# ICR ANNUAL REPORT 2001

## Kyoto University
## Institute for Chemical Research

Volume 8

# Front cover

## [a] Examples of rheological phenomena

Polymeric liquid squeezes and climbs up a rotating rod (upper left) and its flow line shrinks at a die exit (upper right). Polymer chains stretched and aligned along the flow line give elastic force to the liquid and flow lines behave like a stretched rubber band. Injection-molded bodies may be birefringent due to frozen-in alignment of polymer (lower right), which must be avoided for optical devices. The type of cohesive force in the material is guessed from the shape of the broken surface when a cylinder is twisted (lower left); spiral for a chalk implies that it is strong to shear stress and breaks along the surface where the tensile stress is maximum.

## [b] Newly Found Mechanisms of Polymer Crystallization

The figure shows the optical micrographs of poly(ethylene terephthalate) to evidence two new mechanisms involving microphase separation due to orientational fluctuation other than the usual direct crystal nucleation mechanism. Here a sudden change of morphology from spinodal decomposition (SD) to nucleation-and-growth pattern is seen at a spinodal temperature $T_s = 213$ °C.

## [c] Turned-up magnetization cores

The confinement of spins imposed by geometrical restrictions makes various spin structures with a size comparable to their dimensions. In the case of ferromagnetic dots, a magnetic vortex structure with a turned-up magnetization core has been introduced in many textbooks. However the direct observation of such vortex structures has not been achieved. The dot array of permalloy with 1μm diameter and 50 nm thick was prepared by electron beam lithography and lift-off method, and the observation of such vortex structures was attempted by magnetic force microscope (MFM). The figure shows the MFM image of the dot array. In the center of each dot, a white or black contrast corresponding to the turned-up magnetization core is clearly observed.

## [d] Memory of Chirality

The structure of enolates was long believed to be achiral. However, chiral nonracemic enolate **A** with a racemization barrier of 16 kcal $mol^{-1}$ at -78 °C was found to be the crucial intermediate for asymmetric α-methylation of **1** to give **2** in 81 % *ee*. This asymmetric reaction occurs in the absence of any external chiral sources. Chirality of **1** is *memorized* in the enolate intermediate **A** in the form of dynamic C-N axial chirality.

# CONTENTS

# *Preface*

It is a great pleasure for us to publish the ICR Annual Report 2001 which has been refined using color pages and concise research topics in order to represent our research activities much more precisely and vividly than before.

In 2001, the first year of the 21st century, the Institute for Chemical Research of Kyoto University, celebrated its 75th Anniversary. It was the main topics last year that the Bioinformatics Center was launched as the first research center in this field in our country by introduction of a new high-speed super computer system. The center consists of three laboratories, two of them having been newly established. Our institute has now been expanded to a system of 9 divisions and 2 attached research centers, consisting of a total of 29 laboratories and 3 guest-laboratories. In 2001, a new research network between physics and chemistry has started by collaboration of five big institutes in Japan including our institute. Our institute continues to play a key role in the Kyoto University Center of Excellence (COE) Project entitled "Elements Science" started in 2000 as only one center in the engineering science field at Kyoto University.

At the end of March, 2001, Prof. KOBAYASHI Takashi of the Laboratory of Crystal Information Analysis retired from the ICR. At the end of March 2002, the following four professors will retire: The former Director, Prof. SHINJO Teruya of the laboratory of Artificial Lattice Alloys, Prof. FUJI Kaoru of the laboratory of Fine Organic Synthesis, Prof. KAJI Keisuke of the laboratory of Polymer Materials Science, and Prof. OSAKI Kunihiro of the laboratory of Molecular Rheology. On behalf of all staff, I would like to express my heartfelt gratitude to these five leading scientists for their splendid achievements in their research fields. Sadly, Technician Dr. HONMA Takashi suddenly passed away in July; May he rest in peace.

We have appointed four new professors in 2001. Prof. FUKUDA Takeshi and Prof. ISODA Seiji were promoted to succeed the professorship, respectively, of the Laboratory of Polymeric Materials in February and of the Laboratory of Electron Microscopy and Crystal Structure in July. In October, Prof. AKUTSU Tatsuya and Adjunct Prof. MIYANO Satoru moved from the Institute of Medical Science, The University of Tokyo, to chair the two new professorships in the Bioinformatics Center, the laboratory of Biological Information Network and of Pathway Engineering, respectively. In addition, from April, Prof. KANEHISA Minoru was assigned to the Laboratory of Bioknowledge Systems in the Bioinformatics Center. At the present stage, 26 full professors, 27 associate professors, and 44 instructors work in the ICR, and about 220 graduate students and 20 foreign researchers study at the ICR.

The organization of national universities must be significantly changed by transformation into agencies in 2004 at the latest. It is our common knowledge that we must keep and strengthen the vitality for overcoming the forthcoming inevitable turning points and for providing strong leadership in research activities for the development of science and technology. For this purpose, we will continue to devote our efforts to fundamental research and its application in specific fields.

January, 2002

TAMAO Kohei
DIRECTOR

**The Bioinformatics Center was established on 1st April, 2001.**


**The Institute's Supercomputer Laboratory houses SGI Origin 3800 supercomputer systems (left) and SUN Fire 15K server systems (right), which are used for research in computational chemistry and bioinformatics as well as for the Genome Net Service.**

# TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

## Key to headline in the columns

**RESEARCH DIVISION — Laboratory (Subdivision)***

*** See also "Organization and Staff " on pages 96 and 97.**

## Abbreviations used in the columns

| | |
|---|---|
| Prof Em | Professor Emeritus |
| Prof | Professor |
| Vis Prof | Visiting Professor |
| Assoc Prof | Associate Professor |
| Lect | Lecturer |
| Lect(pt) | Lecturer (part-time) |
| Instr | Instructor |
| Assoc Instr | Associate Instructor |
| Techn | Technician |
| Guest Scholar | Guest Scholar |
| Guest Res Assoc | Guest Research Associate |
| PD | Post-Doctral Research Fellow |
| Res(pt) | Researcher (part-time) |
| A Res(pt) | Assistant Researcher |
| RF | Research Fellow |
| RS | Research Student |
| GS | Graduate Student |
| DC | Doctor's Course (Program) |
| MC | Master's Course (Program) |
| UG | Undergraduate Student |
| D Sc | Doctor of Science |
| D Eng | Doctor of Engineering |
| D Agr | Doctor of Agricultural Science |
| D Pharm Sc | Doctor of Pharmaceutial Science |
| D Med Sc | Doctor of Medical Science |

# States and Structures -Atomic and Molecular Physics-

Assoc Prof
ITO, Yoshiaki
(D Sc)

Instr
NAKAMATSU, Hirohide
(D Sc)

**Researcher (pt)**

TOCHIO, Tatsunori

**Students**

SHIGEOKA, Nobuyuki (D2)
OoHASHI, Hirofumi (D1)

## Scope of Research

In order to obtain fundamental information on the property and structure of materials, the electronic states of atoms and molecules are investigated in detail using X-ray, SR. Theoretical analysis of the electronic states and development of new radiation detectors are also performed.

## Research Activities (Year 2001)

### Presentations

The information on $L_{III}$ and $L_{II}$ shell in $K$ x-ray absorption and emission of $Cr_2O_3$, Ito Y, 7th International Conference on Applications of Nuclear Techniques, June 17-23, 2001 Crete, Greece, Oct. 19, 2001.

On $K\alpha_{1,2}$ spectra of Copper, Ito Y, 7th International Conference on Applications of Nuclear Techniques, June 17-23, 2001 Crete, Greece, Oct. 19, 2001.

Fluoride Ion Conduction in Pb1-xSnxF2 Solid Solution System, Yoshikado S. (Doshisha University ), Ito Y, J.M.Reau (Institut de Chimie de la Matiere Condensee de Bordeaux), International Conference on Solid State Ionics, July 8-12, 2001, Australia, July 8, 2001.

Fabrication and evaluation on Battery in Fluorine compounds, Togashi G (Doshisha University), Ito Y, Yoshikado S (Doshisha University), 27th annual meeting in Solid State Ionics, Tokyo, Nov. 12, 2001.

On W $L\beta$ visible satellite, A. M. Vlaicu (NIRM), Fukushima S (NIRM), Ito Y, 37th annual meeting in x-ray analysis, Tsukuba, Oct. 29, 2001.

X-ray spectral measurements using Xe gas sintilation counter with a large window, 30 $cm^2$, Nakanishi Y, Ito Y, Omote K (Rigaku Denki X-ray Lab.), 37th annual meeting in x-ray analysis, Tsukuba, Oct. 30, 2001.

Topics

## Evolution of *K* and *L* satellites of X-ray emission spectra at BL15XU, SPring-8

The existance of two or more holes in atomic inner shells gives rise to satellite lines with energies that are shifted from the corresponding one-hole (diagram) lines. One of the method to study the origins of satellite lines is to find the threshold of the excitation energy. For that experiment it is effective to measure emission spectra, tuning excitation energy used by synchrotron radiation.

In $K\alpha$ spectra of *3d* transition element very weak satellite line appears in the higher energy region for $K\alpha_1$. It is called $K\alpha_{3,4}$, and thought as the transition from multiple hole state. We measured Fe $K\alpha$ spectra at various excitation energy to investigate the origin of the satellite.

The relative intensity of $K\alpha_{3,4}$ looks gentle dependence for the excitation energy. That relative intensity is saturated at the energy higher about 2000 eV than the energy of the threshold. $K\alpha_{3,4}$ satellite is thought the transition from $1s2p$ to $2p^2$. This experiment suggests that shake-off process connects predominantly the creation of the *2p*-spectator hole.

For heavy element we focused on satellite lines of Au $L\beta_2$, which has two satellites in the high-energy side. They are thought to be ascribed to the spectator hole $M_{4,5}$. We measured Au $L\beta_2$ spectra at various excitation energy including $L_1$ edge.

In the spectra excited at 14390 eV and 15000 eV (above $L_1$ edge), we can confirm two satellites at high-energy side of $L\beta_2$. On the other hand satellite doesn't appear in the spectra excited at 14320 eV (below $L_1$ edge). It is clear that $L\beta_2$ satellite lines grow up with $L\beta_3$, which has initial stage with vacancy at $L_1$ subshell.

We did energy scan for the peak intensity of $L\beta_2$" ($L_3M_4$-$M_4N_5$) which is most far distance from main peak. That intensity (red square) grows up with $L_1$ absorption spectra (blue line). So that the present experiment suggests that Au $L\beta_2$ satellite lines are caused mainly by $L_1$-$L_3M_i$ (i=4,5) Coster-Kronig transition.

