoshida, and S. Tagawa, 9th European Particle Accelerator Conference, Lucerne, Switzerland, July 5-9, 2004.

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Generation of Low-emittance Femtosecond Electron Pulse with Laser Photocathode RF Linac, J. Yang, K. Kan, H. Tomosada, K. Takeya, T. Kondo, T. Yamamoto, T. Kozawa, Y. Honda, Y. Yoshida, and S. Tagawa, 8th SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, Dec. 6-7, 2004.

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	6 papers
Linear accelerator Meeting in Japan	4 papers
Physic Society of Japan	1 paper
Atomic Energy Society of Japan	7 papers
Applied Physic Society of Japan	1 paper
Symposium on RF Electron Gun	1 paper
Symposium on TIARA	2 papers

Academic Degrees

Master Degree of Engineering

H. Tomosata Femtosecond pulse radiolysis based on equivalent velocity spectroscopy

T. Shimada Study of positron annihilation in polymers by using AMOC

T. Fujii Development of modulator for slow positron generation

Sponsorship

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

Y. Yoshida	Basic Research on Subfemtosecond and Attosecond Pulse Radiolysis	¥8,900,000

Collaborative Researches

Y. Yoshida	JAERI Tokai	High time resolution study on radiation-induced reaction in nanostructure
	JAERI Tokai	Pulse radiolysis study on Lanthanide solution
	JAERI Takasaki	Mechanism of micro sphere generation in phenol solution
	JAERI Takasaki	Radiation damage of new recycle chemical system
	Sumitomo Heavy Industries, Ltd	Research on photocathode RF gun and high brightness electron beam
	Hiroshima Univ.	Photonic crystal radiation

Department of Quantum Beams for Nanotechnology

Professor, Director: Goro ISOYAMA
Associate Professor: Yoshihide HONDA
Research Associate: Norio KIMURA

Outlines

For the purpose of research and development of quantum beams and their applications, which are expected to form bases for nanotechnology, we conduct research, in this department, on electron linear accelerators (linacs) for pursuing higher performance and development of quantum beams as well as on new measurement methods for the nanometer range and applications using the beams. The pulse radiolysis technique is commonly used for the reason that the understanding of chemical reaction processes induced by incident electrons helps the fabrication in nanometer range. In order to study the ultra high-speed reactions taking place in nanometer range, development of the linac with higher quality is desired. The high-energy linac is also used to produce a slow positron beam. Positrons have the nature to concentrate in holes and free volumes in materials and consequently measurements using positrons are considered to be an effective method to analyze the sizes and distributions of free volumes. The positron beam is highly expected to play an important role in the analysis of not only the sizes but also the distributions of nanometer size spaces and free volumes in porous materials such as polymers. We conduct research on analyses of free volumes, surfaces and interfaces in thin polymer films, which will be useful to develop new materials by promoting better understandings of interactions of positrons and positroniums, which are formed by an electron and a positron as a bound state, with materials. In order to make these analyses practical, we also conduct researches on the production of intense slow positron beam and on the process of making high brightness beam and short-pulsed beam using an electron linac, and on the development of new measurement methods. We take part in management and operation of the Radiation Laboratory, which has the experimental apparatuses for these studies.

Current Research Programs

1. Operation of the S-band Linac

There are two kinds of S-band linacs in Radiation Laboratory. The S-band linac consisting of three acceleration tubes has been used with the energy of about 100 MeV to produce a slow positron beam. In last fiscal year, a new RF-gun equipped S-band linac was installed. The electric power sources were shifted to another room in another floor and the waveguids and related cables were also extended. In this fiscal year, test operation of positron related S-band linac was started. The several troubles were removed during the conditioning, however, the discharges in the waveguides were not so improved in short period. The troubled parts in the waveguides were replaced with the silver-coated ones and the discharges were suppressed. However, we could not start positron experiment as it took a lot of time to suppress the discharges.

One klystron was replaced because of lack of RF power.

2. Generation of the Intense Slow Positron Beam

Positrons have been used by means of positron annihilation lifetime spectroscopy and Doppler broadening measurement of energy spectrum of annihilation γ-ray. The simultaneous measurement of these methods, named AMOC (Age-Momentum Correlation), and coincidence Doppler broadening measurement are effective to study annihilation processes of positrons and positroniums in matter. However the counting rate of annihilation γ-rays becomes low in such the measurements. Thus the intense short-pulsed positron beam is desirable. Furthermore, the small beam size is better for the positron diffraction experiments. Concerning a positron beam based on linac, one of the important factors determining the intensity is the conversion efficiency of a moderator, which moderates kinetic energy of positrons and produces slow positrons. We designed and fabricated a new moderator to improve the conversion efficiency and to reduce beam diameter. This new moderator was equipped and used in this fiscal year. The produced positron beam with this new moderator could be transported to the experimental room for positron experiments. The estimation of the intensity of positron beam is underway.

3. Study of the Annihilation Process of Ortho-Positronium Using AMOC

The lifetime of ortho-positronium (*o*-Ps)is valuable parameter to estimate the size of spaces in polymer, however, there is a possibility that the local electric field mainly introduced by functional groups in polymer, leads to localization of positron and influences on the lifetime of positron and Ps. The information about annihilation electron is very important to investigate a possibility of preferential annihilation in material. The lifetime of positron in polymer is usually divided into three components, i.e. lifetimes of para-positronium (*p*-Ps), free positron and *o*-Ps. The energy spread in the photopeak of annihilation γ-rays, which is represented by S-parameter, consists of these three kinds of annihilation γ-rays in adding to the resolution of detector. The S-parameter is defined by the ratio of central area to whole area of photopeak, e.g. the larger S means the narrower energy spread, leading to the lower electron momentum. These contributions in S cannot be separated in usual measurement, however, AMOC (simultaneous measurement system of the lifetime of positron and the energy spread of annihilation γ-rays) makes it possible and so AMOC is suitable to study the annihilation process of positron and Ps.

The AMOC experiments were carried out in this year for polystyrene related materials using ^{22}Na source to investigate the influence of functional groups on S-parameters. The compressed powders after refinement were used as the samples. Results showed that S-parameters for pick-off annihilation process were greater than those for free annihilation process in all samples. The AMOC data showed remarkable results that the momentum of electrons annihilating with positron is larger even for the samples containing many low energy electrons such as polystyrene and polymethylstyrene. Furthermore, the mapping of S-parameter relating to the pick-off annihilation vs. lifetime showed that the plots could be grouped into halogenated and non-halogenated ones, however, the correlations were the same, i.e. the S-parameters became larger according to the increase of lifetimes in each groups. Direct comparison between two samples can be made by subtracting photopeaks of annihilation γ-rays which are extracted from the energy spectrum relevant only to the o-Ps, using AMOC data.

The estimations of potential distribution in polymers were made using molecular orbital theory. The overall analysis of experimental data and simulation is underway.

4. Influence of Functional Groups on Positronium Formation in Polymers

A positronium (Ps) is produced competitively with electron capture by solvents and additives and recombination of electron and ion pair in spur model. Therefore the reaction rate of electron capture can be inferred from the number of Ps. We examined the effects of substituent on the yield of *o*-Ps in polystyrene and poly(methyl methacrylate) and their derivatives. The results of positron annihilation lifetime spectroscopy (PALS) measurement showed that halogen and benzyl substituents are brought into a lowering of the *o*-Ps yield. These groups are generally called the functional group, since they are always the site of chemical reactivity. These findings suggest that free electrons, generated by the irradiation, react with polystyrenes and poly(methyl methacrylates) containing a functional group. According to the spur model, this reaction is occurred competitively with the formation of Ps. The observed results clearly indicate that free electrons react with functional groups before the formation of *o*-Ps (few ps). It can therefore be presumed that PALS is useful to investigate the radiation chemistry at the early stage.

Publications

Original Papers

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Positron Annihilation Lifetime Spectroscopy as a Novel Method to Investigate the Radiation Chemistry of Resists, N. Kimura, K. Miyamoto, Y. Honda, G. Isoyama, S. Tagawa , 8th SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Dec. 6-7, 2004, Osaka, Japan

Study on Positron Annihilation Process in Nano Vacancy, T. Shimada, N. Kimura, Y. Honda, Y. Yoshida, 8th SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Dec. 6-7, 2004, Osaka, Japan.

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Femtosecond Electron Pulse with Laser Photocathode RF LinacJ. Yang, K. Kan, H. Tomosada, K. Takeya, T. Kondo, T. Yamamoto, T. Kozawa, Y. Honda, Y. Yoshida, and S.

Tagawa, 8th SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Dec. 6-7, 2004, Osaka, Japan.

Equivalent Velocity Spectroscopy for Improvement of Time Resolution on Electron Beam Pulse Radiolysis System, T. Kondoh, H. Tomosada, K. Kan, J. Yang, T. Yamamoto, T. Kozawa, Y. Honda, Y. Yoshida, and S. Tagawa, Third 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" International Symposium. March 9-10, 2004, Makino, Japan.

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Upgrade of the L-band Linac at ISIR, Osaka University for Highly Stable Operation, R. Kato, G. Isoyama, S. Kashiwagi, T. Yamamoto, S. Suemine, Y. Yoshida, Y. Honda, T. Kozawa, S. Seki and S. Tagawa, FREE ELECTRON LASERS 2003, Proc. of the 25th International Free Electron Laser Conference and the 10th FEL Users Workshop, Tsukuba, Ibaraki, Japan, September 8-12, 2003, Elservier 2004, pp.II-43 - II-44.

Publications in Domestic Meetings

Japanese Society of Radiation Chemistry	2 papers
Linear Accelerator Meeting	3 papers
The Atomic Energy Society of Japan	3 papers

Department of Beam Science for Nanotechnology

Professor: Seiichi TAGAWA
Associate Professor: Shu SEKI
Associate Professor: Takahiro KOZAWA

Outlines

The targets of the present department are the establishment of initiatives of quantum beams for nanoscience and nanotechnology. Quantum beams mean both beams such as photons and beams inducing interactions with materials in the nanoscopic level of quantum mechanics. The beams potentially have an applicability for imaging with ultra fine patterns, and the present department aims to use the fine patterns as the probes for nano-structured material sciences and devices.

Current Research Programs

1. Electronic Structure and Physical Properties of Molecular Nano-wires

Polysilanes and polygermanes containing only silicon and germanium in the backbone attracted considerable attention because of their interesting electro-optical properties which are due to conjugated bondings in the main chain. The electronic structure of conjugated skeleton is investigated in the present program, which leads to an improvement the physical properties of the conjugated polymers.

2. Reaction Mechanisms in Polymeric Materials for Micro- and Nano-electronics

Chemically amplified resist system is one of the most practical candidates in the future technology in semiconductor fabrication. Reaction mechanisms in the system are analyzed upon exposure to electron beams, X-rays, and laser beams to design a new lithography technique in the present program.

3. 1-D Nanostructure Formation by Charged Particle

High density energy deposition by charged particles causes non-homogeneous crosslinking reaction of polysilane derivatives within a nano-sized cylindrical area along an ion trajectory, and gives β-SiC based nano-wires of which sizes (length, thickness) and number densities are completely under control by changing the parameters of incident ion beams and molecular sizes of target polymers.

4. Gas Evolution from Nanoelectronic Materials

Gas evolved from resists deposits on optical system during lithographic exposure, leading to serious optical contamination. This is therefore one of the most grave issues in next generation optical lithography. Dependence of gas evolution on resist structure was investigated by using quadrupole mass spectrometer in order to obtain information on design of contamination-free resist.

5. Radiation-Induced Reactions in Nanoscopic Region

Electron beam lithography has the highest resolution among top-down writing

systems. The ultimate spatial resolution is closely related to the reaction mechanism of resist materials. The relation between a spatial resolution and reaction mechanisms was investigated by a subpicosecond pulse radiolysis.

6. Radiation-Induced Reactions in Aromatics

Aromatics have high radiation resistance. The characteristic has been used in electron beam lithography. Especially, the radiation–induced reaction of aromatics is important to improve and understand the resist materials. Primary process of irradiated aromatics from nano- to picosecond time scale is investigated by electron beam pulse radiolysis.

Publications

Original Papers

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157 nm-Induced Resist Outgassing Studied by Films Thickness Loss and in-situ Quadru-pole Mass Spectrometer, Y. Matsui, S. Seki, S. Tagawa, S. Kishimura, and M. Sasago: J. Photo-polym. Sci. Technol. 17 (2004) 671.

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Inhomogeneous Distribution of Crosslinks in Ion Tracks in Polystylene and Polysi-lanes, S. Seki, S. Tsukuda, K. Maeda, Y. Matsui, A. Saeki, and S. Tagawa: Phys. Rev. B 70 (2004) 144203.

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Charged Particle and Photon-Induced Reactions in Polymers, S. Tagawa, S. Seki and T. Kozawa: Charged Particle and Photon Interactions with Matter (Marcel Dekker, New York, 2004) 551-578.