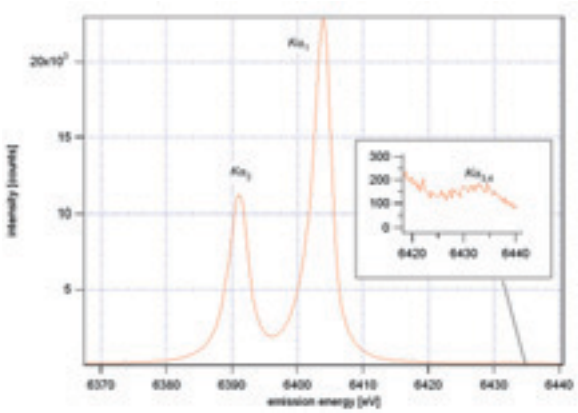

**Figure 1.** Fe $K\alpha$ emission spectra

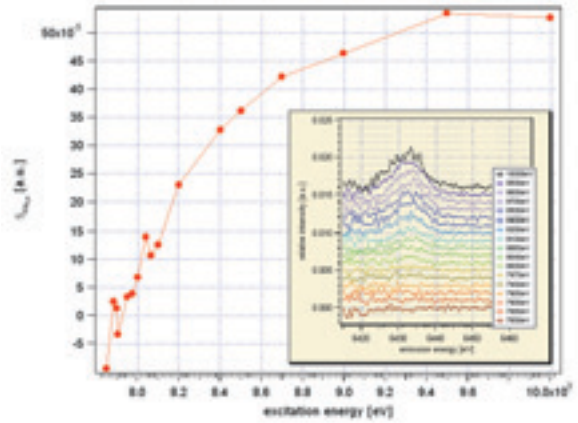

**Figure 2.** Energy dependence of relative intensity Fe $K\alpha_{3,4}$ satellites for $K\alpha_1$

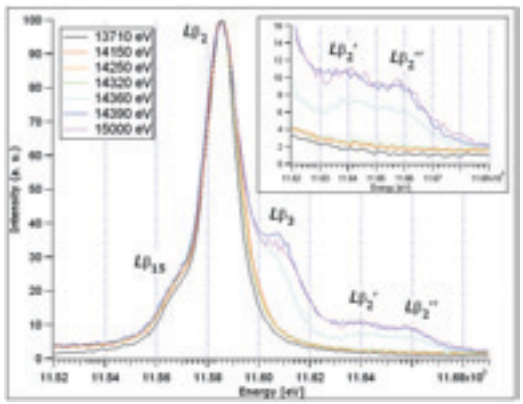


**Figure 3.** Au $L\beta_2$ emission spectra at various excitation energies

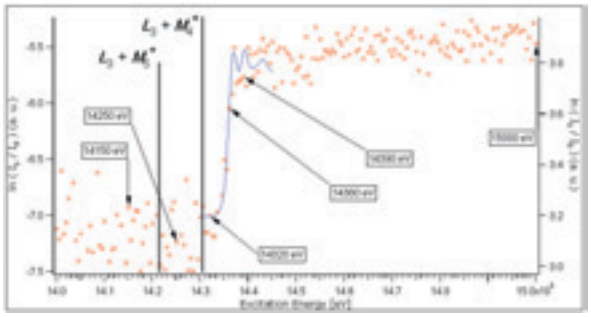

**Figure 4.** Energy scan of Au $L\beta_2$" satellite's intensity and Au $L_1$ absorption spectra

# States and Structures -Electron Microscopy and Crystal Chemistry-

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MINARI, Takeo (M1)
TSUJIMOTO, Masahiko (D3)
TAKAJYO, Daisuke (M2)
YOSHIOKA, Yasutomo (M1)

## Visitors

| | |
|---|---|
| Prof BEKALOGLU Ozer | Technical University of Istanbul, Turkey, 19-21 January 2001 |
| Prof TORRES Thomas | The Autonoma University of Madrid, Spain, 2-3 February 2001 |
| Prof FUCHS Harald | University of Münster, Germany, 4-5 September 2001 |
| Prof ULANSKI Jacek Pawel | Technical University of Lodz, Poland, 19-20 September 2001 |

## Scope of Research

Structures of materials and their structural transition associated with chemical reactions are studied through direct observation of atomic or molecular imaging by high-resolution spectromicroscopic method which realizes high resolution energy-filtered imaging as well as electron energy-loss spectroscopy. It aims to explore new methods for imaging and also obtaining chemical information in thin films, nano-clusters, interfaces, and even in solutions. By combining with scanning probe microscopic methods, the following subjects are studied: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, fabrication of low-dimensional functional assemblies.

## Research Activities (Year 2001)

### Presentations

Correlation between dynamical effect and real thickness of crystal in electron diffraction intensity, Kuwamoto K, Annual Meeting Elec. Micro., 11 May.

Electron radiation damage processes in TCNQ and $F_4$TCNQ studied with an imaging plate, Hasegawa H, Annual Meeting Elec. Micro., 11 May.

Electron radiation damage processes in TCNQ and $F_4$TCNQ studied by EELS, Koshino M, Annual Meeting Elec. Micro., 12 May.

STM study on photopolymerization of 17, 19-hexatriacontadiyne monomolecular layer, Irie S, 13th Intern. Conf. on Crystal Growth, 31 July.

Lattice-lattice interaction in pseudo-commensurate epitaxy at liquid/solid interfaces, Isoda S, 15th Intern. Conf. on Chem. of the Organic Solid State, 1 Aug,.

Formation process of ultrafine platinum particles in an aqueous solution with a surfactant, Hahakura S, 13th Intern. Conf. on Crystal Growth, 2 Aug.

Comparative study on surface morphology by photo- and thermal-polymerization of a diacetylene, Yaji T, 4th Intern. Conf. Non-contact AFM, 2 September.

Bulk, surface and interface polymerized in solid-state, Isoda S, Summer Seminar of Fiber Soc. Jpn., 6 September.

Organic epitaxy mode and two-dimensional packing efficiency, Fujiwara E, Autumn Meeting, Chem. Soc. Jpn., 22 September.

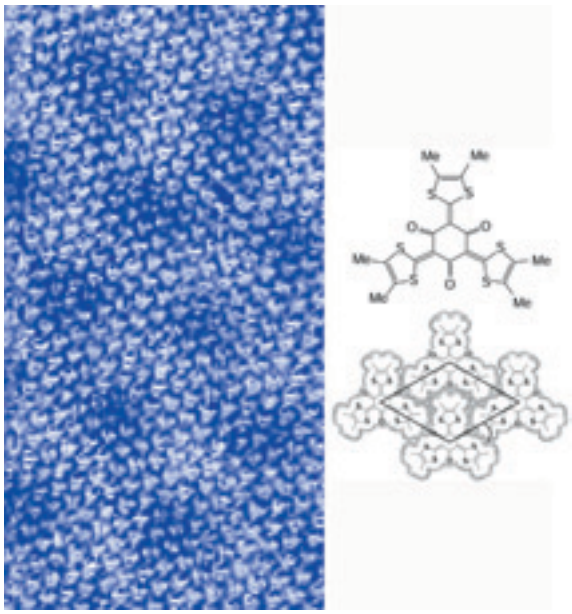
Epitaxial growth of (μ-oxo)bis(phthalocyaninato) aluminium(III), Suga T, Autumn Meeting, Chem. Soc. Jpn., 22 September.

Local charge transfer in iron-phthalocyanine-amine complexes, Isoda S, Meeting, Coordination Chemistry, 28 September.

Topics

## Effect of molecular packing efficiency on the epitaxial growth modes of monomolecular film on graphite studied by STM

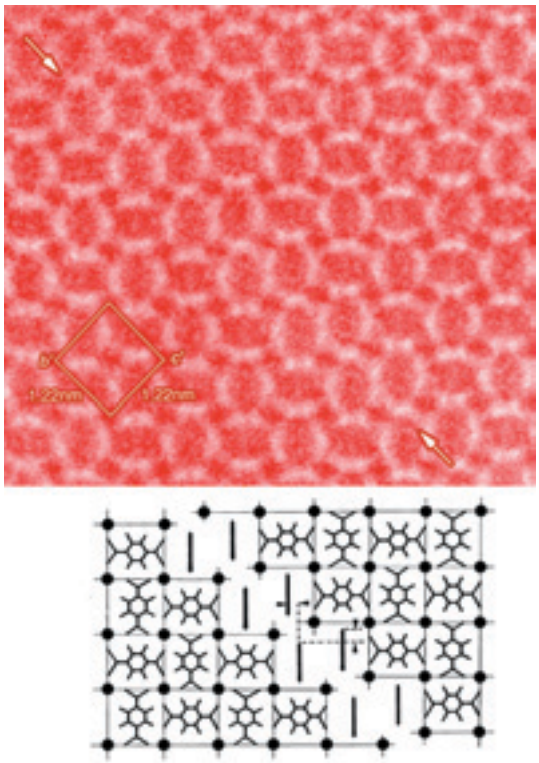
The monomolecular film of a triangular molecule vacuum-deposited on a (0001) surface of graphite was observed by scanning tunneling microscopy, in order to examine its growth mode and structure. The flat lying molecules form an ordered close-pack arrangement in the film on graphite as shown in the figure. The unit lattice of the monomolecular layer was found to be incommensurate to the substrate lattice, judging from two-dimensional moire-like contrast modulation. This result is compared with other cases of molecules reported already from a viewpoint of two-dimensional packing that indicates the intermolecular interaction in monomolecular layer [1]. The packing efficiency, a newly proposed parameter, in the monomolecular layer is concluded to characterize the growth modes of monomolecular layer formed on substrates; commensurate, point-on-line and incommensurate.



1. Fujiwara E, Isoda S, Ogawa T, Kobayashi T and Yamashita Y, Surf. Sci., **487**, 118 (2001).

## Lattice defects in organic crystals revealed by direct molecular imaging

The arrangement of molecules at crystal defects in organic crystals was examined with a high-resolution electron microscope [2], and the results are discussed from molecular interaction around the faults. The stacking fault in a charge transfer complex of $K^{+}TCNQF_4^{-}$ is interpreted to be a defect produced by the deficiency of one molecular plane along the (001) or (010) plane as shown by the arrows in the figure shown below. The expected molecular packing near the stacking fault is shown schematically in the figure. An edge dislocation found in a quaterrylene thin crystal is made by two excess half-planes along the a-axis without forming stacking faults. At the core of the dislocation, some unpaired molecules are located to fill the space produced by the edge dislocation, although the molecules in the perfect crystal are packed in the sandwich herringbone-type arrangement (paired molecules)



2. Maeda T, Kobayashi T, Nemoto T and Isoda S, Phil. Mag., **81**, 1659 (2001).

# States and Structures - Polymer Condensed States -

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TOGAMI, Tadahiro (UG)
OKADA, Yumi (UG)
NAKAO, Toshio (D3)
YOSHIOKA, Taiyo (D1)
UEDA, Masahiro (M2)
TANI, Kenji (M1)
MIKI, Takashi (UG)

### Visitors

Dr HASHIM S Azanam University Sains Malaysia, Malaysia, February 25-March 5, 2001
Dr LOTZ Bernard Institut Charles Sadron, France, April 5-7, 2001

## Scope of Research

Attempts have been made to elucidate the molecular arrangement and the mechanism of structural formation/change in crystalline polymer solids, polymer gels and elastomers, polymer liquid crystals, and polymer composites, mainly by electron microscopy and/or X-ray diffraction/scattering. The major subjects are: synthesis and structural analysis of polymer composite materials, preparation and characterization of polymer gels and elastomeric materials, structural analysis of crystalline polymer solids by direct observation at molecular level resolution, and *in situ* studies on structural formation/change in crystalline polymer solids.

## Research Activities (Year 2001)

### Presentations

Morphological investigation on the formation of fibrillar structure for PEN fibers, Yoshioka T, Tsuji M, Kohjiya S, et al., Annual Meeting, Soc. of Fib. Sci. and Technol., Jpn., 6-8 June, and related 1 presentation.

Structure analysis of polymer solids mainly by transmission electron microscopy, Tsuji M, Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 12-14 September.

Biaxial deformation of endlinked model polydimethylsiloxane networks, Kawamura T, Urayama K, Kohjiya S, Annual Meeting, Soc. Polym. Sci., Jpn., 24 May, and related 5 presentations.

Swelling behavior of liquid crystalline gels in liquid crystalline solvents, Okuno Y, Kawamura T, Urayama K, Kohjiya S, Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 13 September.

Electromechanical properties of thin polymer layers, Urayama K, Neher D (Potsdam Univ.), et al., Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 13 September, and related 3 presentations.

### Grants

Kohjiya S, Urayama K, Murakami S, Ikeda Y, Role of polymers in all solid-state ionic devices, Grant-in-Aid for Scientific Research, Priority Area (B), 1 April 1999 - 31 March 2004

Kohjiya S, Tsuji M, Urayama K, Direct observation of amorphous polymer network structures by TEM, Grant-in-Aid for Scientific Research, (B)(2), 1 April 2001 - 31 March 2003

Urayama K, Dynamics of guest polymers in host polymer networks, Grant-in-Aid for Scientific Research, Encouragement of Young Scientists, 1 April 2001 - 31 March 2003

Topics

## Lamellar and Crystalline-Core Thicknesses of Poly(3-oxotrimethylene) (POK) Crystallized Epitaxially on Alkali Halides

Edge-on lamellar crystals of POK were isothermally grown from a dilute solution in nitrobenzene epitaxially onto KI at various temperatures ($T_c$ = 150–190 °C). The resulting crystals were observed by transmission electron microscopy (TEM) in bright-field (BF) and dark-field (DF) modes and by high-resolution (HR) TEM. The DF images obtained by conventional TEM and the (110) lattice images obtained by HR-TEM showed that the crystalline-core thickness of each lamella is inevitably smaller than the corresponding lamellar thickness. Figure 1 shows the $T_c$-dependence of the crystalline-core thickness obtained by DF- (circle) and HR-TEM (triangle), and also that of the lamellar thickness obtained by BF-TEM of the edge-on lamellae (square) and by small-angle X-ray scattering of the "single crystal" mats (+). Both of the thicknesses increase with increasing $T_c$. For the crystals grown at any $T_c$, the crystalline-core thickness is 50–60 % of the corresponding lamellar thickness. Thus the POK lamella has a surface layer (20–25 % of the lamellar thickness) containing folds on each basal side of the lamella.

1. M. Fujita, et al., *Macromolecules*, **34**, 6147 (2001)
2. M. Fujita, et al., *Macromolecules*, **34**, 7724 (2001)

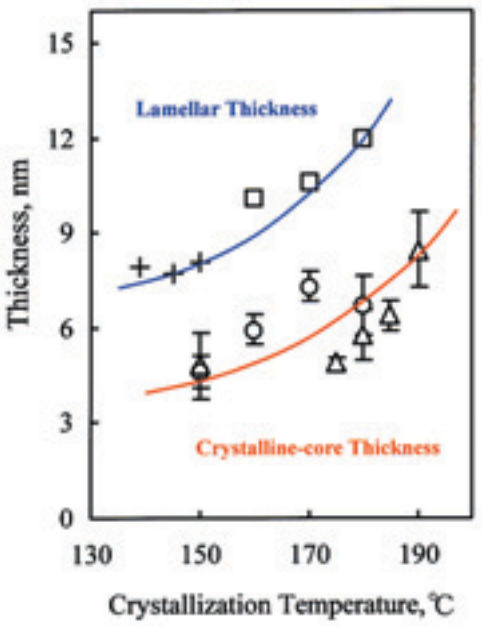


**Figure 1.**

## Multi-Axial Deformations of End-linked Polydimethylsiloxane Model Networks

Molecular interpretation of rubber elasticity of cross-linked amourphous polymer networks still remains incomplete due to the complicated network topology, especially, entanglement couplings of different network chains. A large number of theoretical models with different treatments of entanglement effects have been proposed. We have prepared a model polydimethylsiloxane network which has a well-characterized network chain length and junction functionality via end-linking method. Using this model network, we have carried out the biaxial deformation experiment which achieves all accessible pure homogeneous strains [1,2]. The data obtained enable us to identify the models which account for the entanglement effects most successfully and correctly [2]. Among the five molecular theories tested, the Edwards-Vilgis slip-link model [3] shows the most successful reproducibility over large portions of the experimental data, as shown in Figure 2.

1. T. Kawamura, et al., *Macromolecules*, **34**, 8252 (2001)
2. K. Urayama, et al., *Macromolecules*, **34**, 8261 (2001)
3. S. F. Edwards, et al., *Rep. Prog. Phys.*, **51**, 243 (1988)

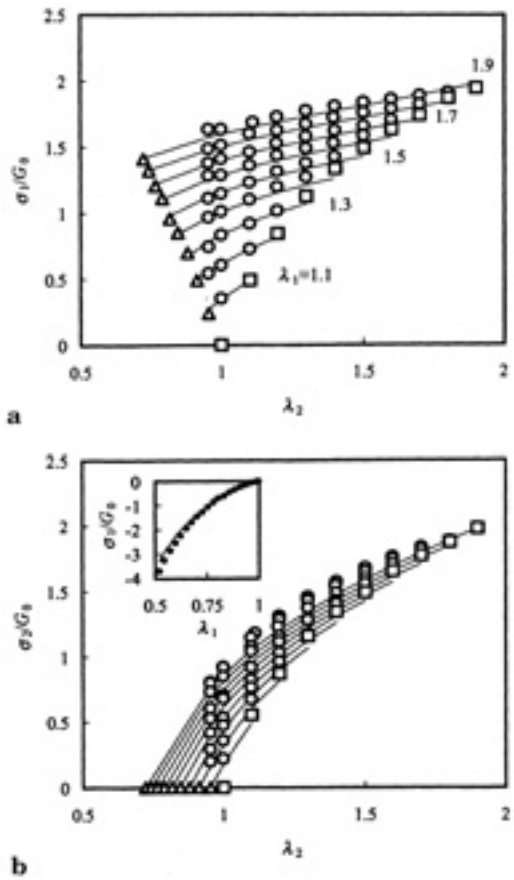


**Figure 2.** Comparisons of the experimental reduced principal stresses (a) $\sigma_1/G_o$ and (b) $\sigma_2/G_o$ - principal elongations ($\lambda_1$ and $\lambda_2$) relations with the predictions of the slip-link model (solid lines). The inset of part b shows the comparisons for uniaxial compression.

# Interface Science - Solutions and Interfaces -

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MATUBAYASI, Nobuyuki
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NAGAI, Yasuharu (D1)
TAKIZAWA, Takeyuki (M2)
TSUNASHIMA, Hiroyuki (M1)
KIMURA, Tomohiro (D4)
KONISHI, Hirofumi (D3)
TSUJINO, Yasuo (D3)
IWASA, Masaki (M2)
MIKAWA, Kohei (M1)
USUI, Yuma (M1)

## Visitors

Prof LEVY Ronald M — Rutgers University, USA, 15 October 2001 - 16 October 2001
Prof LEBLANC Roger M — University of Miami, USA, 14 October 2001 - 16 October 2001

## Scope of Research

Structure and dynamics of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are systematically studied by NMR under extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Vibrational spectroscopic studies are carried out to elucidate structure and orientations of organic and water molecules in ultra-thin films. Static and dynamic aspects of membrane-drug and membrane-protein interactions, crystallization of protein monolayers, and advanced dispersion systems are also investigated.

## Research Activities (Year 2001)

### Presentations

#### *Water and Solutions under Extreme Conditions*

NMR and computer simulation studies of structure, dynamics, and reaction of supercritical water, Matubayasi N, 2001 International Association for the Properties of Water and Steam, 9-14 September.

NMR study of aqueous solutions of electrolytes at high temperature and high pressure, Matubayasi N, Nakao N, Kubo M, Tsunashima H, and Nakahara M, High-pressure meeting, 20-22 November.

NMR analysis of hydrothermal decomposition of formic acid: competitive processes into carbon monoxide and water and carbon dioxide and hydrogen, Tsujino Y, Wakai C, Matubayasi N, and Nakahara M, High-pressure meeting, 20-22 November.

#### *Ultra-thin Films*

Simultaneous evaluation of refractive-index dispersion and molecular orientation in a ultrathin film by oscillator model simulation and infrared external-reflection spectrometry, Hasegawa T [Kobe Pharm Univ], Umemura J, and Leblanc R M [Univ of Miami], The Pittsburgh Conference, 8 March.

#### *Advanced Dispersion Systems*

Surface forces in presence of nano-meter size particles in solution, McNamee C, Matsumoto M, and Nakahara M, 54th Annual Meeting of Division of Colloid and Interface Science, Chem Soc., Jpn, 16 September.