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Philadelphia, USA, May 20-22, 2004.

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Modelling and Simulation of Chemically Amplified EB, X-ray and EUV Resist Processes, *T. Ko-zawa, A. Saeki and S. Tagawa, 48th International Conference on Electron, Ion and Pho-ton Beam Technology and Nanofabrication 2004, June 1-4, San Diego, USA.

Subpicosecond Pulse Radiolysis Study on Geminate Ion Recombination Process in n-Dodecane, *Y. Yoshida, A. Saeki, T. Kozawa, J. Yang and S. Tagawa, 14th International Conference on Ultrafast Phenomena, 25-30 July, 2004, Niigata, Japan.

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Dynamics of Positive Charge Carriers on Si Chains of Polysilanes, *S. Seki, Y.

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Formation of Nanowires Based on π-Conjugated Polymers by High-Energy ion Beam Irradia-tion, S. Tsukuda, S. Seki, M. Sugimoto, S. Tagawa, Microprocess and Nanotechnology Confer-ence2004, Osaka, Japan, October 26-29, 2004.

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Contributions to International Conferences and Journals

	(Conference Organizer)	
S. Tagawa	Microprocess and Nanolithograph Conference	(Organizing Committee)

Publications in Domestic Meetings

The Japan Society of Radiation Chemistry	7 papers
Chemical Society of Japan	6 papers
Atomic Energy Society of Japan	5 papers
The Japan Society of Applied Physics:	6 papers
Society of Polymer Science, Japan	4 papers

Sponsorship

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

S. Tagawa	Femtosecond Pulse Radiolysis Study on Radiation-Induced Reactions in Nanoscopic Region	¥7,200,000

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

S. Seki	Isolated Nanowire Formation along Ion Projectiles	¥3,200,000

Grant-in-Aid for Scientific Research, Encouragement of Young Scientist (B)(2)

S. Seki	Development of Plateless Conductivity Measurement in Iosolated Nanostructure and Molecular Element	¥1,700,000
T. Kozawa	Creation of Ultimate Nano Process by Femtosecond Pulse Radiolysis	¥1,300,000

Entrusted Research

S. Tagawa	Advanced Semiconductor Engineering and Technology	Development of Color Film Dosimeter Based on Advanced

		Radiation Chemistry
S. Tagawa	Advanced Semiconductor Engineering and Technology	Reaction Mechanism in Chemically Amplified Resist Materials
S. Tagawa	Semiconductor Leading Edge Technology Inc.	Study on Solvent for Immersion Lithography

Cooperative Research

S. Tagawa, S. Seki	Japan Atomic Energy Research Institute	Ion Beam Pulse Radiolysis in Condensed Matter

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: El Mustapha MOUADDIB (2004.6.28 – 2004.10.4)

Outlines

The studies focus on theoretical analysis of compounded omnidirectional stereo vision system which consists of a single camera and multiple omnidirectional mirrors.

Achievements

We defined the criteria and the methodology for evaluating the compounded omnidirectional vision. The omnidirectional vision simulator was built on a standard personal computer. The result was published on the proceeding of international conference on Robotics and Automation 2005.

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

The following lectures were given.

“Computer Vision in the CREA lab: Some results” (July.28, 2004).

The summary of the lecture is as follow.

Perception is a central question for autonomy of humans and animals and of course for the machines and more particularly for mobiles robots. From all different approaches to perceive the world, vision is the most important. Specific means of perception were developed by engineers, given more precision in perception (Coded and structured light vision for instance) and especially a better adapted and more complete perception (like omnidirectional vision). Mouaddib showed his research work done in this approach based on the using of integral invariants calculated starting from the images (omnidirectional images) and from the movement of the robot. Outline of his talk is presentation of the laboratory, omnidirectional vision, and structured and coded light projection system.

Department of Ultrafast Spectroscopy of Nanostructures

Guest Associate Professor: Marek NOWICKI (2004.11.6. – 2005.1.11.)

Outlines

Understanding of structure and property of materials in nanoscale is one of important targets for nanotechnology. The STM-induced luminescence spectroscopy provides an optical spectroscopy with a nanometer scale resolution afforded by STM. This technique is also useful to study the operation of an organic light-emitting diode, in which one of the cathode is the tip, at nanometer dimensions. In this study, we have developed a system of STM-induced luminescence measurement, and carried out spectroscopic measurements of molecular luminescence on the metal surfaces.

Achievements

In a STM system, photons emitted from the tip-sample tunnel junction were collected using an optical fiber (core diameter 1 mm, numerical aperture 0.5), which was placed near the tip-sample junction (about 1 mm) and oriented 45° relative to the sample surface normal. Then the collected photons were guided into a spectrograph (HoloSpec f/2.0, Kaiser Optical Systems, Inc.) through the optical fiber. The spectra were recorded with an ICCD detector (intensified charge coupled device, ICCD-1024E, Princeton Instruments, Inc.). Using this spectrograph and ICCD, the photon detection system was capable of covering a wavelength range of 400 ~ 900 nm. To cut the background lights, a double-light-shielding box was made. The STM-induced luminescence on a nanometer scale has been successfully measured in air by using the system. This is achieved in collaboration with professor H. Iwasaki.

Department of Ultrafast Spectroscopy of Nanostructures

Guest Professor: Werner SCHLEGEL (2005.1.12 – 2005.3.11)

Outlines

The department aims to analyze the nanoscale structure functioning at ultra-fast speed.

Achievements

The ENH1-PKCε-PKD1 signaling complex involving cardiac hypertrophy was analyzed using neonatal rat cardiomyocytes.

The following lecture was given.

"Intracellular Signaling and Gene Expression. Immediate early response gene transcription is dynamically controlled at the level of elongation." (Feb. 15, 2005)

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.

- Solidification of Sn-Ag-Cu solder balls
- Reliability establishment of Sn-Zn solder in humid atmosphere
- TEM of Ni-P plating interfaces and identification of nano-structure
- Synthesis and characterization of calcium phosphate-AMP composite material
- HREM observation and simulation of BCN fullerene materials

Mizoguchi Lab.

- Extension of the preliminary nanotech-ontology developed last year.
- Development of prototype system for supporting creative design of nanomaterials at the functional level.
- Development of function decomposition trees for material design of nano-particles/films
- Revision of Cell Signaling Networks Ontology (CSNO), and reorganization of the related knowledge using CSNO

Yoshida Lab.

- Development of ab initio molecular dynamics simulation (OSAKA-2003-Nano)
- Electronic excitation induced nano-structure-process design (From graphite to Nano-diamond)
- Tc-enhanced Co-doping and Nano-scale delta-doping method for diluted magnetic semiconductors.
- Materials design of high-efficient thermo-electric Nano-materials.
- Design of nano-structure gettering center in silicon.
- Mechanism of CN-treatment of dangling-bond in amorphous silicon and high efficient photovoltaic solar cels.

Department of Nanomaterials and Environmentally Conscious Technology

Professor:	Katsuaki SUGANUMA
Associate Professor:	Takeo OKU
Research Associates:	Shunro YAMAGUCHI, Masahiro INOUE
Research Assistant:	Kimiaki TANIHATA
Post Doctoral Fellow:	Kim KEUN-SOO, Yamato HAYASHI
Research Promotion Staff:	Mariko HATAMURA
Graduate Students:	Kim YOUNG-SUN, Masayuki NAKATA, Ichihito NARITA, Jeono LEE, Motoki KANENO, Toshiko NAKAGAWA, Kimihiro YAMANAKA, Takayuki IMANISHI, Atsushi NISHIWAKI, Yuusuke YAMASAKI, Naruhiro KOI
Support Staff:	Naomi URAYAMA, Kozue IDE

Outlines

Through nanotechnologies and knowledge for organic/inorganic materials, we are conducting the development of environmentally conscious fine technologies for electronics packaging area, i.e., lead-free soldering and conductive adhesives, the composite materials based on metals and intermetallic compounds, the structural characterization of BCN fullerenes, and the bio mimetic bone structures. We set our route towards contributions to our society in near future.

Current Research Programs

1. Environmentally Conscious Electronics Packaging

The development of environmentally conscious fine technologies for electronics packaging area, i.e., lead-free soldering and conductive adhesives, and the establishment of scientific basis required for those technologies are our goals. For lead-free soldering, we found that solidification phenomena become critical rather than the conventional leaded alloys. By using simulation and the in-situ observation method for soldering solidification, the mechanisms and the various factors influencing on CSP defect formation became clear. The suppression method of solidification defects was proposed. Sn-Zn alloy is one of the candidates as low temperature solder. The degradation mechanism of the joint under humid atmosphere was clarified. The composite mixture rules were adopted for understanding the properties of nanopaste and conductive adhesives and it was proved that the interface bonding nature has key role for understanding the practical conductive adhesives.

2. Atomic Structure Analysis and Electronic Properties of New B-C-N Fullerene Materials

Synthesis and HREM structure analysis of the new B-C-N 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 by self-assembled monolayers

Publications

Original Papers

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Molecular orbital calculations of hydrogen storage in carbon and boron nitride clusters, N. Koi and T. Oku: Sci. Tech. Adv. Mater., 5 (2004) 625-628.

Formation and atomic structure of $B_{12}N_{12}$ nanocage clusters studied by mass spectrometry and cluster calculation, T. Oku, A. Nishiwaki and I. Narita: Sci. Tech. Adv. Mater., 5 (2004) 635-638.

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Microstructures and magnetic properties of boron nitride- and carbon-coated iron nanoparticles synthesized by a solid phase reaction, H. Tokoro, S. Fujii and T. Oku: J. Mater. Chem., 14 (2004) 253-257.

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Contributions to International Conferences and Journals

K. Suganuma	TMS Annual Meeting, Committee of Phase Stability, Phase Transformation, and Reactive Phase Formation in Electronic Materials
K. Suganuma	Electronics Goes Green 2004 International Advisory Board
K. Suganuma	Electronic Components and Technology Conference (ECTC), Materials Processing Committee
K. Suganuma	High Density Packaging and Components Failure Analysis(HDP'04), International Advisory Board

Publications in Domestic Meetings

Japan Institute of Electronics Packaging	4papers
Japan Institute of Metals	3papers
Others	4papers

Academic Degrees

Doctor Degree of Engineering

I. Narita	Synthesis, structure analysis and magnetic properties of BN nanocapsules encaging magnetic nanoparticles

Master Degree of Engineering

T. Imanishi	Study on interconnect Reliability of low temperature lead-free solders in Sn-Ag-In system.
A. Nishiwaki	Structure and propecties of BN nanomaterials
Y. Yamazaki	Development of super-flexible wiring technology for realizing soft skin sensor of humanoid robots.

Sponsorship

Grant-in-Aid for JSPS Research Fellowships for Young Scientists

I.Narita	Structures and Properties of New BCN Nanoclusters.	¥1,000,000
K-S. Kim	Development and curing characteristics of metal nano paste for fine printed circuits.	¥1,200,000

Other Allocations

K. Suganuma	21st Century COE Program	¥4,000,000
I. Narita	21st Century COE Program for Young Scientists	¥1,000,000

Entrusted Research

Japan Society for the Promotion of Science

K. Suganuma	Investigation on academic research trends in the field of metallic material engineering.	¥3,500,000

NEC Corporation

K. Suganuma	Study on interconnect and wiring technologies using	¥1,050,000

conductive adhesives.

Other Research Fund

The Foundation for Technology Promotion of Electronic Circuit Board

K. Suganuma	Investigation on present states and perspectives of electronic packaging technology using conductive adhesives.	¥100,000

The foundation Kinki area invention center

T. Oku	Study in synthesis and properties of new BN nanotubes and nanocage materials.	¥150,000

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Outlines

The primary activities of this department are theoretical study of electronic properties of nanomaterials, which are different from those of bulk crystals. The first-principles calculations based on the density-functional theory are used, in order to exclude any empirical parameters. More importantly, we wish to predict unknown features of new nanostructure and design novel nanomaterials. Lead of the area of material research from the theoretical viewpoint is one of our goals.

At the same time, efforts are continued to keep development in the methodologies in order to solve difficult problems encountered in this field, because nanoscience is different from study of bulk materials with many respects.

Current Research Programs

Spintronics and Materials Design using Semiconductor Nanostructures

We have developed hybrid method for calculating Curie temperature (T_C)of dilute magnetic semiconductors (DMS) by combining first-principles electronic structure calculations and Monte Carlo simulation. Curie temperature of several DMS systems is well reproduced by the present method. From electronic structure calculations, it is found that magnetic exchange interactions are very short ranged if impurity bands are formed in the gap and double exchange dominates. In this case, for small concentrations percolation effect is very important and it is indispensable to take disorder into account in T_C calculations. To these impurity band systems belong (Ga, Mn)N, (Ga, Cr)N, (Zn, Cr)Te, (Zn, Cr)Se and (Zn, Cr)S and many others. On the other hand, if impurity d states are well below the valence band and p-d exchange dominates, exchange interactions are weak but long ranged. To these localized moment systems belong (Ga,

Mn)As, (Ga, Mn)Sb and so on. Even in these systems, the percolation effect is still important for small concentrations. For both systems, it is found that Curie temperatures calculated by the present hybrid method show almost perfect agreement with experimental values if homogeneous impurity distribution is achieved in experiments.

We have also developed electronic structure descriptions of DMS systems beyond local density approximation. First, we calculate electronic structures (Ga, Mn)N and (Ga, Mn)As by LDA+U method. It is found that in (Ga, Mn)As LDA predicts Mn d-states at too high energy and p-d exchange interaction is more important in LDA+U calculations. In (Ga, Mn)N, LDA+U predicts unoccupied Mn d-states at higher energy. This effect suppresses anti-ferromagnetic super-exchange interaction and calculated Curie temperatures are higher than LDA results for large concentrations. More '*ab initio*' implementation for beyond-LDA method is developed by using pseudo-SIC prescription proposed by Filippetti et al. Electronic structure of Co-doped ZnO is calculated by this method. Calculated density of states well corresponds to recent photoemission experiment.

We have also proposed materials design for new DMS systems. Based on first-principles electronic structure calculations, ferromagnetism of transition-metal doped $CuAlO_2$ is discussed for realizing transparent half-metallic ferromagnetic semiconductor. It is also shown that B- or P-doped diamond shows ferromagnetism by co-doping with H. For this kind of exotic DMS systems, C- or N-doped BaO, CaO, MgO, SrO and SiO_2 are proposed. Carrier co-doping method with size compensation in Mn-doped nitrides is shown to be very effective for enhancing their Curie temperature.

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. We have simulated the enhancement of the atomic diffusion of boron (B), hydrogen (H), and oxygen (O) in silicon under the electronic excitation.

Materials Design 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 thermo-electric material ($ZT>3$) and transparent superconductivity upon slightly p-type or heavily p-type doped CuAlO2.

Fermiology of Highly Correlated Electron Systems by FLAPW-LSDA+U Method

The new *ab initio* method for the electric structure calculation of highly correlated electron systems are developed by using the FLAPW-LSDA+U method and taking into account the spin-orbit interactions. We have calculated the Fermi surface of ferromagnetic CeSb and $CeRh_3B_2$, and analyzed the Fermi surfaces and compared with detail of the experimental data. We have understand the complex Fermi surfaces of

these highly correlated electron systems.

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, generalized-gradient approximation was implemented. This improves in many cases accuracy for the cohesive properties of solids. For molecular dynamic simulation, a bias technique has been applied in order to accelerate the processes. This method is particularly suitable for simulation of diffusion.

Material Design for Superconductivity of Icosahedron-based Boron

Growing interests are addressed to solid boron and its compounds because of its superconducting transition at high pressures. We have succeeded to make the phase diagram of boron in the pressure-temperature space, and determined the transition pressure and temperature of a and b phases. For b phase, a disorder in the atom arrangement is known. This property is also reproduced in our calculation. Those results form the foundation for superconductivity-material research.

Material Design for Light-induced-degradation Proof Amorphous Silicon

Application of amorphous silicon to solar cells encounters a big problem of light-induced degradation. In order to overcome this problem, a new technique of CN incorporation has been proposed. By simulating the formation of bonds of CN in *a*-Si, we found that insertion of CN ion near dangling bonds has additional role to recover a broken network, which should be responsible to depress light-degradation. Further study on stability of the bond at high temperatures was examined, with result that the CN bond is quite stable.

Material Design for Cu Gettering in Crystal Si

Cu atom exhibits very fast diffusivity in crystal Si. This is a serious problem in Si technology, *i.e.*, impurity contamination. In order to solve this problem, gettering method by introducing dopant atoms is frequently used. The mechanism of fast diffusion of Cu and gettering by B has been clarified. Our dynamic simulation well reproduces experimental data on the gettering efficiency. This constitutes the basis of surveying more efficient gettering centers.

Material Design for Selective Diffusion of Dopant Atoms in Crystal Si

In Si processes, as the device size is small, the demand for accurate controlling diffusion of impurities becomes more severe. An idea of controlling diffusion of individual dopant atoms is use of IR irradiation with the frequency tuned with the local vibration mode of impurity atoms. How effective this method is not yet clear. Our simulation can effectiveness of this method. It is shown that the resonant effect on the vibration is found for B and O, while not for P.

Publications

Original Papers

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"Thermoelectric materials using natural super-lattices and its control method" H. Katayama-Yoshida, H, Funashima, I. Hamada, H. Harima, A. Yanase, JP2004-085615

"Transparent Ferromagnetic Alkali-chalcogene Compound Containing Transition Metal or Rare-earth Metal, and Control Method of Ferromagnetic Properties." H. Katayama-Yoshida, M. Seike, K. Sato, A. Yanase, PCT/JP04/003373

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"Magnetic Random Access Memory (MRAM)" H. Katayama-Yoshida, K. Sato, JP Patent Registered No. 3571034

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“Ferromagnetic p-type single crystalline ZnO and production method” H. Katayama-Yoshida, K. Sato, EP Patent No.1219731

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Ferromagnetism and Curie Temperature of V-doped Nitrides, *V. A. Dinh, K. Sato and H. Katayama-Yoshida, International Symposium on the Creation of Novel Nanomaterials (ISCNN04), Osaka, Japan, January 20-22, 2004

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Hyperfine Interactions and Magnetism of 3d impurities in magnetic semiconductors (invited), *K. Sato, International Workshop on Nanomaterials, Magnetic Ions and Magnetic Semiconductors studied mostly by Hyperfine Interactions (IWNMS - 2004), Vadodara (Baroda), Gujarat, India, February 10-14, 2004

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Enhancement of Tc by Carrier Codoping Method with size compensation for Nitride (GaN), *V. A. Dinh, K. Sato and H. Katayama-Yoshida, Internaional Conference on Nanospintronics Design and Realization (ICNDR 2004), May 24-28, 2004. Kyoto, Japan

Computer modeling and simulation for nanospintronics: prediction vs. experiment (Invited), *H. Katayama-Yoshida, 3rd International Conference "Computational Modeling and Simulation of Materials" & Special Symposium "Modeling and Simulating Materials Nanoworld" (CIMTEC), Sicily, Italy, May 30- June 4, 2004.

Exchange interactions and Curie temperatures in diluted magnetic semiconductors (Invited), *K. Sato, P. H. Dederichs, H. Katayama-Yoshida, 3rd International Conference "Computational Modeling and Simulation of Materials" & Special Symposium "Modeling and Simulating Materials Nanoworld" (CIMTEC), Sicily, Italy, May 30-June 4, 2004.

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Ab initio Study of Native Point Defects in Delafossite $CuAlO_2$, *I. Hamada and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Theoretical Prediction of Curie Temperature in (Zn, Cr)S, (Zn, Cr)Se and (Zn, Cr)Te by First Principles Calculations, *T. Fukushima, K. Sato, H. Katayama-Yoshida and P. H. Dederichs, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Self-interaction Corrected First Principles Calculations for ZnO-based Diluted Magnetic Semiconductors, *M. Toyoda, H. Akai, K. Sato and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Theoretical Investigation on the Electronic Structure of Alq_3/Al Interface, *S. Yanagisawa and Y. Morikawa, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Ferromagnetism and magnetic Transition Temperatures *Tc* of Nitride Ternary-based Dilute Magnetic Semiconductors, *V. A. Dinh, K. Sato and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004

Tc-enhanced without Codoping by Avoiding Nearest Neighbor Mn-Mn Site in (Ga, Mn)N, (Ga, Mn)P, (Ga, Mn)As and (Ga, Mn)Sb, *Y. H. Chang, K. Sato, H. Katayama-Yoshida and C. H. Park, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Low Temperature Ferromagnetism in (Ga, Mn)N, *K. Sato, P. H. Dederichs and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Pressure Dependence of Band Gap in Solid Boron, *A. Masago, K. Shirai and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Bandstructure Calculations and Fermi Surfaces of Ferromagnetic CeSb, *K. Yamauchi, A. Yanase, H. Harima and H. Katayama-Yoshida, SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, December 6-7, 2004.

Contributions to International Conferences and Journals

H. Katayama-Yoshida	3rd International Conference on Physics and Application of Spin-related Phenomena in Semiconductors: PASPS3 (International Advisory Committee and Program Committee)
H. Katayama-Yoshida	1st International Conference on Nanospintronics Design and Realization: ICNDR (Organizing Committee and Program Committee and Proceedings Editor)
H. Katayama-Yoshida	23rd International Conference on Defects in Semiconductors

	: ICDS23 (Conference Chair)
K. Shirai	23rd International Conference on Defects in Semiconductors : ICDS23 (Organizing Committee)
H. Katayama-Yoshida	The third international school and conference on spintronics and quantum information technology: Spintech III (Conference Chair)
K. Sato	The third international school and conference on spintronics and quantum information technology: Spintech III (Organizing Committee)
H. Katayama-Yoshida	International Conference on Magnetism: ICM2006 (Organizing Committee)

Publications in Domestic Meetings

The Physical Society of Japan	17papers
The Japan Society of Applied Physics	5papers

Academic Degrees

Doctor Degree of Science

K. Yamauchi	Theoretical Study on Electronic Bandstructure of Ferromagnetic Ce Compounds

Master Degree of Science

M. Toyoda	Development of self-interaction corrected electronic structure calculation method and study on electronic and magnetic state in ZnO-based dilute magnetic semiconductors"
T. Fukushima	Theoretical Prediction of Curie temperature in (Zn,Cr)S, (Zn,Cr)Se and (Zn,Cr)Te by First Principles Calculations.

Master Degree of Engineering

H. Kizaki	First-principles materials design of $CuAlO_2$ based dilute magnetic semiconducting oxide
K. Kenmochi	Materials Design of Transparent and Half-Metallic Ferromagnetic Semiconductors without Transition Metal Elements

Sponsorship

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

Entrusted Research

Special Coordination Funds for Promoting Science and Technology

H. Katayama-Yoshida	Design and Fabrication of Nanospintronics Computational Nanomaterials and Device Design	¥27,164,000

Ministry of Education, Culture, Sports, Science and Technology
Grant-in-Aid for the Creation of Innovations through Business-Academic-Public Sector Cooperation

H. Katayama-Yoshida	Research on selective and low-temperature impurity diffusion in semiconductor by infra-red laser excitation	¥4,500,000

Japan Science and Technology Corporation

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

Japan Science and Technology Corporation

H. Katayama-Yoshida	Research and development Applying Advanced Computational Science and Technology (H. Akai) Computational Nano-materials Design

New Energy and Industrial Technology Development Organization (NEDO)

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

Cooperative Research

H. Katayama-Yoshida	Institute for Materials Research, Tohoku Univ.	Spintronics in II-VI based ferromagnetic semiconductors
H. Katayama-Yoshida	SPring8	Mechanism of New Materials Fabrication Using Electronic Excitation
H. Katayama-Yoshida	International Institute of Advanced Study	Materials Science and System Design
H. Katayama-Yoshida	Jülich Institute (Germany)	Computational Materials and Devices Design for Nanospintronics

Department of Nano-Bio Intelligent Systems Science

Professor: Riichiro MIZOHUCHI
Research Associate: Kouji KOZAKI

Outlines

The research on development of Nano-Bio intelligent help system, data mining from the nano-bio data, systematization of nano-bio knowledge, ontology engineering is conducted aiming at amalgamation of knowledge research and nano-biotechnology. Special emphasis is placed on systematization of nanotechnology.

It is highly expected that bridging the gap between several domains of nanotechnology to facilitate creative design by enabling reuse of knowledge across these domains. Ontology engineering is an advanced AI technology which has a great potential to achieve the goal. This is why we have been intensively involved in ontology engineering. The concrete objectives include development of nanotechnology ontology, development of function achievement ways for nanomaterials and development of a system for supporting creative design of nanomaterials at the functional level together with an ontology engineering environment.

Current Research Projects

1. Development of 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. Its brief explanation is given below.

(a)Four top-level categories

－Top-level categories are composed of *Process, Structure, Function and Matter*

(b)Distinction between *Structure* and *Shape*

－*Shape*: figure or form attributed to a primitive and concrete thing such as sphere.

－*Structure*: abstract concept representing topological relation among elements

(c)Function and quality

－*Quality*: Characteristics attributed to matters

－*Function*： Teleological conceptualization of a role played by thing

2. Development of a System for Supporting Creative Design of Nanomaterials

Aiming at bridging required functions stated by engineers in industries and basic functions(or quality) and at facilitating the creative design, systematization of function achievement ways in a particular domain and development of a support system of

functional design of materials are currently conducted in parallel.