# Topics

## Water acts as an effective acid at hydrothermal conditions

Water in its neutral form is quantitatively demonstrated at hydrothermal conditions to promote a chemical reaction that proceeds at ambient conditions under the presence of strong acid. By focusing on the dehydration of 1,4-butanediol into tetrahydrofuran, the noncatalytic and acid-catalyzed rate constants are separately determined by varying the hydronium ion concentration. Over a wide range of temperature from moderate to subcritical, neutral water was found to promote the reaction at an effective acid concentration of $10^{-4}$ -$10^{-5}$ M. Actually, the role of neutral water as an effective acid appears operative even at ambient conditions and becomes manifest at high temperatures. [Fig. 1]

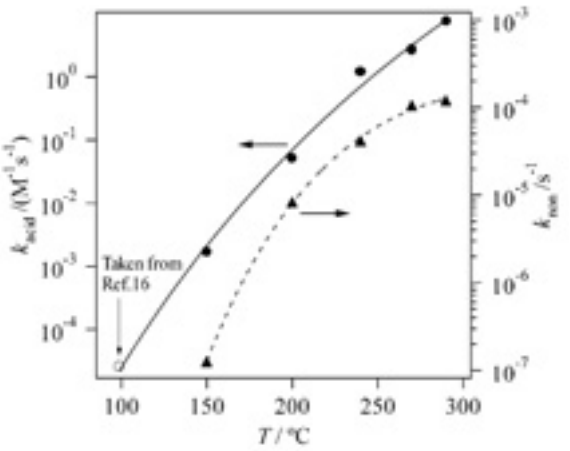


Fig. 1

## $^{13}$C NMR method for determining peptide and protein binding sites in membranes[1]

Reliable NMR criteria for the location and depth of peptides and proteins in membranes were shown by the natural abundance $^{13}$C NMR method, which reproduced not only the deep penetration of a channel peptide gramicidin A but also the superficial binding of 18A, a model peptide of apolipoprotein A-I (apoA-I) in plasma. The NMR reliability was ensured by the recent X-ray diffraction data. Our method first provided the atomic-level evidence for native apoA-I binding in egg lecithin (EPC) vesicles (SUV, LUV) and emulsions as model lipoproteins. The result showed not deep but shallow penetration of apoA-I into the membrane interface whose polarity is intermediate between water and the hydrophobic core. [Fig. 2]

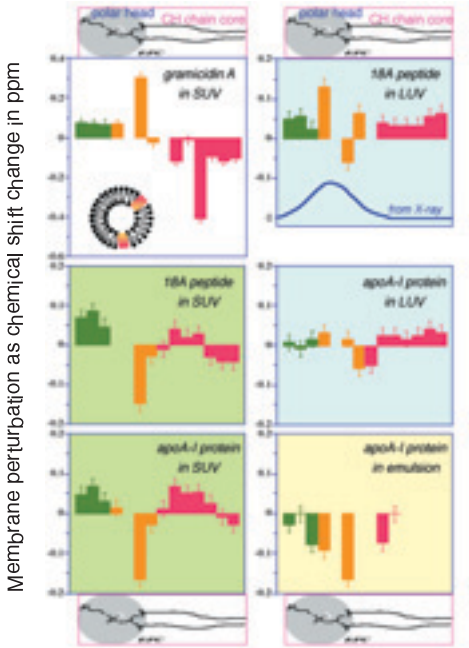


Fig. 2

1. Okamura E et al., *J. Phys. Chem. B*, **105**, 12616-12621 (2001).

## Grants

Nakahara M, Collaboratory on Electron Correlations - Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2001 - 31 March 2006.

Nakahara M, Element Organic Reactions in Super- and Subcritical Water, Grant-in-Aid for Creative Scientific Research (B) (2), 1 April 2001 - 31 March 2003.

Nakahara M, Theoretical and Experimental Studies of Aqueous Solutions under Extreme Conditions, The Japan-USA Joint Research Projects, 1 April 1999 - 31 March 2002.

Umemura J, Study of Spread Monolayers on Liquid Surface by Polarization Modulation Infrared External Spectroscopy, Grants-in-Aid for Scientific Research (B) (2), 1 April 1999 - 31 March 2002.

Hasegawa T and Umemura J, Study of Molecular Recognition Formed in Systematic Molecular Assemblies, The Japan-USA Joint Research Projects, 1 April 2000 - 31 March 2003.

Matubayasi N: Theory of Solutions in the Energy Representation from Ambient to Supercritical, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

## Awards

Matubayasi N: Helmholtz Award, NMR and computer-simulation studies of supercritical water, International Association for the Properties of Water and Steam, 9 May.

Matubayasi N: Promotion Award, Structure, dynamics, and reactions of supercritical water, Japan society of high-pressure science and technology, 21 November.

# Interface Science - Molecular Aggregates -


Prof
SATO, Naoki
(D Sc)

Assoc Prof
ASAMI, Koji
(D Sc)

Instr
KITA, Yasuo
(D Sc)

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YOSHIDA, Hiroyuki
(D Sc)


## Students

TSUTSUMI, Kiyohiko (D3) KITA, Hiroki (M2) SAKOU, Machiko (M2) YAMAMOTO, Daisuke (M2)
HIRAMATSU, Takaaki (M1) TSUTSUMI, Jun'ya (M1) YOSHIDA, Tadashi (M1)

## Visitor

Prof ZHAO, Kongshuang South China Normal University, China, 26 December 2000-25 March 2001.

## Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectroscopies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous structures in microcapsules, biopolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

## Research Activities (Year 2001)

### Presentations

Characterization of biological cells by dielectric spectroscopy, Asami K, 1st International Conference on Dielectric spectroscopy in Physical, Chemical and Biological Applications (Jerusalem, Israel), 13-15 March.

Unoccupied states of organic semiconductor thin films examined by inverse photoemission spectroscopy, Sato N, Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications (Glumslöv, Sweden), 4-7 June.

Dielectric monitoring of cell growth in culture using an inductive probe, Asami K, Zhao KS, XI International Conference on Electrical Bio-Impedance (Oslo, Norway), 17-21 June.

Electronic structures of unoccupied states in metallophthalocyanine thin films studied by inverse photoemission spectroscopy, Sato N, Yoshida H, Tsutumi K, The 7th China-Japan Joint Symposium on Conduction and Photoconduction in Organic Solids and Related Phenomena (Guangzhou, China), 18-22 November.

Thin film growth of bis(1,2-dimethylglyoximato)-platinum(II) on pseudo-Ag(111) studied by X-ray photoemission spectroscopy, Yoshida H, Takahashi R, Kita H, Sato N, The 7th China-Japan Joint Symposium on Conduction and Photoconduction in Organic Solids and Related Phenomena (Guangzhou, China), 18-22 November.

### Grants

Sato N, Precise analyses of extended electronic structures in organic thin films by means of in situ normal and inverse photoemission spectroscopies, Grant-in-Aid for Scientific Research (A) (2), 1 April 1999 - 31 March 2002.

Asami K, Bio-impedance imaging by scanning dielectric microscopy, Grant-in-Aid for Scientific Research (C)(2), 1 April 2000-31 March 2002.

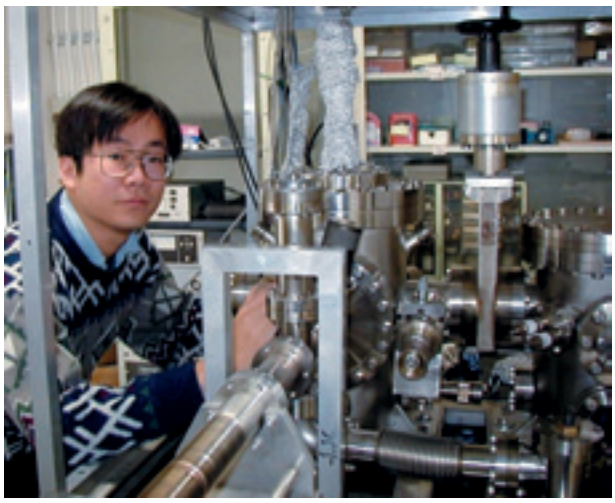
Topics

## Unoccupied electronic states of 3d-transition metal phthalocyanines (MPc: M = Mn, Fe, Co, Ni, Cu and Zn) studied by inverse photoemission spectroscopy

Unoccupied electronic states of thin films of 3d-metal phthalocyanines (MPc: M = Mn, Fe, Co, Ni, Cu and Zn) were systematically investigated in the energy range from the Fermi level to the vacuum levels using inverse photoemission spectroscopy: obtained spectra are shown in Fig. 1. The spectra obtained for NiPc and CuPc were in good agreement with spectra previously reported. Overall the features of the observed spectra were similar to each other, regardless of the substitution of the central metals. This is explained by the dominant contribution to the spectra from the macrocyclic π orbitals of the Pc framework.

Changes in the contribution of the central metal, however, cause small variations in the spectra. In our analysis of the metal contribution, we examined the difference spectra obtained by subtracting a ZnPc reference spectrum (as shown as purple-colored areas in Fig. 1). The choice of ZnPc as a reference was made because the d orbitals of the zinc ion in ZnPc are fully occupied.

The difference spectra of MnPc, FePc, NiPc and CuPc were found to agree well with the reported X-ray absorption spectra. It is thus concluded that the difference spectra reflect the density of unoccupied states derived from the central metals. The difference spectra of MnPc, FePc, CoPc, NiPc and CuPc were further tentatively assigned with the help of reported results from extended Hückel and density functional calculations.



K. Tsutsumi working on our home-built inverse photoemission apparatus; the bellows coupling seen in the front of the apparatus accommodates a low-energy electron source.

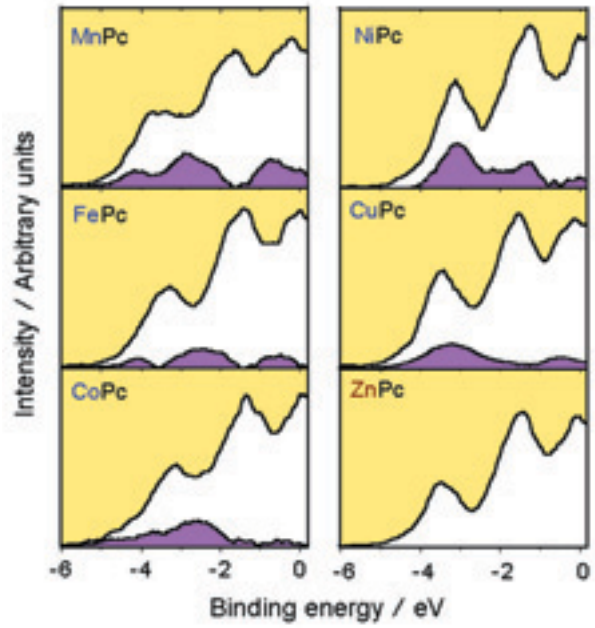



**Fig. 1.** Inverse photoemission spectra observed for evaporated thin films of MPc (M = Mn, Fe, Co, Ni, Cu and Zn). Purple-colored areas show difference spectra obtained by subtracting the ZnPc spectrum from the MPc spectra.