In general, a function is achieved by performing multiple sub-functions. The achievement is supported by a physical principle and/or structure of the device or materials which is conceptualized as *Function achievement way.* The decomposition is continued concerning each sub-function to eventually form a function decomposition tree for each device/material. There exist multiple ways of functional decomposition so that the computer can help device/material designers to help their design process by giving possible alternative ways stored in a function achievement way server.

We have conducted the cross-over collaboration between us and Niihara & Kawai Labs. The concrete results on this collaboration include development of functional decomposition trees of Nano-film and nano-particle together with a prototype system of creative design support system using a function achievement way server we developed. In addition we investigate effects and problems of the framework and the system through some real examples.

3. An Environment for Ontology Development and its Use

We developed ***Hozo,*** an ontology engineering environment, which enables a user to build and use an ontology and instance models. It consists of Ontology editor, Concept factory and ontology server.

Ontology editor

It provides a friendly user interface as well as powerful functions necessary for ontology building and editing.

Concept factory

A guidance system based on AFM(Activity-First Method) has been implemented to guide ontology developers who build an ontology from technical documents.

Ontology server

A server for ontologies and models has been developed. It is based on the client-server architecture and enables human/computer agents to access them through internet.

We improved the Graphical User Interface of Ontology editor and published the software at the web site (http://www.hozo.jp).

Publications

International Conferences

A Success Story of Ontological Engineering in a Japanese Company - Engineering Knowledge Management Based on Functional Ontology (Invited), *R. Mizoguchi, KEST04, Beijin, P.R.China, September 17-19, 2004

Ontological integration ofdata models for cell signaling pathways, *T. Takai-Igarashi,

and R. Mizoguchi, GIW2004, Tokyo, Dec.13-15, 2004.

Contributions to International Conferences and Journals

Riichiro Mizoguchi	The 3rd International Semantic Web Conference (ISWC2004) （Organizing committee chair）
Riichiro Mizoguchi	European Project on SEKT(Steering committee member)
Riichiro Mizoguchi	International Conference on Intelligent Tutoring Systems(ITS2004)(PC member)
Riichiro Mizoguchi	The 9th Ibero-American Conference on Artificial Intelligence IBERAMIA'04(PC member)
Riichiro Mizoguchi	European Semantic Web Conference (ESWC2004) (PC member)
Riichiro Mizoguchi	The Fifth International Symposium on Tools and Methods of Competitive Engineering (TMCE 2004) (PC member)
Riichiro Mizoguchi	Workshop on Applications of Semantic Web Technologies for E-learning (Workshop Co-Chair)
Riichiro Mizoguchi	The 2004 IFIP International Conference on Intelligence in Communication Systems (INTELLCOMM 04) (PC member)
Riichiro Mizoguchi	The World Congress on Computers, AIAI2004 (PC member)
Riichiro Mizoguchi	European KAW Conference (EKAW 2004) （PC member）
Riichiro Mizoguchi	Secretary of International Artificial Intelligence in Education Society
Riichiro Mizoguchi	Asia-Pacific Society for Computer in Education (APSCE) (Board member)
Riichiro Mizoguchi	International Journal of Applied Ontology (Editorial board)
Riichiro Mizoguchi	International Journal of Artificial Intelligence in Education （Editorial board）
Riichiro Mizoguchi	International Journal of Advanced Engineering Informatics （Editorial board）
Riichiro Mizoguchi	International Journal of Web Semantics（Editorial board）
Riichiro Mizoguchi	International Journal of Computer and Engineering Management（Editorial board）
Riichiro Mizoguchi	International Journal of Web Engineering and Technology (Editorial board)
Kouji Kozaki	Evaluation of Ontology-based Tools 3rd International Workshop (EON2003) (PC member)

Publications in Domestic Meeting

Japanese Society for Artificial Intelligence	2 papers
Information Processing Society of Japan	1 papers

Sponsorship

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

R. Mizoguchi	Management and Utilization of Knowledge Contents of Design and Manufacturing based on Function	¥4,900,000

Cooperative Research

R. Mizoguchi	The Society of Chemical Engineers, Japan	New Energy and Industrial Technology Development Organization Nanotechnology Materials Program "Structuralization of Materials Technology Know-How" Nanotechnology ontology studies and development of an ontology server	¥5,250,000

Department of Nanotechnology Transfer

Guest Professor: Ramasamy RAMARAJ (2004.5. - 2004.9.)

Outlines

The electron transfer reaction from nucleophilic anions to the 1-pyrenesulfonic acid radical cation generated via a resonant two-photon ionization process in the Nafion membranes was investigated with transient absorption measurements. The decrease in electron reaction rate, compared with that obtained in bulk water, was interpreted in terms of the anionic Hofmeister effects. The effects of hydrophobic organic cations such as tetrabutylammonium ion and tetraethylammonium ion exchanged into the Nafion membranes were also examined.

Achievements

The electron transfer reaction from nucleophilic anions such as SCN^-, N_3^-, I^-, and Br^- to 1-pyrenesulfonic acid radical cation ($Py^{\bullet+}SA^-$) generated via a resonant two-photon ionization process in the Nafion membranes was investigated with transient absorption measurements. The apparent quenching rates observed in Nafion (k_q^{Nf}) were almost 2-4 orders smaller than those observed in the bulk solutions (k_q^{bulk}). The attenuation factor (AF), which is defined as log (k_q^{Nf}/k_q^{bulk}), decreased in the order $SCN^- > N_3^- > I^- > Br^-$. According to the anionic Hofmeister effects, the hydrophobic ions such as SCN- are more likely to be found in the vicinity of $Py^{\bullet+}SA^-$ in the fluorocarbon-ionic cluster interfacial region. Hydrophobic organic cations such as tetrabutylammonium ion and tetraethylammonium ion exchanged into the Nafion membranes inhibit the incorporation of anions into the Nafion membrane.

This work has been published in *J. Phys. Chem. B.*

"Hofmeister Effects on the Electron Transfer Reactions of 1-Pyrenesulfonic Acid Radical Cation with Nucleophilic Anions in Nafion Membrane"

T. Tachikawa, R. Ramaraj, M. Fujitsuka, and T. Majima

J. Phys. Chem. B **2005**; *109*(8); 3381-3386.

Department of Nanotechnology Transfer

Guest Professor: Thomas WIRTH (2004.9.-10.)

Outline

The aim of this department is to transfer research results to the industry, and to create new industrial field.

Achievements

In order to develop novel methods and reagents for stereoselective oxidative functionalizations, the following research topics have been discussed.

1. **Design and synthesis of new chiral selenium electrophiles and their application in selenenylation reactions of alkenes.**
2. **Synthesis of efficient chiral electrophilic reagents on solid support.**
3. **Development of new chiral hypervalent iodine reagents and their use in stereoselective reactions.**
4. **Total synthesis of furofuran lignans.**
5. **Investigations on reagent controlled stereoselective halocyclization reactions.**
6. **Computational chemistry: Calculations of reaction pathways, mechanistic transition states and intermediates.**

Department of Nanotechnology Transfer

Guest Associate Professor: Jay A. LAVERNE (2004.10.-11.)

Outlines

The aim of this department is to elucidate the physico-chemical processes in condensed media by use of ultrafast spectroscopic techniques associated with whort pulses of quantum beams.

Achievements

Heteroaromatic compounds are not only the universal organic materials but also high-functional reagents which promote efficiently the catalytic reactions of organic systems. Neutral radicals, anionic and cationic species of the heteroaromatic compounds were produced quantitatively by electron pulse irradiation, and the entire reaction scheme of the species was clarified not only by transient spectroscopy and kinetic traces of the species but also by analysis of the final products. The present study clarified the yields, dynamics, and reactions of the intermediates at every stage of the reactions, giving new insights into the potentials of the heteroaromatic compounds as matrices of new efficient organic reaction systems.

Department of Nanotechnology Transfer

Guest Associate Professor : Dae Won CHO (2004.12. - 2005.2.)

Outlines

Molecular switch with ultra-fast response is an important component of nanotechnology. For the characterization of the response of the molecular switch, ultra-fast spectroscopy is important. In the present study, development of the system, which measures sub-picosecond fluorescence lifetime, was attempted. Switching behavior of molecular dyad composed of oligothiophene and acceptor was also investigated by the fluorescence lifetime measurements.

Achievements

The fluorescence lifetime in sub-picosecond region was measured by observing sum-frequency generation of fundamental light of Ti:Sapphire laser and sample fluorescence, which was generated by excitation with the second harmonic generation. The resolution of the system was 300 fs. By employing this system, fluorescence lifetime of the dyad composed of oligothiophene and acceptor was successfully estimated to be 600 fs. Since the conventional time-correlated single photon counting method cannot measure the lifetime in sub-picosecond region, the present estimation system is quite powerful tool to estimate fluorescence lifetime of ultra-fast molecular switch. Furthermore, the present system is applicable to the other functional molecular systems such as dendritic light energy harvesting systems.

Department of Nanotechnology Transfer

Guest Associate Professor: Mohamed El-MAGHRABY (2005.3.–2005.6.)

Outlines

The purpose of this work is development of Nano-structure formation process which is the new approach (bottom-up technique), opposite to the old top-down technique that uses the electron beam lithography and the forcused ion beam method.

We are going to control the array of metallic corpuscles which works as catalyst sites, make it possible to control the crystal growth (nuclear formation) of the wide gap semiconductor.

Furthermore, we aim at the realization of the DOS (density of states) localization and appearance of quantum fuction with controlling the diameter of metallic catalyst corpuscles which can change the diameter of nanorod.

In addition, we will try to application of spintronics devices by doping the magnetic elements and by heterostructure band engineering with the band gap adjustment etc..

Achievements

I have prepared to set up a Hot Wall Pulsed Laser Deposition system in order to deposit ZnO, ZnMgO and ZnCoO nanometer thin films. These films are very important for applications in light emitting diodes devices, and expected to low its working voltage with better performance.

Publications

Original Papers

Influence of Gamma Radiation on the Absorpion Spetra and Optical Enrgy of Li-Doped ZnO Thin Films, A. Abu EL-Fadl, El-Maghraby Mohamed , Galal A. Mohamed : Cryst. Res. Technol., 39 (2004) 143-150.

High Quality Growth of TiO_2 Thin Films from Its Precursor Solution by New Sol-Gel Method, El-Maghraby Mohamed, Y. Nakamura, Y. Fujii, M. Kamiya, S. Rengakuji : Electrochemistry, 72 (2004) 455-457.

International Conference

Preparation and Characterization of Phosphoric Acid-doped Triglycine Sulphate Crystals, *El-Maghraby Mohamed, The fourth International Conference on Solid State Crystals, Zakopane, Poland, May 16-20, 2004

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.

Achivements

- 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.
- XAFS and Raman nano-structural characterization of ferromagnetic semiconductors.
- Time-resolved characterization of PL emission from ferromagnetic semiconductors.
- SPM nano-characterization of sub-micron Si devices.

Department of Advanced Nanostructural Characterization

Professor: Yoshihiko HIROTSU
Research Associates: Muneyuki NAITO

Outlines

The purpose of this department is to develop new electron microscopy methods to characterize atomic structures, atomic bonding and electronic structures of functional nanomaterials in order to contribute to the development and realization of novel functional materials and devices.

Current Research Programs

Development of comprehensive structure analysis of amorphous materials using advanced transmission electron microscopy

The precise structure analyses of amorphous materials have been performed using high-resolution transmission electron microscopy, energy filter, nanobeam electron diffraction and imaging plate techniques. Structure models of amorphous materials have been constructed taking advantage of computer calculation such as reverse Monte Carlo calculation on the basis of structural information of both real and reciprocal spaces obtained by advanced TEM techniques.

Transmission Electron Microscopy Study on Amorphous Ge-Sb-Te Thin film

Phase-change optical recording provides rewritable data storage, such as DVD-RW and DVD-RAM optical disks, taking advantage of the differences in reflectance and transmittance of amorphous and crystalline phases of recording materials. Crystalline clusters were frequently observed in the high resolution TEM images of as-deposited amorphous Ge-Sb-Te thin film. Autocorrelation function analysis of the TEM image indicated the similarity between the structures of crystalline clusters and rhombohedral Sb. Atomic pair-distribution functions obtained from halo NBED intensity showed a development of local structure whose atomic configuration is similar to that of the rhombohedral Sb.

Electron Diffraction Study on Soft Phonon Mode in Ge-Sb-Te thin film

We have found nonradial diffuse streaks in electron diffraction patterns from laser-induced crystalline phase of Ge-Sb-Te thin film using nanobeam electron diffaraction. Considering the crystal structure of Ge-Sb-Te, three equivalent zigzag atomic chains exist with chain directions of $[2\bar{2}01]$, $[\bar{2}021]$ and $[02\bar{2}1]$. The directions of diffuse streaks were always perpendicular to those of zigzag atomic chains. In addition, the intensities of diffuse streaks depended on the angles between the directions of incident electron beam and zigzag atomic chains. These results coincide with the features of nonradial diffuse streaks explained by the viewpoint of lattice dynamics. The conspicuous diffuse streaks show a softening of atomic chains in the Ge-Sb-Te crystal, which would influence rapid phase transition of this material.

Publications

Original Papers

Nanoscale Phase Separation in an $Fe_{70}Nb_{10}B_{20}$ Glass Studied by Advanced Electron Microscopy Techniques, T. Hanada, Y. Hirotsu and T. Ohkubo: Mater. Trans. 45 (2004) 1194-1198.

Nanoscale Phase Separation in Metallic Glasses Studied by Advanced Electron Microscopy Techniques, Y. Hirotsu, T. Hanada, T. Ohkubo, A. Makino, Y. Yoshizawa and T. G. Nieh: Intermetallics 12, 1081-1088 (2004).

Local Structure Analysis of Ge-Sb-Te Phase Change Materials Using High-resolution Electron Microscopy and Nanobeam Diffraction, M. Naito, M. Ishimaru, Y. Hirotsu and M. Takashima: J. Appl. Phys. 95 (2004) 8130-8135.

Local Structural Change of Amorphous Ge-Sb-Te Thin Film during Annealing, M. Naito, M. Ishimaru, Y. Hirotsu and M. Takashima: J. Non-Cryst. Solids 345/346 (2004) 112-115.

Review Papers

Nanoscale Phase Separation in amorphous Fe-B alloys, T. Hanada, A. Hirata, Y. Hirotsu, T. Ohkubo and V. Bengus, Materia Japan 43 (2004) 1002 (in Japanese).

Books

Nanostructure of amorphous alloys, Y.Hirotsu, T.Ohkubo and M.Matsushita:
"Novel Nanocrystalline Alloys and Magnetic Nanomaterials", Edited by B.Cantor, Series in Materials Science and Engineering, Institute of Physics Publishing, Bristol, 2004, p 16-41.

International Conferences

Two dimensionally dispersed Fe/FePd nanocomposite particles synthesized by electron beam deposition (Invited), *Y. Hirotsu, K. Sato and J. Kawamura, Int'l Conf. New Frontiers of Process Science and Engineering in Advanced Materials, Kyoto, November 24-26, 2004.

Growth and atomic ordering of hard magnetic $L1_0$-FePt, FePd and CoPt alloy nanoparticles studied by transmission electron microscopy (Invited), *Y. Hirotsu and K. Sato, ICCG&D2004, Seoul, November 10-14, 2004.

Fabrication and Structural Analysis of Oriented $L1_0$-FePt and FePd Nanoparticles (Invited), *Y. Hirotsu and K. Sato, The First Asia Forum on Magnetics, Okinawa, September 21-24, 2004.

Local Structure Analysis of Metallic Glasses Using HREM and Electron Diffraction (Invited), *Y. Hirotsu, T. Ohkubo and T. Hanada, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Structure and metallurgy of alloy nanoparticles in Fe-Pd system (Invited), *Y. Hirotsu and K. Sato, $L1_0$ Ordered Intermetallic and Related Phases for Permanent Magnet and Recording Applications, Colorado, USA, August 15-20, 2004.

Nanostructures of binary and ternary Fe-B based glasses studied by HREM and electron diffraction (Invited), *Y. Hirotsu, Akihiko Hirata, Tadakatsu Ohkubo and A.Makino, 5th Polish-Japanese Symposium on Advanced Methods of Materials Characterization, Niedizca, Poland, August 29-September 1, 2004.

Structural Analysis of As-sputterd and Melt-quenched Ge-Sb-Te Thin Film (Poster), *M. Naito, M. Ishimaru, Y. Hirotsu, and M. Takashima, 8th Asia-Pacific Conference on Electron Microscopy, Kanazawa, June 7-11, 2004.

Contributions to International Conferences and Journals

Y. Hirotsu	8th Asia-Pacific Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	16th International Conference on Electron Microscopy (Organizing Committee)
Y. Hirotsu	International Conference on New Frontiers of Process Science and Engineering in Advanced Materials (Advisory Committee)
Y. Hirotsu	5th Japan-Polish Joint Seminar on Materials Analysis (Organizing Committee)
Y. Hirotsu	11th International Symposium on Metastable, Mechanically Alloyed and Nanocrystalline Materials (Advisory Committee)

Publications in Domestic Meetings

The Japan Institute of Metals	4 papers
The Japan Society of Applied Physics	1 paper

Sponsorship

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

Y. Hirotsu	In situ observation of atomistic structures in metallic liquid and metallic glass	¥30,100,000

Grant-in-Aid for Scientific Research (S)

Y. Hirotsu	Fabrication and characterization of hard magnetic alloy nanoparticles produced by vapor quenching	¥33,400,000

Entrusted Research

Y. Hirotsu	Special Coordination Funds for Promoting Science and Technology on "Nanohetero Metallic Materials" from the Ministry of Education,	Electron Diffraction Local Structure Analysis of Nanohetero Metallic Materials	¥15,057,000

Y. Hirotsu	Culture, Sports, Science and Technology, Japan NEDO (Advanced Materials Technology Utilizing Glassy Metals for Commercial Uses)	Nano-structure Analysis for the Evaluation of Mechanical Properties in Glassy Metals	¥3,150,000

Department of Advanced Characterization for Nano-Processing

Professor: Katsumi TANIMURA
Associate Professor: Jun'ichi KANASAKI

Outlines

Electronic excitations often induce structural instability on solid surfaces, such as structural changes, diffusion, and desorption of constituent atoms. The electronic excitations, which induce and promote atomic processes with site-sensitive rates, can be a promising methods for creating surfaces and nano-scaled structures possessing new properties and functions that are not achieved by conventional thermal processes. Our targets are to understand completely the fundamentals of underlying physics, and finally to establish advanced surface- and nano-processing technologies fully exploiting unique features of electronic-excitation effects.

Current Research Projects

Structural Instability of Semiconductor Surfaces Induced by Electron-Beam Irradiation

It has been demonstrated that laser beam removes individual atoms on semiconductor surfaces, triggered by localization of two holes generated by photo-induced interband electronic transitions. Structural instability of the surfaces is also induced by low-energy electron-beam irradiation, but its mechanism is still controversial. Whether the mechanisms of electronic bond breaking under laser excitation and under electron beam irradiation are the same or qualitatively different is an important problem to be studied for a general understanding of the structural instability under electronic excitation.

Our group conducted scanning tunnelling microscopic studies of electron-irradiated Si(111)-(7x7) surfaces and have revealed that excitation with 15-50 eV electron beams removes adatoms from individual surface sites, resulting in the formation of vacancies. The site-sensitivity of electron-induced vacancy formation is essentially the same as that for laser excitation, suggesting strongly that the final process of the bond breaking is the same for the two excitation sources. The rate of vacancy formation is proportional to the excitation intensity, which is quite different from the case for laser-excitation, and the cross section of bond breaking depends strongly on the primary energy of incident electrons. We have elucidated an important role of surface plasmon excitation on the electron-induced bond breaking process.

Structural Instability of Graphite Surfaces Induced by Pulsed Laser Excitation

Graphite is a quasi two-dimensional material made of sp_2-bonded hexagonal carbon layers that are weakly coupled to neighboring layers. To investigate characteristic features and mechanisms of structural changes induced by electronic excited states on this surface can be a key for understanding the dimensionality dependence of structural instabilities by electronic excitations.

Our group carried out STM observations of structural changes on Highly Oriented Pyrolytic Graphite (HOPG) surfaces induced by $\pi - \pi^*$ transitions under femtosecond

laser irradiation. We have shown a definite threshold intensity above which structural changes are induced, indicating multiple excitation effects are included for the electronic process. It has been found that plane fragments are removed above the threshold intensity, resulting in the formation of nano-scaled vacancy-clusters on the surface. We have also observed quite a new surface phase around the vacancy-clusters, which has never been found. These results indicate a strong relationship between the surface phase transition and removal of plane fragments under excitation.

Creation of Defect-Free Surface New Phase by Electronic Excitations

Our approach is based on recent investigations of laser- and electron-induced structural changes on semiconductor surfaces: electronic excitations can induce emission of atoms selectively from the topmost layer of the surfaces. The techniques can be of use for creating defect-fee surfaces of atomic-scale smoothness by removing surface top layer, which generally contains much more atomic-scaled defects compared to the bulk layers.

Laser-induced atomic removal from Si(001) 2x1 surface reveals a relatively defect-free layer, with a '1x1'periodic structure, which has been never produced by conventional thermal process. So far we could remove surface atoms up to 95 % of total atomic sites of the surface. Now we are searching the excitation conditions of wavelength, flux, and pulse width, for completely removing remaining surface atoms and for preparing the defect-free surface.

Development of Novel Methods for Characterizing Physical Properties of Atomic-Scale Defects on Semiconductor Surfaces

As the dimension of electronic devices is reduced towards nano-scale regime, it becomes of greater importance to understand the structural and electronic properties of atomic-scaled defects on surfaces. Our group developed a novel method to analyse quantitatively charge transfer around point defects on semiconductor surfaces.

We introduce differential image (ΔI) analysis, where difference between images of a unit cell including an adatom-vacancy and those of a perfect unit cell has been analysed as a function of sample-bias voltage. The differential image provides a map of the changes in surface charge densities at respective surface sites induced by the defect. The analysis has revealed three important features. First, the adatom vacancy induces prominent change in ΔI in the filled-state images, while little in the empty-state images. Second, the vacancies induce significant changes in the un-faulted half (UFH) unit but not in the faulted half (FH) unit. Third, the spatial range of vacancy-induced change is limited at most to neighboring atoms. Since the change of charge density distribution is not observed in the empty-state images, the results can be due to electronic charge transfer between dangling bonds around the vacancies, not due to lattice distortion that would induce the change in images of both biases. Therefore, the clear difference in ΔI between the two half units demonstrates a direct evidence that significant amount of charge transfer is operative among dangling bonds of atoms around the vacancies in UFH unit, while the charge transfer is negligible in FH unit.

Publications

Original Papers

Electronic Bond Rupture of Si-Dimers on the Si(001)-(2x1)., J. Kanasaki, K. Katoh, Y. Imanishi, and K. Tanimura: Applied Physics A79 (2004) 865-868.

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Femtosecond Time-Resolved Reflection Spectroscopy of Photoinduced Ionic-Neutral Phase Transition in TTF-CA Crystals, K. Tanimura: Physical Review B70 (2004) 144112-1-11.

Temperature-Dependent Yield of Frenkel Pairs Generated by Valence Excitation in NaCl., K. Tanimura and W. P. Hess: Physical Review B69 (2004) 155102-1-7.

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Review Papers

Local bond breaking on semiconductor surfaces induced by laser beam (in Japanese): J. Kanasaki and K. Tanimura: OYO BUTURI 74 (2004) 485-489.

International Conferences

Site-Selective Yields of Laser-Induced Bond Rupture of Si-Dimers on Si(001)-(2x1) Surface, *J. Kanasaki, K. Katoh, Y. Imanishi, and K. Tanimura, The 16th International Vacuum Congress / The 12th International Conference on Solid Surfaces / The 8th international Conference on Nanometer-Scale Science and Technology, Venice, Italy June 28-July 2, 2004.

Photoinduced Structural Instability on Si(111)-(2x1), *E. Inami and K. Tanimura, The 10th International Workshop on Desorption Induced by Electronic Transitions (DIET10), Susono, Japan, Nov. 8-11, 2004.

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Contributions to International Conferences

K. Tanimura 10th International Workshop on Desorption Induced by Electronic Transitions (DIET-10) (Susono, 2004.11-3-8) (Chairman, International Steering Committee)

K. Tanimura SANKEN International Symposium on Scientific and Industrial Nanotechnology 2004(SISSIN-2004)(Osaka, 2004.12.6-7) (Organizing Committee)

J. Kanasaki 10^{th} International Workshop on Desorption Induced by Electronic Transitions (DIET-10) (Susono, 11.3-8)
(Local Organizing Committee)

Publications in National Meetings
The Physical Society of Japan 10 papers

Sponsorship

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

(B)(2)

K. Tanimura	Mechanisms of Photoinduced Structural Phase Transitions of Quasi One-Dimensional Organic Crystals Studied by Time-Resolved Raman-Scattering Spectroscopy	¥5,300,000
J. Kanasaki	Photo-Induced Bond Breaking and New Phase Formation on Si(001) Surface	¥3,900,000

Department of Quantum Materials and Devices Characterization

Professor: Hajime ASAHI
Research Associate: Yi-Kai ZHOU

Outlines

The department of quantum materials and devices characterization makes researches on the new characterization methods and the characterization of the 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 nanocharacterization methods for the physical properties of quantum materials.

・ Development and application of nanocharacterization methods for the structural and physical properties of quantum devices including next generation LSIs.

・Development and application of nanocharacterization methods for the device properties of quantum devices.