## Ion channels of alamethicin dimers N-terminally linked by disulfide bond

Because of structural resemblance, the helix-bundle type channels formed by alamethicin, 20-residue antibiotic peptide, in lipid bilayers are available as a model of biological channels. The channels, however, have drawbacks in single channel analysis: the multi-conductance behavior that are due to transient changes in molecularity of peptides in a helix bundle, and the voltage-gated channel formation preventing characterization of the current-voltage relation.

To overcome the drawbacks we adopted covalent alamethicin dimers, that restrict the peptide molecularity and form long lasting channels that allow us to measure the current-voltage relations by applying a fast voltage ramp during channel opening. The dimers, N-terminally linked by a disulfide bond, revealed the relationship between the channel conductance and the peptide molecularity, and demonstrated that negative fixed charges at the narrowest part of the pore much more enhanced cation-selectivity in ion permeation than those at the pore mouth.

# Interface Science - Hydrospheric Environment Analysis -


Prof
SOHRIN, Yoshiki
(D Sc)

Assoc Prof
UMETANI, Shigeo
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Instr
SASAKI, Yoshihiro
(D Sc)

Instr
OKAMURA, Kei
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NORISUYE, Kazuhiro


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KINUGASA, Masatoshi (M2)
KURAHASHI, Kensuke (M1)
MATSUMOTO, Hirofumi (M1)
NAITO, Kanako (D3)
KISHIDA, Koichi (M2)
YOSHIMOTO, Shinichi (M2)
MIKATA, Michi (M1)

## Visitor

Dr Rudolf Durny — Slovak Technical University, Slovakia, 1 December 2000

## Scope of Research

Research activities are concerned with geochemistry, oceanography, limnology and analytical chemistry, which are important basic sciences in order to realize the sustainable society. Major research subjects are as follows: (i) Biogeochemistry of trace elements in the hydrosphere. (ii) Hydrothermal activity and deep biosphere on the ocean floor. (iii) Fe-uptake mechanism of phytoplankton. (iv) Ion recognition. (v) Simulation of non-linear chemical reaction.

## Research Activities (Year 2001)

### Presentations

Determination of trace metals in the ocean by MAF-8HQ column extraction-ICP-MS, Sohrin Y, Kinugasa M, Okamura K, et al., International Congress on Analytical Sciences 2001, 8 August.

Determination of $^{240}Pu/^{239}Pu$ ratio in the ocean by using HR-ICP-MS, Norisuye K, Okamura K, Sohrin Y, et al., International Congress on Analytical Sciences 2001, 8 August.

Separation of transition metals with poly(pyrazolyl)borates by solvent extraction technique, Kitano T, Wada H (Kanazawa U.), Mukai H (Kyoto U. Educ.), et al., International Congress on Analytical Sciences 2001, 8 August.

The pursuit of siderophore secreted by marine phytoplankton *Rhodomonas ovaris*, Naito K, Suzuki M, Mito S, et al., International Congress on Analytical Sciences 2001, 10 August.

Steric control of selectivity in metal ion-selective membrane electrode based on polypyrazolylmethanes, Yoshimoto S, Mukai H (Kyoto U. Educ.), Sohrin Y, International Congress on Analytical Sciences 2001, 10 August.

Novel acylpyrazolones having crown ether moiety as intramolecular synergist, Umetani S, Ogura K (Ube Nat. C. Tech.), Yamazaki S (Nara U. Educ.), International Congress on Analytical Sciences 2001, 10 August.

### Grants


Sohrin Y, Dynamics of trace bioelements in the ocean and its effect on ecosystem, Grant-in-Aid for Scientific Research (B) (1), 1 April 2001 - 31 March 2004.

Umetani S, Design of highly selective recognition and separation system of metal ions, Grant-in-Aid for Scientific Research (C) (1), 1 April 2001 - 31 March 2003.

Okamura K, Development of *in situ* measurment system of $CO_2$ related matter in seawater for gloval warming control, NEDO Grant, 1 April 2001 - 31 March 2004.

# Topics

## Development of a deep-sea *in situ* Mn analyzer and its application for hydrothermal plume observation

This paper [1] presents the first *in situ* flow-through chemical analyzer using a chemiluminescence (CL) method in the deep sea to a depth of 5,200 m. The analyzer, called GAMOS (Geochemical Anomalies MOnitoring System), successfully determines concentration of dissolved manganese continuously *in situ* using a $H_2O_2$-luminol CL method. A detection limit of 0.23 nM was obtained. Continuous measurements of manganese performed *in situ* with the GAMOS in a hydrothermal vent plume yielded high-resolution chemical data in near real time. This detection capability will provide a more representative sampling of hydrothermal plumes over larger concentration ranges than have been possible using most previous methods and instrumentation.

1. K. Okamura, H. Kimoto, K. Saeki, J. Ishibashi, H. Obata, M. Maruo, T. Gamo, E. Nakayama and Y. Nozaki, *Mar. Chem.*, **76**, 17-26 (2001).

**Figure 1.** The *in situ* chemical analyzer GAMOS attached on the submersibel "Shinkai 6500"

## Distribution of trace bioelements in the subarctic North Pacific Ocean and the Bering Sea (the R/V Hakuho-Maru Cruise KH-97-2)

A column concentration-high resolution ICP-MS determination was applied to measuring the total dissolved concentrations of Fe, Co, Ni, Cu and Zn in seawater collected from the subarctic North Pacific (~45°N) and the Bering Sea in July–September [2]. The vertical profiles for Fe, Ni and Zn were nutrient-like. The deep water concentration of Fe was ~0.5 nM in the northeast Pacific and increased to ~1 nM in the northwest Pacific and ~2 nM in the Bering Sea. The deep water concentrations for Ni and Zn in the Bering Sea were also 1.3–2 times higher than in the North Pacific. Fe and Zn were depleted in surface water of the subarctic North Pacific. The relationship between these trace elements and nutrients suggests that these elements could be a limiting factor of phytoplankton productivity. In the Bering Sea, surface water contained ~0.3 nM of Fe. The Zn concentration, which was less than the detection limit in surface water, increased at shallower depths (~30 m) compared with the subarctic North Pacific. These results imply a higher flux of Fe and Zn to surface water in the Bering Sea. This in turn may cause the Bering ecosystem characterized by a dominance of diatoms and high regenerated production.

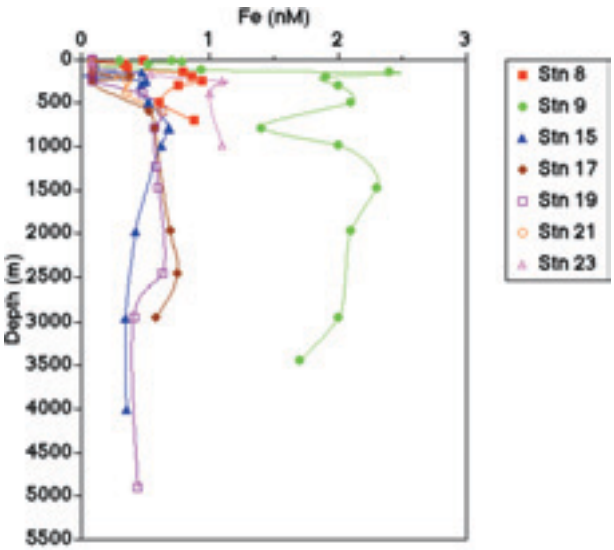


**Figure 2.** Vertical profiles of dissolved Fe in the Bering Sea (Stn. 8 and 9) and the subarctic North Pacific (Stn. 15-23).

2. Y. Fujishima, K. Ueda, M. Maruo, E. Nakayama, C. Tokutome, H. Hasegawa, M. Matsui and Y. Sohrin, *J. Oceanogr.*, **57**, 261-273 (2001).

## Award

Okamura K, The ICR Award for Young Scientists.

# Solid State Chemistry - Artificial Lattice Alloys -

Prof
SHINJO, Teruya
(D Sc)

Assoc Prof
HOSOITO, Nobuyoshi
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### Students

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OHKOUCHI, Takuo (M1)
MIZUTANI, Masahiro (M1)
OKUNO, Takuya (D1)
SHINGAKI, Yukihiro (M2)
JIKO, Norihiro (M1)

### Visitors

Assoc Prof SUN Huiyuan Hanbei Normal University, China, 1 October 2000 – 30 September 2001

Dr BACZEWSKI Lech Tomaz Institute of Physics, Polish Academy of Sciences, Poland, 1 April 2001 - 30 June 2001

## Scope of Research

Metallic multilayer films have been prepared by ultrahigh vacuum deposition method. Magnetic and electric transport properties of metallic multilayers have been studied by various techniques including $^{57}$Fe and $^{119}$Sn Mössbauer spectroscopy , x-ray magnetic scattering, and neutron diffraction. Microstructured films such as wires and dots have been successfully prepared by electron beam lithography and novel magnetic and transport properties are investigated.

## Research Activities (Year 2001)

### Presentations

Magnetic structure of Gd layers in Fe/Gd multilayer films by resonant x-ray magnetic scattering, Hosoito N, Hashizume H (NAIST), Ishimatsu N (JAERI), et al., MML2001, 26 June, Annual Meeting of Phys. Soc. Jpn., 17 September.

Field dependent orientation of sublattice magnetizations in FeRh/NiFe bilayers by Mössbauer spectroscopy, Hosoito N, Nyvlt M (Charles Univ.), Suzuki Y (AIST), et al., Annual Conf. on Magnetics, 25 September.

Spin density wave with the modulation commensurate to the superlattice period in Cr(001)/Sn Multilayers, Mibu K, Takeda M (Tohoku), Suzuki J (JAERI), et al., MML2001, 27 June, Annual Meeting of Phys. Soc. Jpn., 17 September.

Control of magnetic properties by nano-structural engineering, Mibu K, Shinjo T, Int. Conf. on Materials for Advanced Technologies, 4 July.

Magnetism of Cr-based multilayered Films studied using $^{119}$Sn Mössbauer spectroscopy, Mibu K, Almokhtar M, Shinjo T, ICAME2001, 7 September.

Temperature dependence of switching field distribution in a NiFe wire with a pad, Shigeto K, Ono T (Osaka), Mibu K, et al., Annual Meeting of Phys. Soc. Jpn., 29 March, MML2001, 28 June, Annual Conf. on Magnetics, 27 September.