Current Research Programs

Nanocharacterization 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, our group succeeded in the growth of GaCrN and observed the room temperature ferromagnetism as well as the PL emission. In 2004, we have investigated their optical and structural properties to clarify the origin of this PL emission. Time-resolved PL measurements showed that the emission from GaCrN is originated from the band-to-band (exciton) transition in GaCrN. On the other hand, the PL emission from GaGdN is due to the f-f atomic level transition at Gd atoms. EXAFS measurements on GaCrN revealed that Cr atom substituted the Ga site for the GaCrN with Cr concentration of 1%-2.6% and that for the GaCrN with Cr concentration of larger than 3% the NaCl-type CrN is formed. Raman scattering experiment suggested that the coexistence of cubic GaCrN, which was confirmed with the TEM experiment.

Nano-Characterization of Structure and Functions of GaN Nanorods

GaN is expected to be promising to the application to the electric field emission electron sources because of a small electron affinity. In 2004, we have made clear the structural properties and the electric field emission characteristics of the GaN grown on Si substrate. AFM observation showed that the grown GaN has a nanorod structure with a diameter of about 50 nm and a roughness of about 12 nm. Furthermore, the cross sectional TEM revealed that GaN grows as columnar-like and is well-elongated along c-axis with a good crystallinity. It also showed that there exist sharp tip-like structures on the surface of some nanorods. We observed the very small threshold voltage of 1.25 V/μm and a high field emission current density as high as 2.5 mA/cm^2 at an applied

field of 2.5 V/μm for the electron emission.

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. We have demonstrated that the STM has the potential to characterize the 2D potential profile for the cross sections of 100 nm MOSFETs with nanometer scale resolution.

Publications

Original Papers

Observation of photoluminescence emission in ferromagnetic semiconductor GaCrN, M. Hashimoto, H. Tanaka, R. Asano, S. Hasegawa, and H. Asahi: Appl. Phys. Lett. 84 (21) (2004) 4191-4193.

Growth and characterization of new III-V-based magnetic semiconductors for application to semiconductor spintronics devices (Invited), H. Asahi, Y.K. Zhou, M. Hashimoto, H. Tanaka and S. Emura: Proceedings of 12th International Workshop on The Physics of Semiconductor Devices (Eds. by K.N. Bhat and A. DasGupta, 2004 Narosa Publishing House, New Delhi, India) 1095-1100.

Migration Enhanced Epitaxy (MEE) Growth of Five-Layer Asymmetric Coupled Quantum Well (FACQW) and Its Cross-sectional STM Observation, J.H. Noh, S. Hasegawa, T. Suzuki, T. Arakawa, K. Tada and H. Asahi: Physica E 23 (2004) 482-486.

Wavelength control of 1.3-1.6 μm light emission from the quantum dots self-formed in GaAs/InAs short-period superlattices grown on InP (411)A substrates, J. Mori, T. Nakano, T. Shimada, S. Hasegawa and H. Asahi: J. Appl. Phys. 96 (3) (2004) 1373-1375.

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1.3-1.5-μm-wavelength GaAs/InAs superlattice quantum-dot light-emitting diodes grown on InP(411)A substrates, J. Mori, T. Nakano, T. Shimada, S. Hasegawa and H. Asahi: Jpn. J. Appl. Phys. 43(7A) (2004) L901-L903.

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Optical properties of GaN-based magnetic semiconductors, Y.K. Zhou, M.S. Kim, X.J. Li, S. Kimura, A. Kaneta, Y. Kawakami, Sg. Fujita, S. Emura, S. Hasegawa and H. Asahi: J. Phys.: Condens. Matter. 16 (48) (2004) S5743-S5748.

Magnetic, optical and transport properties of GaN-based ferromagnetic/nonmagnetic heterostructurtes, M.S. Kim, Y.K. Zhou, X.J. Li and H. Asahi: J. Phys.: Condens. Matter. 16 (48) (2004) S5711-S5716.

Ramana scattering characterization of GaN-based spintronics materials, N. Hasuike, H. Fukumura, H. Harima, K. Kisoda, M. Hashimoto, Y.K. Zhou and H. Asahi: J. Phys.: Condens. Matter. 16 (48) (2004) S5811-S5814.

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Review Papers

Temperature-independent lasing wavelength TlInGaAs/InP semiconductor laser diodes, H. Asahi: in *Investigation Report on Power Semiconductor Laser Application Technology*, IEE Japan Technical Report 961 (IEE Japan, 2004) 36-39.

Ferromagnetic semiconductors and their synthesis, H. Asahi: in *From Introduction to Magnetism to Spintronics Materials and Devices*, Introductory Seminar to Spintronics 3 (2004) 53-61.

Books

Structural and optical characterization of self-formed quantum dots, S. Gonda and H. Asahi: in *Encyclopedia of Nanoscience and Nanotechnology*, Eds. by J.A. Schwarz, C. Contescu and K. Putyera (Marcel Dekker, Inc., 2004) 3227-3235.

International Conferences

New III-V-based magnetic semiconductors and their optical and magnetic properties (Invited), *H. Asahi, Y.K. Zhou, M. Hashimoto, R. Asano and H. Tanaka, SPIE Optoelectronics 2003 International Symposium, San Jose, CA, USA, January 25-31, 2003.

Temperature-stability of lasing wavelength for TlInGaAs/InP DH laser diodes and 77K CW operation, *A. Fujiwara, H.J. Lee, A. Imada, K. Mukai, S. Hasegawa and H. Asahi, Second 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" and 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, January 13-14, 2004.

Luminescence from Gd Site in Dilute Magnetic Semiconductor GaGdN, *S. Emura, Y.K. Zhou, M. Hashimoto, H. Tanaka, M.S. Kim, S. Kimura, S. Shanthi, X.J. Li, N. Teraguchi, A. Suzuki, A. Yanase, and H. Asahi, Second 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" and 7th SANKEN International Symposium on

Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, January 13-14, 2004.

Tunneling magnetoresistance effect in magnetic semiconductor heterostructure DyN/GaN, *M.S. Kim, Y.K. Zhou, X.J. Li and H. Asahi, Second 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" and 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, January 13-14, 2004.

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GaN-based magnetic semiconductors for nanospintronics (Invited), *H. Asahi, Y.K. Zhou, M. Hashimoto, M.S. Kim, X.J. Li, S. Emura and S. Hasegawa, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

Optical properties of GaN-based magnetic semiconductors, *Y.K. Zhou, M.S. Kim, X.J. Li, S. Kimura, A. Kaneta, Y. Kawakami, Sg. Fujita, S. Emura, S. Hasegawa and H. Asahi, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

Magnetic, optical and transport properties of GaN-based ferromagnetic/nonmagnetic semiconductor heterostructures, *M.S. Kim, Y.K. Zhou, X.J. Li and H. Asahi, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

Raman scattering characterization of GaN-based spintronics materials, *H. Fukumura, N. Hasuike, H. Harima, K. Kisoda, M. Hashimoto, Y.K. Zhou and H. Asahi, International Conference on Nanospintronics Design and Realization, Kyoto, Japan, May 24-28, 2004.

Gas source MBE growth of Tl-containing semiconductors and their application to temperature–insensitive wavelength laser diodes (Invited), *H. Asahi, H.J. Lee, A. Fujiwara, A. Imada, K. Mukai and S. Hasegawa, 16th International Conference on Indium Phosphide and Related Materials, Kagoshima, Japan, May 31-June 4.

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GaAs-InAs short-period superlattice/InP(411)A self-formed quantum dot light emitting diodes with 1.3-1.5 μm light emission, *T. Shimada, J. Mori, S. Hasegawa and H. Asahi,

16th International Conference on Indium Phosphide and Related Materials, Kagoshima, Japan, May 31-June 4.

Photoluminescence emission from room temperature ferromagnetic semiconductor GaCrN, *H. Asahi, M. Hashimoto, H. Tanaka and S. Hasegawa, International Workshop on Nitride Semiconductors 2004, Pittsburgh, USA, July 19-23, 2004.

Electric field emission characteristics of GaN nanorods grown on Si substrates with native oxides, *T. Yamashita, S. Nishida, S. Hasegawa and H. Asahi, International Workshop on Nitride Semiconductors 2004, Pittsburgh, USA, July 19-23, 2004.

Magnetic, optical and transport properties of GaCrN-based ferromagnet/nonmagnet/ferromagnet trilayer structure, *M.S. Kim, Y.K. Zhou, S. Kimura, S. Emura, S. Hasegawa and H. Asahi, 13th International Conference on Molecular Beam Epitaxy, Edinburgh, UK, August 22-27, 2004.

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Polycrystalline GaN for field electron emitter application (Invited), *S. Hasegawa, S. Nishida, T. Yamashita and H. Asahi, International Conference on Polycrystalline Semiconductors 2004, Potsdam, Germany, September 5-10, 2004.

Formation of local ferromagnetic area on GaAs by focused Mn ion beam implantation, *M. Kasai, J. Yanagisawa, H. Tanaka, S. Hasegawa, H. Asahi, K. Gamo, and Y. Akasaka, 14th International Conference on Ion Beam Modification of Materials, Monterey, California, USA, September 5 - 10, 2004.

Magnetoresistance in GaCrN-based ferromagnet/nonmagnet/ferromagnet trilayer structures, *Y.K. Zhou, M.S. Kim, H. Kimura, S. Emura, S. Hasegawa and H. Asahi, 13th Semiconducting and Insulating Materials Conference, Beijing, China, September 20-25, 2004.

Magnetic, electric and optical properties of AlN and GaN doped with rare-earth element Gd, *S.W. Choi, Y.K. Zhou, M.S. Kim, S. Kimura, S. Shanthi, S. Emura, S. Hasegawa and H. Asahi, 3rd Asian International Symposium on the Science of Engineering Ceramics, Osaka, Japan, October 31-November 3, 2004.

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Emission spectra from AlN and GaN doped with rare earth elements (Invited), S. Emura, *S.W. Choi, S. Kimura, M.S. Kim, Y.K. Zhou, N. Teraguchi, A. Suzuki, A. Yanase, and H. Asahi, International Conference on Rare Earths in Nara, Nara, Japan, November 7-12, 2004.

Electron field emission from polycrystalline GaN nanorods (Invited), *S. Hasegawa and H. Asahi, 2004 Fall International Symposium on Crystal Growth and Devices, Seoul, Korea, November 10-13, 2004.

Evaluation of device configurations through different cross-sectional planes of 0.1 μm MOSFETs by scanning tunneling microscopy/spectroscopy, *S. Hasegawa, W. Doi, A. Yabuuchi and H. Asahi, 12th International Colloquium on Scanning Probe Microscopy, Izu-Atagawa, Shizuoka, December 9-11, 2004.

Luminescence properties of GaN and AlN doped by rare earth elements, *S. Emura, S.W. Choi, S. Kimura, S. Kobayashi, M.S. Kim, S. Shanthi, Y.K. Zhou, N. Teraguchi, A. Suzuki and H. Asahi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, December 6-7, 2004.

Effect of chromium doping on the luminescence properties of GaCrN on sapphire, *S. Shanthi, M. Hashimoto, S. Kimura, Y. K. Zhou, S.W. Choi, M. S. Kim, S. Emura, S. Hasegawa and H. Asahi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, December 6-7, 2004.

Cross-sectional scanning tunneling microscopy study of 100 nm MOSFETs through the different cross sections, *W. Doi, A. Yabuuchi, S. Hasegawa and H. Asahi, Sanken International Symposium on Scientific and Industrial Nanotechnology 2004 -Advanced Characterization for Nanomaterials, Nanodevices and Nanoprocessing-, Osaka, Japan, December 6-7, 2004.

Contributions to International Conferences and Journals

H. Asahi	16th International Conference on Indium Phosphide and Related Materials (International Steering Committee member)
H. Asahi	International Conference on Nanospintronics Design and Realization (Organizing Committee member)
H. Asahi	International Workshop on Nitride Semiconductors 2004 (International Advisory Committee member)
H. Asahi	12th International Colloquim on Scanning Probe Microscopy (Steering Committee member, Publication Committee member)
H. Asahi	14th International Conference on Molecular Beam Epitaxy (Organizing Committee Vice-Chair, Program Committee Chair)
H. Asahi	17th International Conference on Indium Phosphide and Related Materials (International Steering Committee member, Program Committee member)
H. Asahi	SANKEN International Symposium on Scientific and Industrial Nano-Technology 2004 (Organizing Committee member, Local Arrangement Chair)
H. Asahi	Third International Symposium on 21st Century COE "Towards Creating New Industries Based on Inter-Nanoscience" (Organizing Committee member, Publicity and Publication Chair)

H. Asahi	International Workshop on Nitride Semiconductors 2006 (International Advisory Committee member)
H. Asahi	SpinTech III (Organizing Committee member)
H. Asahi	2005 International Conference on Solid State Devices and Materials (Program Committee member)
H. Asahi	Japan. J. Appl. Phys. (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	22 papers
Electronic Materials Symposium	2 papers
Symposium on PASPS	3 papers

Sponsorship

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

Y.K. Zhou	Study on Synthesis of GaN-Based Transparent Ferromagnetic Semiconductors	¥2,600,000

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

H. Asahi	Study on Applications of Polycrystalline Nitride Semiconductors to Field Emission Electron Source and Visible Fluorescent Substance	¥4,200,000

Other Research Fund

H. Asahi	MEXT Special Coordination Funds for Promoting Science and Technology (H. Kasai)	Design and Invention of Spintronics ¥18,717,000

Open Laboratory

Professor:	Hitoshi TABATA (chair) Hideo NAKAJIMA Katsuyuki TANIZAWA Yasushi YAGI
Technical Staff:	Akira YOSHIDA, Kimihiro NORIZAWA
Supporting Staff:	Manami HASE

Outlines

Open Laboratory supports to 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. This Open Laboratory is shared by the researchers engaged in nanotechnology in Osaka University.