Behavior of the vortex core in the magnetic dot under an external magnetic field, Okuno T, Shigeto T, Suzuki Y (AIST), et al., Annual Meeting of Phys. Soc. Jpn, 29 March, Annual Meeting of Phys. Soc. Jpn, 18 September.

Magnetization Configuration of domain wall injected to small contact between two NiFe sub-micron wires, Miyake K, Shigeto K, Suzuki Y (AIST), et al., Annual Meeting of Phys. Soc. Jpn, 18 September.

Conttol of magnetic structure of trilayer film –spin fan of NiFe array-, Shingaki Y, Shigeto K, Mibu K, et al., Annual Meeting of Phys. Soc. Jpn, 17 September.

# Topics

## Magnetic domain wall in a nano-contact

We report here the magnetic structure and electric resistance of a domain wall (DW) in a nano-contact between two NiFe wires. The sample was fabricated by an electron beam lithography and lift-off method (Fig. 1). The size of the prepared contact in Fig. 1 is 15 × 20 nm$^2$. The thickness of the sample is 10 nm. Figure 2 shows a magnetic force microscopy image of the trapped DW in the contact. The dark signals indicate magnetic charge distribution. The magnetization configuration inferred from a micromagnetics simulation indicates that a small 180 degree Bloch wall is confined in the nano-contact area. The magnetoresistance (MR) curves dropped abruptly when the DW was trapped in the small contact (Fig. 3). García et al. [1] experimentally observed large positive resistance change up to 300 % at room temperature by the confined domain wall in a point contact between two macroscopic Ni wires. On the other hand, we observed the negative DW contribution to the MR, which is understood on the basis of anisotropic magnetoresistance effect around the contact.

1 García et al., Phys. Rev. Lett. **82**, 2923 (1999).

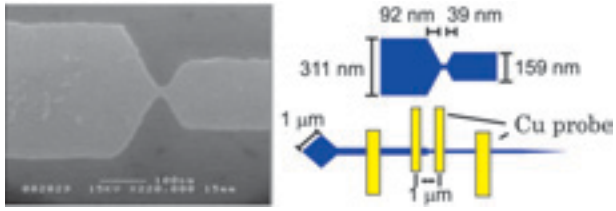


**Fig. 1** Illustration of sample structure and SEM image.

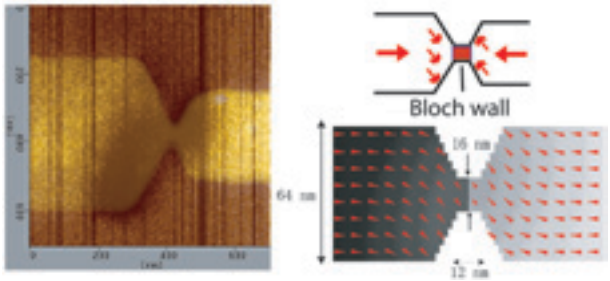


**Fig. 2** MFM image and schematic illustration of the magnetic structure.

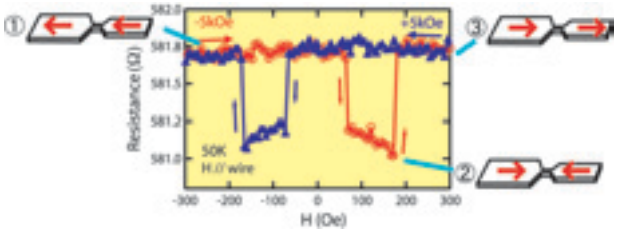


**Fig. 3** MR curves of the prepared sample at 50K.

## Magnetic structures of Fe/Gd multilayer films investigated by resonant x-ray magnetic scattering technique

Now it becomes possible to investigate magnetic structures of ferromagnetic multilayers by x-ray diffraction technique. Using a resonant x-ray magnetic scattering at Gd $L_3$ edge, magnetic depth profiles of Gd layers in the [Fe(3.53 nm)/Gd(4.85 nm)]×15 multilayer were determined. The depth-dependent average Gd magnetizations parallel and perpendicular to the applied field are shown in Figs. 4a and 4b. The external field is applied parallel to the film plane and the Gd magnetizations always stay in the film plane. While in a weak field (0.5 kOe), the depth-dependent Gd magnetizations are parallel to the applied field, the perpendicular components are observed in the field of 5.0 kOe. Such behavior is qualitatively understandable by Camley model [1]. However the model predicts a uniform magnetization profile of the parallel component in the weak field region at 10 K. The discrepancy may come from the magnetic anisotropy of the Gd layer, which is not considered in the model. The non-uniform magnetization depth profile in the field of 0.5 kOe indicates that there are depth-dependent distributions in the orientation of the Gd magnetizations and the distribution width is narrower in the interface parts of the Gd layer.

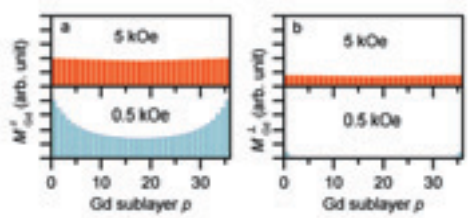


**Fig.4** Magnetic depth profiles of Gd layer in an Fe/Gd multilayer at 10K determined by resonant x-ray magnetic scattering.

1 R.E.Camley, Phys. Rev. B**35**, 3608(1987).

## Grants

Shinjo T, Magnetic fluctuation of microfabricated magnets, Grant-in-Aid for Scientific Research (C) (2), 1 April 2000 - 31 March 2002.

Hosoito N, Magnetic structures of metallic multilayers by resonant magnetic scattering of circularly polarized synchrotron X-rays, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

Mibu K, Control of Magnetic Properties of Nanoscale Magnet by Structural Engineering, Research for the Future Program of Japan Society for the Promotion of Science, 1 September 2000 - 31 March 2001, 1 September 2001 - 31 March 2002.

# Solid State Chemistry - Quantum Spin Fluids -

Prof
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## Students

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## Scope of Research

Quantum spin oxide system such as high-$T_c$ superconducting cuprates, $La_{2-x}(Ba,Sr)_xCuO_4$, $Nd_{2-x}Ce_xCuO_4$ and $Pr_{1-x}LaCe_xCuO_4$ are synthesized in the form of single crystals using traveling-solvent-floating-zone method. Detailed equilibrium phase diagram of Bi cuprate systems is investigated. Main subjects and techniques are: mechanism of high-$T_c$ superconductivity: origin of quantum phase separation in strongly correlated electron systems: spin excitations in quantum spin systems: interplay between spin and charge flow in doped spin systems: neutron scattering by using triple-axis as well as time-of flight-techniques.

## Research Activities (Year 2001)

### Presentations

Magnetic phase diagrams of electron-doped high-$T_c$ cuprates studied by μSR measurements, T. Kubo, M. Fujita, T. Uefuji, K. Yamada, I. Watanabe, K. Nagamine, Autumn Meeting, Phys. Soc. Jpn., 18 Sep., ISS 2001, 26 Sep.

Preparation of electron-doped superconductor by electrochemical reduction, K. Kawashima, M. Fujita, T. Kubo, K. Yamada, Autumn Meeting, Phys. Soc. Jpn., 18 Sep., ISS 2001, 26 Sep.

Structural effect on the stability of magnetic order in $La_{1.875}Ba_{0.125-x}Sr_xCuO_4$, H. Goka, T. Kubo, T. Uefuji, M. Fujita, K. Yamada, M. Matsuda, I. Watanabe, K. Nagamine, Autumn Meeting, Phys. Soc. Jpn., 18 Sep., ISS 2001, 26 Sep.

Electron-doping effect on magnetic order and superconductivity in $Nd_{2-x}Ce_xCuO_4$, T. Uefuji, K. Kurahashi, M. Fujita, M. Matsuda, K. Yamada, Autumn Meeting, Phys. Soc. Jpn., 17 Sep., ISS 2001, 26 Sep.

### Grants

Yamada K, Study of quantum phase separation in the transition metal oxides, Grant-in-Aid for Scientific Research on Priority Areas (Novel Quantum Phenomena in Transition Metal Oxides), 1 April 2000 - 31 March 2003.

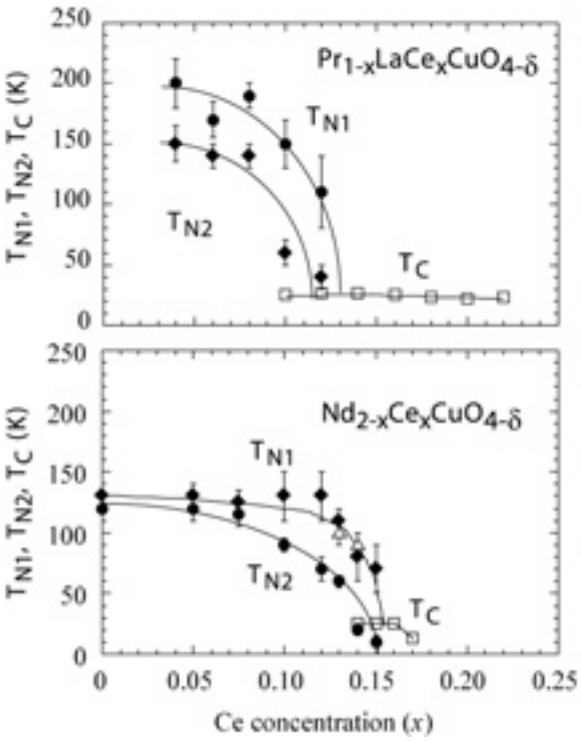
Yamada K, Study of magnetic correlation and cooperative/competitive phenomena of electronic conductivity in the localized/itinerant electron systems, Grant-in-Aid for Scientific Research (A), 1 April 2000 - 31 March 2002.

Fujita M, Study of High-$T_c$ superconductivity mechanism in the electron-doped cuprates, Grant-in-Aid for Encouragement of Yong Scientists, 1 April 2001 - 31 March 2003.