Achievements

In this year, 17 research groups were accepted at the 1st application and 5 groups were accepted at the 2nd application. Following is the list of accepted 22 groups.

Prof. Tomoyuki KAKESHITA Graduate School of Engineering
Prof. Masahiko YAMAMOTO Graduate School of Engineering
Prof. Takatomo SASAKI Graduate School of Engineering
Associate Prof. Yusuke MORI Graduate School of Engineering
Prof. Katsumi YOSHINO Graduate School of Engineering
Prof. Yasufumi FUJIWARA Graduate School of Engineering
Prof. Kenjiro OURA Graduate School of Engineering
Prof. Tomoji KAWAI The Institute of Scientific and Industrial Research
Prof. Tomoji KAWAI The Institute of Scientific and Industrial Research
Associate Prof. Seiichi MURASUGI Nanotechnology Process Foundry, The Institute of Scientific and Industrial Research
Prof. Hiroshi MASUHARA Graduate School of Engineering
Associate Prof. Tsuyoshi ASAHI Graduate School of Engineering
Prof. Satoshi KAWATA Graduate School of Engineering
Associate Prof. Takuo TANAKA Frontier Research Center
Prof. Yoshimitu YAMASAKI Graduate School of Medicine
Prof. Shun-ichi FUKUZUMI Graduate School of Engineering
Prof. Yukichi UMAKOSHI Nanoscience and Nanotechnology Research Center
Associate Prof. Takehiko WADA Graduate School of Engineering
Prof. Susumu KUWABATA Graduate School of Engineering
Prof. Mitsuru AKASHI Graduate School of Engineering
Prof. Osamu NAKAMURA Graduate School of Frontier Biosciences
Prof. Kiichi FUKUI Graduate School of Engineering

Radiation Laboratory

Professor, Director:	Goro ISOYAMA
Professors	Seiichi TAGAWA, Tetsuro MAJIMA, Yoichi YOSHIDA
Associate Professors:	Yukio YAMAMOTO, Ryuko KATO, Yoshihide HONDA, Shu SEKI, Mamoru FUJITSUKA, Takahiro KOZAWA
Research Associates:	Toshiji IKEDA, Norio KIMURA, Kazuo KOBAYASHI, Sachiko TOJO, Kiyohiko KAWAI, Masayuki ENDO, Shigeru KASHIWAGI, Jinfeng YANG, Akinori SAEKI
Technical Staff:	Tamotsu YAMAMOTO, Kumiko BABA
Support Staff:	Naoko KAWAGUCHI

Outlines

The Radiation Laboratory was newly established in the fiscal year 2002 in the Nanoscience and Nanotechnology Center as a successor of the *Radiation Laboratory*, which was a facility directly attached to the Institute but had been reorganized to be 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 γ-ray irradiation facility with ^{60}Co. Among them, the L-band linac and the 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 a related Department of the Institute. They run the Radiation Laboratory and care for outside users.

Achievements

After the large-scale remodeling of the L-band linac and the new installation of the RF-gun linac begun in the fiscal year 2002, we have been improving these accelerators, optimizing operation conditions, and measuring their performances. We completed commissioning of these accelerators in the first half of the fiscal year 2005. An application was approved to modify the license to use radioactive isotopes and radiation-generating equipment in the same period and also the RF-gun linac passed the pre-service inspection, so that we began to use these accelerators. In the latter half of the fiscal year 2004, we resumed user service with the L-band linac.

1. L-band linac

We installed a new timing system with an RF master oscillator for the L-band linac this fiscal year, and proceeded further to optimize operation of the linac. The problem left till the end was minute and random fluctuations of unknown origin in the RF power for acceleration, but the instability disappeared when the new timing system was used and consequently stabilization of the electron beam was realized. We could reduce the intensity fluctuation of the electron beam to one tenth of the previous value before the

remodeling. We had a trial to change operation modes of the linac twice in a day for two different users, which was only made possible with the computer control system. We have appended a new mode of operation called the multi-bunch mode. In the machine time for user experiments beginning in October, 100 days are allotted to 22 research subjects.

2. S-band linac

The S-band linac has been used for production of the slow positron beam. After the long shutdown, we made commissioning of the S-band linac again, including parts changed for installation of the RF-gun linac. Since discharges occurred frequently in wave-guides, we improved them, so that we could produce the slow positron beam again.

3. RF-gun linac

We conducted beam tests with the RF-gun linac and succeeded in producing an electron beam with the pulse duration shorter than 100 fs. We injected two laser beams with a time delay at two different points on the photocathode and we have succeeded in generating two electron beams with the linac.

4. γ-ray irradiation facility with ^{60}Co

The γ-ray irradiation facility with ^{60}Co was used by users of our institute and by others coming from the Graduate School of Science, the Graduate School of Engineering, and the Research Institute for Microbial Diseases. The number of research subjects and the total utilization time are approximately same as those in the previous year. Maintenance and repair of the facility were made in the summer shutdown period, as usual.

Electron Microscope Laboratory

Professor: 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 2004, the 300kV TEM served as an important equipment for the nano-structure characterization researches of 6 laboratories in ISIR with operation times as many as 268.

Electronic Processing Laboratory

Professor: Hajime ASAHI
Associate Professor: Shigehiko HASEGAWA
Associate Professor: Takuya MATSUMOTO
Associate Professor: Tatsuo YOSHINOBU
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 photolithography system, a high vacuum evaporation system, an electron beam evaporation system, a sputter deposition system, a reactive ion etching system, a crystal cleaving system, a wire bonding system, a double crystal X-ray diffractometer, an atomic force microscope 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.

Materials Analysis Center

Professor, Director: Hiroaki SASAI
Associate Professor: Masami SAWADA

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 analytical methods coupled with various analytical instruments.

Current Research Programs

1. Novel Analytical Methods: Host-Guest Chiral Recognition Mass Spectrometry

Until recently, various methods were used for determining chiral recognition of the chiral host compounds such as crown ethers, cyclodextrins, porphyrins, etc. Examples are the methods of extraction/NMR, extraction/polarimetry, titration NMR, induced circular dichromism, liquid chromatography (LC), capillary electrophoresis, transport, etc. Mass spectrometry (MS) is highly sensitive but not generally considered as sensitive to chiral difference and convenient for detecting host-guest chiral recognition properties because of the absence of mass differences between their host-guest diastereomeric isomers.

We have proposed a new technique of the mass spectrometry (MS)/enantiomer labeled (EL) Guest method. In this method, one of the enantiomeric guests is isotopically labeled, and a 1/1 mixture of a labeled and an unlabeled enantiomeric guest is complexed with a chiral host. Therefore, the new method has been called the EL-guest method. The method can be used for the detection and quantitative evaluation of chiral recognition ability of the hosts toward the guests.

The other one, which we have proposed, is another new technique of the MS/EL-Host method. In this method, one of the enantiomeric hosts is isotopically labeled, and a 1/1 mixture of a labeled and an unlabeled enantiomeric host is complexed with an ee-unknown guest. Therefore, the new method has been called the EL-Host method. The method can be used for the determination of enantiomeric excess (ee) of a given chiral guest.

Quantitative chiral analysis, that is enantiomeric excess determination, of organic chiral carboxylic acids has been examined using a new "Host-Metal-Guest Complexation System" by an electrospray ionization (ESI) mass spectrometry (MS)/ enantiomer labeled (EL)-Host method.

After several trials (screenings) by the use of our EL-Guest method, we finally selected a 1/1 mixture of an unlabeled and a labeled enantiomeric host compound ((R,R)-Ph_2-Pybox (**1**) and (S,S)-Ph_2-Pybox-d_4 (**2**), respectively) as a host-pair reagent. The latter labeled compound was synthesized via (S)-phenylglycinol-d_2. Further, we selected a lanthanum ion (La^{3+}) as a transition metal ion. Then, 2-methoxy-2-(1-naphthyl)propionic acid (MNPA) was chosen as a chiral guest carboxylic acid.

The relative peak intensity value (IRIS value) of the two Host-Metal-Guest complex

ions, which simultaneously appear with n=4 mass-unit differences in an ESI mass spectrum, becomes a measure of the chiral analysis of the carboxylic acid. The findings that the IRIS values change with the enantiomeric content of the carboxylic acid guest are the fundamental basis of the present ee-determination.

The obtained Ie-ee plot showed an excellent linear relationship (R^2=0.9994, n=7), indicating that the ee-value of ee-unknown carboxylic acid compounds can be determined by the simple ESIMS coupled with the EL-Host method within the error of ±2 % ee.

Publications

Original Paper

Depression of the Apparent Chiral Recognition Ability Obtained in the Host-Guest Complexation Systems by Electrospray and Nano-Electrospray Ionization Mass Spectrometry. Masami Sawada, Yoshio Takai, Hitoshi Yamada, Muneyoshi Yoshikawa, Ryuichi Arakawa, Hiroyuki Tabuchi, Mikio Takada, Juichi Tanaka, Motohiro Shizuma, Hiroshi Yamaoka, Keiji Hirose, Kazuo Fukuda, Yoshito Tobe, Eur. J. Mass Spectrom., 2004, 10, 27-37.

Chiral Recognition of Carboxylic Acids by ESI Mass Spectrometry. Masami Sawada, Sachiyo Nomura, Yoshitaka Miyamoto, Natsu Egawa, Motohiro Shizuma, Hitoshi Yamada, Yoshio Takai, Juichi Tanaka, and Hiroshi Yamaoka, J. Mass Spectrom. Soc. Jpn., 52(2004), 154-157(in Japanese).

Enantiomer Excess Determination of Amines and Dipeptides by ESI and FAB Mass Spectrometry Coupled with the Enantiomer-Labeled Host Method. Masami Sawada, Akihiro Kamei, Hirotaka Ueno, Hitoshi Yamada, Yoshio Takai, Motohiro Shizuma, Hiroshi Yamaoka, juichi Tanaka, and Ryuichi Arakawa, J. Mass Spectrom. Soc. Jpn. 52(2004), 289-294(in Japanese).

Review Paper

Structure Determination of Organic Compounds: Chiral Compounds,
Masami Sawada, "The Encyclopedia of Mass Spectrometry", Vol. 4, ed. by N. M. M. Nibbering, Elsevier, 2004, Part H06, 740-748.

International Conferences

Quantitative Chiral Recognition in Host-Guest Complexations by Mass Spectrometry (Poster), *M. Sawada, Y. Takai, 2nd 21st Century COE Program: 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, Jan.13-14, 2004

Inclusion of Permethylated Inulin with Alkali Metal Ions (Poster), *Y. Takai, M. Sawada, 2nd 21st Century COE Program: 7th SANKEN International Symposium on Hybridization of Chemistry, Biology, and Material Science, Osaka, Japan, Jan.13-14, 2004

Quantitative Chiral Recognition in Host-Guest Complexations using Mass Spectrometry Coupled with the Enantiomer-Labeled Method (Invited), *M. Sawada, Y. Takai, M. Shizuma, H. Yamaoka, International Symposium on "Stereodynamics of Chemical Reactions 2004", Osaka, Japan, Nov.28-Dec.3, 2004

Chiral Recognition of Amines and Carboxylic Acids by Mass Spectrometry (Poster), M. Sawada, *Y. Takai, M.Shizuma, H. Yamaoka, 8th SANKEN International Symposium & 3rd International Symposium on Scientific and Industrial Nanotechnology, Osaka, Japan, Dec.6-7, 2004

Contributions to International Conferences and Journals

M. Sawada European Journal of Mass Spectrometry (Editor)

Publications in Domestic Meetings

The Chemical Society of Japan	4 papers
The Mass Spectrometry Society of Japan	3 papers
Others	2 papers

Sponsorship

Entrusted Research

M. Sawada	Research of Materials Analysis	¥200,000

Nanotechnology Process Foundry

Professor:	Tomoji KAWAI
Visiting Associate Professor:	Masakazu MURASUGI
	Toshio KAWAHARA (from Jul. 1)
Visiting Research Associates:	Yoshinori MATSUI
	Kazumasa OKAMOTO
	Takahiro OHNO
	Teruo KANKI (from Apr.1 to Jun. 30)
Supporting Staff:	Keiko ENMI (from Apr. 1)

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 3rd year of this project in 2004, and most of our efforts resulted in supporting 23 research themes.