Topics

## Magnetic phase diagrams of NCCO and PLCCO investigated by means of μSR measurements

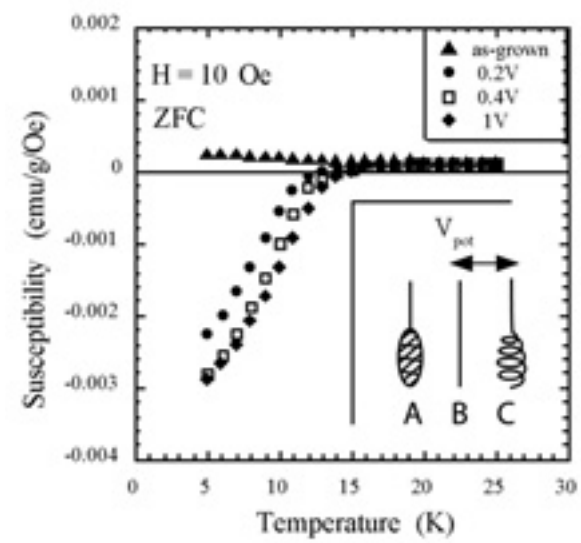
Magnetic phase diagrams of electron-doped high-temperature superconducting cuprates $Nd_{2-x}Ce_xCuO_{4-\delta}$ (NCCO) and $Pr_{1-x}LaCe_xCuO_{4-\delta}$ (PLCCO) have been studied by means of muon spin relaxation and rotation (μSR) measurements. Two characteristic temperatures $T_{N1}$ and $T_{N2}$ are defined in the zero-field μSR (ZF-μSR) measurements for both NCCO and PLCCO. Below $T=T_{N1}$, which approximately corresponds to the previously reported Néel temperature, an exponential type muon spin relaxation firstly appears in the time spectra and upon cooling below around $T_{N2}$ another faster component of relaxation or muon spin rotation is observed similarly. Although critical concentration for the superconductivity is different between the two systems, antiferromagnetic (AF) phase commonly contacts with the superconducting phase. In contrast to the hole-doped superconductivity the electron-doped superconductivity is more drastically terminated by the AF order.




Magnetic phase diagrams of PLCCO and NCCO.

## Preparation of electron-doped superconductor by electrochemical reduction

Electrochemical reduction processes were performed using the opposite chemical reactions to the electrochemical oxidation. As shown in the right figure, we succeeded in preparing superconducting $Nd_{1.85}Ce_{0.15}CuO_4$ samples from the insulating as-grown samples using electrochemical reduction, though the obtained $T_c$ ~15K is lower than that of the heat-treated sample, $T_c$ ~24K. In this figure, we show the dependence on $V_{pot}$ of magnetic susceptibilities for samples treated with different $V_{pot}$ values, $V_{pot} = V_{count} - V_{ref}$ between the counter and reference electrodes in the range of 0 ~ 1V as shown in the inset. We, furthermore, performed the electrochemical reduction under various conditions as functions of $V_{pot}$ and treating time. However, the maximal diamagnetism at 5K and $T_c$ were nearly the same. One of the reasons for such small diamagnetic signal and low $T_c$ compared to heat-treated samples may be due to a small mobility of oxygen atoms inside the sample, which causes the inhomogeneous distribution of oxygen atoms.




Magnetic susceptibilities of $Nd_{1.85}Ce_{0.15}CuO_4$ samples reduced at various $V_{pot}$ for 1day. The inset shows a schematic drawing of the configuration of three electrodes. A, B and C denote a working electrode, a reference electrode and a counter electrode, respectively.

# Solid State Chemistry -Solid State Chemistry-

Prof
TAKANO, Mikio
(D Sc)

Assoc Prof
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Res (pt)
ICHIKAWA, Noriya
(D Eng)

Res (pt)
HAYASHI, Naoaki
(D Sc)

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YAMAMOTO, Masamichi (M2)
KAN, Daisuke (M1)
YAMADA, Ikuya (M1)
CHU, Shucheng (RS)
ISHIWATA, Shintaro (D2)
NINJBADGAR, Tsedev (D1)
YOSHIDA, Hirohumi (M2)
KOBINO, Masashi (M1)
TANAKA, Kazunori (RS)

### Visitors

Alexei Belik NIMS, Japan, 6 November 2001

## Scope of Research

Novel inorganic materials that have new, useful or exotic features such as superconductivity, ferromagnetism and quantum spin ground state are synthesized by novel methods. Recent topics are:

· High-$T_c$ superconducting copper oxides with higher $T_c$ or $J_c$.
· Perovskite-based compounds with unusual magnetic and electronic properties.
· Low-dimensional spin system showing dramatic quantum effects.

## Research Activities (Year 2001)

### Presentations

Epitaxial films of perovskite-type oxides containing 3d transition metal ions in unusually high valence states, Terashima T, Hayashi N, Takano M, The 2nd International Workshop on Novel Quantum Phenomena in Transition Metal Oxides, 25 August.

Material search and single crystal growth at high pressures of several GPa -0,1,2,3 dimensional compounds, Azuma, M, Takano M, Spring Meeting, Phys. Soc. Jpn., 29 March.

Single crystal growth of transition metal oxides at high pressures of several G Pa, Azuma M, Saito T, Takano M et al., AIRAPT, 24 July.

Pressure induced structural transition of spin ladder compound $SrCu_2O_3$, Azuma M, Yoshida H, Takano M, et al., AIRAPT, 26 July.

### Grants

Terashima T, Preparation and properties of epitaxial thin films of oxides containing transition-metal ions in unusually high-valence states, Priority Area Grants from the Ministry of Education, Science, Culture and Sport of Japan, 1 April 2000 - 31 March 2003.

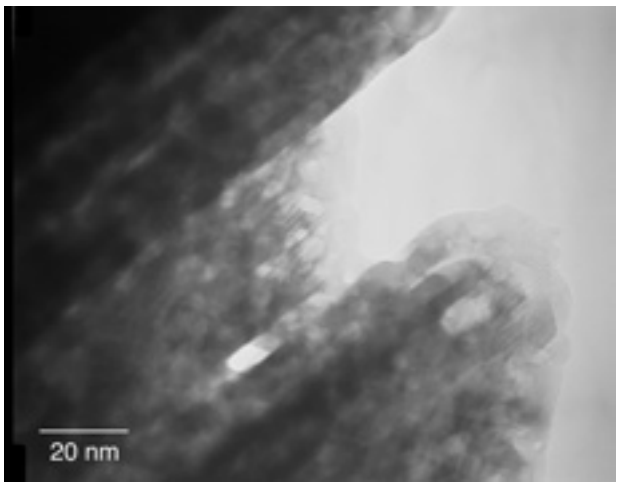
Azuma M, Physical properties of oxychloride superconductor crystals grown at high pressures. Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2003.

Azuma M, Exploration of photo-functions in strongly correlated electron systems of transition metal oxides, PRESTO, 1 December 2001 - 31 November 2004.

Topics

## $Na_xCoO_2$ with nano-sized pores

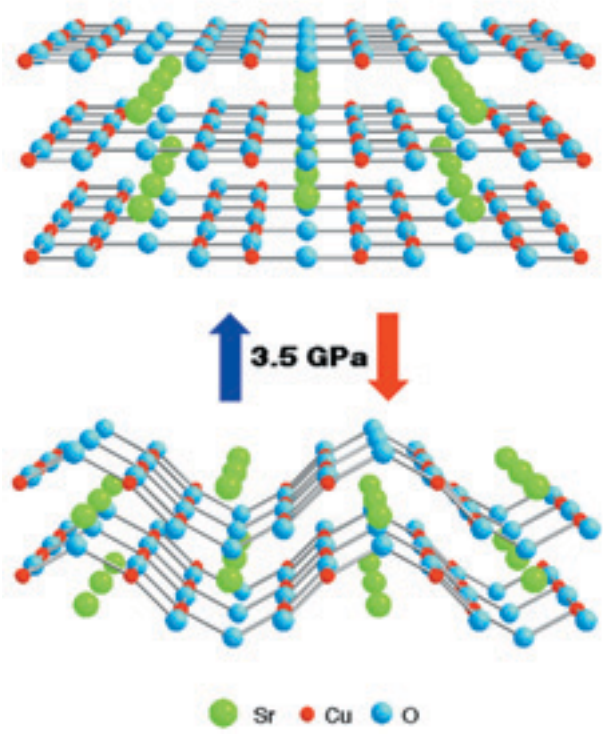
A series of studies of oxides containing "late" 3d transition metals (M's) in high valence states like $Fe^{4+}$, $Fe^{6+}$, $Co^{4+}$, $Ni^{3+}$, and $Cu^{3+}$ are in progress. The d levels of these ions are very deep because their effective nuclear charges are high, and this makes the metal-oxygen bond strongly covalent. As a result, oxides containing tight M -O- M networks like perovskites show metallic conductivity, ferromagnetism, superconductivity, high thermoelectric performance, and other intriguing properties which are dominated by oxygen p-hole character. Usually these oxides are prepared under strongly oxidizing atmospheres such as an oxygen pressure of a few GPa for $CaFeO_3$, typically, generated with a costly apparatus. However, we have noticed very recently that a novel brucite-like oxide, $Co^{4+}O_2$, can be obtained with a simple flux method under mild conditions of ambient pressure and a relatively low temperature of about 600°C. Shown in the photo are the particles thus obtained. Of particular interest is the presence of nano-sized pores (~10 nm in diameter), which might find applications in the future.




## Pressure induced structural transition of $SrCu_2O_3$

$SrCu_2O_3$ is a well-known compound as typical example of quantum spin ladder synthesized at 4 GPa [1]. On the course of X-ray diffraction (XRD) study at high pressure with the aim of single crystal growth, an unexpected pressure induced structural transition at room temperature was found.

The figure shows the structures of $SrCu_2O_3$ at ambient and high pressures refined by Rietveld analysis of powder XRD data taken with a diamond anvil cell and synchrotron radiation X-ray. The structure of the high-pressure phase was similar to that of $CaCu_2O_3$. Application of an external pressure had the same effect as "chemical pressure", substitution of smaller Ca ions for Sr ions.




1. M. Azuma, Z. Hiroi, M. Takano, K. Ishida and Y. Kitaoka, Phys. Rev. Lett., **73** (1994) 3463.

# Solid State Chemistry - Amorphous Materials-

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MIZUNO, Megumi (M1)
YOSHIKAWA, Yu (B4)
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## Visitor

Dr HEO Jong Pohang University of Science and Technology, Korea, 15 January 2000 – 14 Feburary 2001

## Scope of Research

Amorphous and polycrystalline inorganic materials with various optical functions such as photorefractivity, optical nonlinearity, and photo-catalysis are the target materials in this laboratory, which in the forms of thin film and bulk are synthesized mainly by sol-gel, multi-cathode sputtering and sintering methods. The detailed correlation between structure and properties is extensively investigated to obtain highly functional materials by using X-ray diffraction techniques, high-resolution NMR, thermal analyses, various laser spectroscopies and ab initio molecular orbital calculations, and so on.