The Nanotechnology Support Project system was organized to realize the requests that researchers in private laboratories and R&D projects needed opportunities to use special facilities and equipments for their Nanotechnology R&D.

Institute of Science and Industrial Research, Osaka University has played an important role in Nanotechnology field by means of providing technology and information. In particular, thin film deposition works covering oxides and organic materials were presented a lot of impressed results. Based on the excellent works, Nanotechnology Process Foundry focuses the following supports.

(1) Thin film deposition of oxides, organic materials, and high melting point metals.
(2) Nanofabrication for oxide and organic material devices.
(3) Characterization of thin films and devices made of oxides and organic materials.

Achievements

The 68 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 are three points on our achievements in FY2002 in the followings:

1. Bring-up Nanotechnology Process Foundry.

The foundry was founded to support Nanotechnology researchers through thin film deposition, nanofabrication, and characterization. These supports are provided in the type of (a) consulting, (b) collaboration, (c) equipment use, and (d) research support.

2. Break-through toward functional Nanotechnology R&D.

The foundry supports advanced Nanotechnology R&D as well as fundamental research. The research on functional integration and system building based on

nanomaterials is acceptable in the foundry.

3. Fusion between top-down and bottom-up Nanotechnologies.

Many useful equipments for top-down and bottom-up Nanotechnologies are in operation. The fusion between top-down and bottom-up Nanotechnologies will bring a lot of important progresses on Nanotechnology in the near future.

Publications

Original Papers

Coordination Number Constraint Models for Hydrogenerated Amorphous Si Deposited by Catalytic Chemical Vapour Deposition, T. Kawahara, N. Tabuchi, T. Arai, Y. Sato, J. Morimoto and H. Matsumura: Journal of Physics: CONDENSED MATTER, 17 (2005) S103-S110.

157-nm-Induced Resist Outgassing Studied by Film Thickness Loss and In-Situ Quadrupole Mass Spectrometry, Y. Matsui, S. Seki, S. Tagawa, S. Kishimura and M. Sasago: J. Photopolym. Sci. Technol, 17 (2004) 671.

Photoacourstic Spectra from Co doped ZnO with Different Grain or Cluster Sizes, Y. Inoue, Y. Miyauchi, A. Kimura A, T. Kawahara, Y. Okamoto and J. Morimoto: Jpn. J. Appl. Phys., 43 (2004) 2936-2939.

Electron Dynamics in Chemically Amplified Resists, T. Kozawa, H. Yamamoto, A. Nakano, A. Saeki, K. Okamoto and S. Tagawa: J. Photopolym. Sci. Technol, 17 (2004) 449-452.

Estimation of Schottky to Porous Si by Photoacourstic Spectroscopy, T. Kawahara, S. Fukunai, M. Okamoto, Y. Inoue, K. Tahira, Y. Okamoto and J. Morimoto: Jpn. J. Appl. Phys., 43 (2004) 2932-2935.

Inhomogeneous Distribution of Crosslinks in Ion Tracks in Polystylene and Polysilanes, S. Seki, S. Tsukuda, K. Maeda, Y. Matsui, A. Saeki and S. Tagawa: Phys. Rev., 70 (2004) B144203-144210.

Development of Structual Analysis Method Based on Reverse Monte Carlo Simulation and Its Application to Catalytic Chemical Vapor Deposition Hydrogenated Amorphous Silicon, N. Tabuchi, T. Kawahara, T. Arai, J. Morimoto and H. Matsumura: Jpn. J. Appl. Phys., 43(2004) 6873-6879.

Formation of Benzene Trimer Radical Cation in g-irradiated Low Temperature 2-methylpentane Matrices, M. Todo, K. Okamoto, A. Seki and A. Tagawa: Chem. Phys. Lett., 399 (2004) 378-383.

Substrate Dependence of Photoacourstic Spectra on 3,4,9 10-Perylenetracarboxylic Dianhydride(PTCDA) Film, M. Okamoto, Y. Inoue, K. Yoshihara, T. Kawahara and J. Morimoto: IEICE Trans. Electron, E87-C (2004) 2108-2111.

Dependence of Acid Generation Efficiency on the Protection Ratio of Hydroxyl Groups in Chemically Amplified Electron Beam, X-ray and EUV Resists., H. Yamamoto, T. Kozawa, A. Nakano, K. Okamoto, S. Tagawa, T. Ando, M. Sato and H. Komano: J. Vac. Sci. Technol. B, 22(2004) 3522-3524.

Polymer Screening Method for Chemically Amplified Electron Beam and X-ray Resists, H. Yamamoto, A. Nakano, K. Okamoto, T. Kozawa and S. Tagawa: Jpn. J. Appl. Phys., 43 (2004) 3971-3973.

Proton Dynamics in Chemically Amplified Electron Beam Resists, H. Yamamoto, A. Nakano, A. Saeki, K. Okamoto, T. Kozawa, T. Tagawa, T. Ando, M. Sato and H. Komano: Jpn. J. Appl. Phys., 43 (2004) 848-850.

Proton Dynamics in Chemically Amplified Electron Beam Resists., H. Yamamoto, A. Nakano, A. Saeki, K. Okamoto, T. Kozawa, S. Tagawa, T. Ando, M. Sato and H. Komano: Jpn. J. Appl. Phys., 43 (2004) L848-L850.

Pulse Radiolysis Study on Proton and Charge Transfer Reactions in Solid Poly (Methyl Methacrylate), A. Nakano, K. Okamoto, T. Kozawa and S. Tagawa: Jpn. J. Appl. Phys., 43 (2004) 4363-4367.

Effects of Ester Groups on Proton Generation and Diffusion in Polymethacrylate Matrices, A. Nakano, K. Okamoto, T. Kozawa and S. Tagawa: Jpn. J. Appl. Phys., 43 (2004) 3981-3983.

The Study for the Annealing Effects on the Si and Ge Amorphous Thin film by Using Photoacourstic Spectroscopy, A. Miyata, Y. Okamoto, H. Takiguchi, T. Kawahara and J. Morimoto: Transactions of the MRS-J, 29 (2004) 2801-2804.

Review Papers

Substrate Temperature and Anneal Cycle Dependence of the Optical Properties for Thermoelectric Materials Si-Ge-Au Thin Films, A. Miyata, K. Morita, Y. Okamoto, T. Kawahara and J. Morimoto: Memories of the National Defense Academy, Japan, 44 (2004) 15-20.

Size Estimation of the Calcined $Zn_{1-X}Co_XO(x=0.03)$Powders by Photoacoustic Spectroscopy, T. Kwahara, Y. Miyauchi, A. Kimura, Y. Inoue, Y. Okamoto and J. Morimoto: Memories of the National Defense Academy, Japan, 44 (2004) 1-5.

Studies of Deep Levels in $Al_{0.75}Ga_{0.25}As$: Sn by Isothermal Capacitance Transient Spectroscopy, Y. Inoue, K. Yoneda, T. Kawahara, Y. Okamoto and J. Morimoto: Memories of the National Defense Academy, Japan, 44 (2004) 7-13.

Books

Inductively Coupled Plasma Etching of GaN and the Micro Photoluminescence, T. Kawahara, F. Fälth, L. Xinyu, R. Nunes, Tg.Anderson, V., H.Zirath, Pp.Paskov and Po.

Holts, Eds.Ka. Khor, Y. Watanabe, K. Komeya and H. Kimura: Materials Processing for Properities and Performance (MP3), Institute of materials (East Asia), Yokohama, 2(2004) 548-555.

International Conferences

157nm in Duced Resist Outgassing Studued by Film Thickness Loss and *in-sitsu* Quadrupole Mass Spectrometer (oral), Y. Matsui, S. Saki, S. Tagawa, S. Kishimura and M. Sasago. The 21st Conference of Photopolymer Science and Technology/The International Symposium 2004 Materals & Processes for Advanced Microlithography and Nanotechnology, Chiba, Japan, Jun. 22-25, 2004.

Sub-picosecond Pulse Radiolysis in Benzane Derivatives (poster), K. Okamoto, A. Saeki, T. Kozawa, S. Tagawa. Gordon Research Conferences (2004 GRC on Radiation Chemistry), Waterville, USA, Jun. 20-25, 2004.

Activities of the Support for the Nanotechnology in Osaka University (poster), M. Murasugi, T. Kawahara, T. Ohno, Y. Matsui, K. Okamoto, and T. Kawai. 8th Sanken International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, Dec. 6-7, 2004.

Fabrication of Ferroelectric $Ba(Zr_xTi_{1-x})O_3$ Superlattices with Different Symmetry by Pulse Laser Deposition (poster), T. Kawahara, T. Ohno, M. Murasugi, H. Tabata, T. Kawai, and T. Hino. 8th Sanken International Symposium on Scientific and Industrial Nanotechnology 2004, Osaka, Japan, Dec. 6-7, 2004.

Tunneling Spectroscopy Analysis for the Observation of the HEX- fluorescent Dye Attached DNA (poster), T. Kawahara, T. Takahashi, H. Tanaka and T. Kawai. The 12th International Colloquium on Scanning Probe Microscopy, Sizuoka, Japan, Dec. 9-11, 2004.

Publications in Domestic Meetings

The Institute of Electrical Engineers of Japan 1 paper

Sponsorship

Entrusted Research

T. Kawai	MEXT (RR2002)	Nanotechnology Support Project	¥94,000,000

Service Facilities

Workshop

Director Professor: Tetsuro MAJIMA
Technical Staff
Metal Processing Shop: Michiaki KAKUICHI, Masayoshi OHNISHI
Glass Blowing Shop: Hiroaki MATSUKAWA, Noriyuki OGAWA

Outlines

The workshop consists of a metal processing shop and a glass blowing shop. In the former, various apparatuses made from metallic materials are designed and assembled for experiments. It is equipped with lathes and fraises in addition to drilling, rolling, and welding machines. In 2000-2001 academic year, a computer-controlled machine (machining center) was newly equipped. In the latter, sophisticated glass apparatuses are made according to researcher's requirements. It is equipped with an electric furnace, glass lathes, and glass cutting machines.

Office of Information Network

Professor: Akihito YAMAGUCHI

Outlines

Office of Information Network was inaugurated in March, 1999, to organize the operation of the information network in ISIR, which had been started with support by volunteers, because of the rapid spread of the information network and the growth of its importance in the research environment. The information was constructed as a prototype by the departments in the division of Intelligent System Science in the late 1980's and has been expanded to the whole of ISIR with the development of ODINS (Osaka University Information Network System). Recently it has played an important role in ISIR to release/access the information available in the Internet. Office of Information Network is now supporting researchers and students on the variety areas.

Laboratory for Radio-isotope Experiments

Professor: Katsuyuki TANIZAWA

Outlines

This laboratory is specially designed for biochemical and molecular biological experiments using radioactive compounds labeled with ^{3}H, ^{14}C, ^{32}P, ^{35}S. The main equipments are liquid scintillation counters and 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: Yasushi YAGI
Staff: Taiko FURUTA

Outlines

The ISIR Library houses only technical books and journals for researchers. Most materials are on open shelves directly available to faculty and students. The library has two reading rooms and a workroom with photocopiers on the second floor of the administration building, and the storage facility on the first floor of the research building.

The library office offers the following services; orders for books and magazines, survey and inquiry of literature, Interlibrary Loan services, photocopy request, and so on. Guide to the Library could be found on its home page (http://www.sanken.osaka-u.ac.jp /labs/lib-web/).

(As of April 1, 2005)

	Number of books	Journals	Newspapers
Japanese	12,549	292 titles	4 titles
Foreign	46,941	979 titles	1 title

Technical Division

Head: Hitoshi YAMADA

Outlines

The Technical Division was established in 1982 to deal with professional duties providing better service for researchers. In the ISIR organization, the technician group is independent of the management and the research groups. The organization was the first one among similar organizations established in the national universities of Japan. The Division consists of two groups: Group of Machine and Group of Measurement, in which each group has two sections: Section of Machine/Circuit, Section of Glass in Group of Machine and Section of Measurement/Information, Section of Analysis/Data in Group of Measurement. The technicians work at various places: the Analysis Center, the Workshop, the Office of Information network, the Electronic Processing Laboratory and the Nanotechnology Center. The Division gives not only high-quality service to research groups but technical training to the researchers and students. The annual report is published to help and encourage training and activities of the members of the Division. In addition, the Division has started the safety lecture for utilizing various machines in the ISIR since 2004. The Technical division makes every effort to promote the ISIR more important development under an independent administration system.

Publications in Domestic Meetings

Symposium of Technology and Engineering in Instrumental Analysis Technique 1paper

Japanese Society of Radiation Safety Management 1paper

Meeting on Engineering & Technology at Osaka Univ. 1paper