## Research Activities (Year 2001)

### Presentations

Preparation of organic-inorganic hybrid low-melting glasses, Niida H, Masai M, Takahashi M, Yoko T, Winter, Spring & Fall Meeting Ceramic Soc. Jpn 19 January, 23 March, 27 September, ICG, 2 & 3 July.

Photocatalysis in thin film $TiO_2$ electrodes, Takahashi M, Enkhtuvshin D, Mori R, Akita Y, Yoko T, Winter & Spring Meeting Ceramic Soc. Jpn 19 January, 23 March,Sol-Gel2001, 15 September. PacRim4, 6 November.

Photoresponce of doped and undoped silica glasses, Ichii K, Sako A, Takahashi M, Uchino T, Yoko T, Spring meeting, JSAP., 3 March, LPM2001, 17 May, Meeting on Glasses and photonics materials, 2 November, PacRim4, 6 November. BGPPGW, 4 July, ICG, 6 July

Dispersion of nonlinear absorption coefficients of tellurite glasses by nonlinear transmission spectroscopy, Tokuda Y, Takahashi M, Yoko T, ICG, 3 July, Fall meeting Ceramic Soc. Jpn, 27 September.

Novel pressure-induced polymorphic transition from fumed silica to transparent amorphous $SiO_2$ at room temperature Uchino T, Sakoh A, Azuma M, et al. AIRAPT-18 & HPCC-11, 24 July

### Grants

Yoko T, Photochemical reactivity of glasses, Grant-in-Aid for Scientific Research (A) (2), 1 April 2001 - 31 March 2005.

Uchino T, Mechanism of defect formation and optical functions of silica glasses under irradiation of light, Grant-in-Aid for Scientific Research, Promotive Research (A) (2), 1 April 1999 - 31 March 2001.

Uchino T, Microstructure modification and photo-induced functions of amorphous silica, Precursory Research for Embryonic Science and Technology (PRESTO), 1 April 2001 - 31 March 2004.

Takahashi M, Development of photorefractive low-melting glasses, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2005.

Takahashi M, Transient transition state of Ge-doped silica glass, Grant-in-Aid for Scientific Research Promotive Research (A) (2), 1 April 1999 - 31 March 2001.

Takahashi M, Development of active optical integrated

# Topics

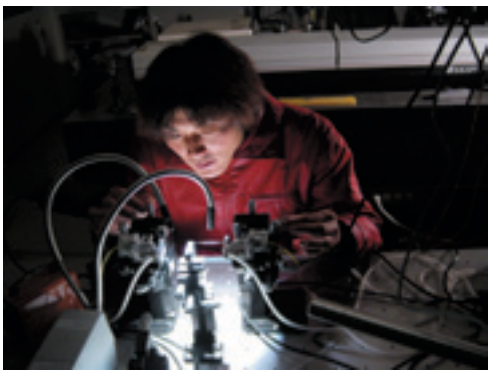
## Preparation of low-melting hybrid glasses through non-aqueous acid-base reaction

Organic-inorganic hybrid glasses of new type low-melting glasses with a melting temperature of less than 200°C have been successfully prepared through a non-aqueous acid-base reaction. Such a low-melting hybrid glass has a bright prospect of finding many applications as advanced active photonics devices in addition to conventional low temperature glass-to-metal sealant because of the easy fabrication in the forms of optical fiber and waveguide and the high solubility of optically active organics.

Preparation of low-melting glass inside the dry-box.

## Large photoreftactivity in Ge-doped silica glasses waveguide

High photorefractive glasses based on silicon dioxide are of great importance as materials for active/passive optical devices in the field of dense and rapid information processing systems. Glasses have long been playing a crucial role in the optical telecommunicating systems as optical fibers. All optical signal processing is, however, strongly required. For this reason, the development of glass materials with large photorefractivity is now the most vigorous field in the photonics community.



Measurements of transmission loss in waveguide by using fiber-coupling apparatus.

Very recently, we have succeeded in the preparation of high Ge-doped $SiO_2$ thin film with a very large photorefractivity of $\Delta n > 10^{-3}$ by the p-CVD process, which is one order of magnitude larger than the value reported so far. Based on the precise investigation of defect photochemistry in the Ge-doped silica glass by means of spectroscopy and computer simulations, it is clarified that the photosensitivity of $Ge^{2+}$ species embedded in the glass during preparation process is the origin of photoactivity such as photorefractive and induced nonlinearity.

## Photocatalysis in advanced $TiO_2$ film electrodes

Since the discovery of water decomposition on the illuminated $TiO_2$, a large number of works on the application and fundamental aspects of photo-catalytic effect of the $TiO_2$ electrode have been reported. They are mainly related to the self-cleaning, chemical energy generation, and photovoltaic devices. In order to realize $TiO_2$-based photocatalytic devices with a visible photo-response, we are trying to apply a new concept of effective carrier separation in the space charge layer to the preparation of $TiO_2$-based film electrode by using the sol-gel process and the multi-cathode helicon sputtering method.

Multi-cathode helicon sputtering apparatus and the preparation chamber (top view).

## Grants (continued)

circuit based on oxide glasses, Industrial Technology Research Grant Program, NEDO, 1 November 1999 – 31 March 2003.

Takahashi M, Development of low-melting glasses with large photorefractivity, Nippon Sheet Glass foundation, 1 April 1999 – 31 March 2002.

Tokuda Y, Structure and optical nonlinearity of chalcogen-containing glasses, Grant-in-Aid for Scientific Research, Promotive Research, 1 April 1999 – 31 March 2003.

Donations from three companies and four private company foundations

## Awards

Uchino T, Vittorio Gottardi Prize, Studies on the structure and properties of glasses, International Commission on Glass, 2 July.

Takahashi M, Award for young scientists, Studies on the optical properties and structure of photonic glasses, Ceramics Society of Japan, 17 May.

Niida H, A E Owen Student Poster Award First Prize, Preparation, properties and structure of organic-inorganic hybrid low-melting glasses, Society of Glass Technology, 6 July.

# Fundamental Material Properties - Molecular Rheology -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### Visitor

Dr Geoff R. Davies — University of Leeds, UK, 12 January 2001

## Scope of Research

The molecular origin of various rheological properties of materials is studied. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluids while heterogeneous polymeric systems exhibit plasticity in addition to these features. For a basic understanding of the features, the molecular motion and structures of various scales are studied for polymeric systems in deformed state. Measurements are performed of rheological properties with various rheometers, of isochronal molecular orientation with flow birefringence, and of autocorrelation of the orientation with dynamic dielectric spectroscopy.

## Research Activities (Year 2001)

### Presentations

Investigation of entanglement dynamics of flexible polymer chains, Watanabe H, Matsumiya Y, APS, 13 March, 3rd PRCR, 9 July, ICAPP, 30 October, 2nd ISAR, 15 November.

Viscoelasticity of polymer solutions, Osaki K, Inoue T, 4th IDMRCS, 22 and 24 June, 3rd PRC R, 9 July.

Rheo-optical studies on amorphous polymers, Inoue T, Osaki K, 3rd PRCR, 10 July.

Rheology of block copolymers, Watanabe H, Matsumiya Y, 3rd PRCR, 10 July, ICAPP, 30 October

### Grants

Osaki K, Molecular rheology of amorphous polymer studied by electric birefringence, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2003

Watanabe H, Rheo-dielectric behavior of entangled chains, Grant-in-Aid for Scientific Research (C) (2), 1 April 2000 - 31 March 2002

Inoue T, Molecular rheology of polymer solids, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003

Osaki K, Viscoelasticity of living anionic systems, Grant-in-Aid for Scientific Research, , 1 April 2000 - 31 March 2002

Matsumiya Y, Effect of branching and molecular weight distributions on entanglement relaxation, Grant-in-Aid for Scientific Research, , 1 April 2001 - 31 March 2003

Watanabe H, Development of platform for designing high functional materials, JCII, 1 April 1998 - 31 March 2002

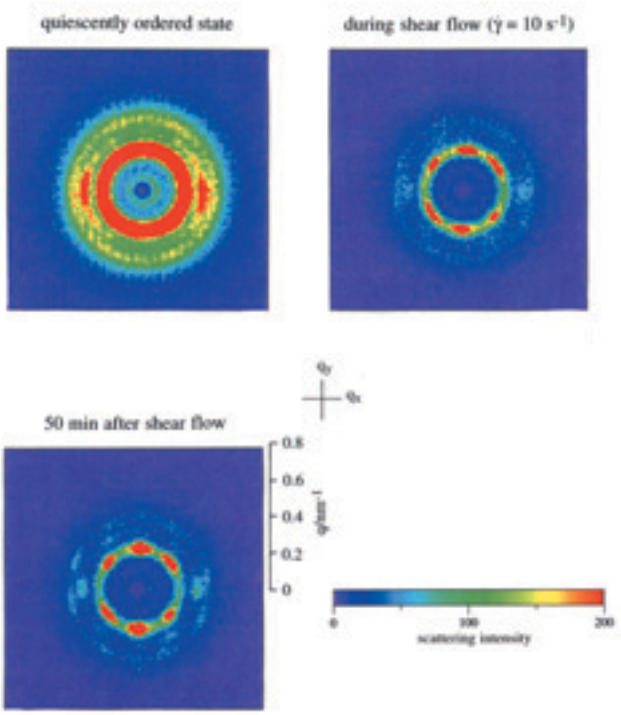
### Award

Osaki K, SROJ Award for 2001, Nonlinear rheology of polymeric systems, Society of Rheology, Japan, 17 May 2001

Topics

## Equilibrium elasticity of diblock copolymer micellar lattice.

In concentrated solutions of styrene-butadiene (SB) diblock copolymers in a B-selective solvent, n-tetradecane (C14), spherical micelles with S cores and B corona form cubic lattices because of the osmotic constraint for the corona conformation. The equilibrium modulus $G_e$ of the micellar lattice is proportional to the number density $\nu$ of the corona blocks but the magnitude of $G_e$ is smaller, by a factor ~ 10, than the modulus $G_e^o$ (= $\nu k_B T$; $k_B T$ = thermal energy) expected for the simplest case of the entropic elasticity of the corona [1]. The origin of this difference between $G_e$ and $G_e^o$ was examined in this study [2]. The $G_e$ of a model SB/C14 micellar lattice (having deutrated S cores) was measured before and after imposition of steady shear. SANS measurements revealed that the quiescently ordered, polycrystalline lattice was orientated after the shear to have less defects; see Figure. This structural change hardly affected $G_e$, suggesting that the defects were not the main factor raising the large difference between $G_e$ and $G_e^o$. Thus, this difference was attributed to the osmotic constraint for the corona conformation [2]: This constraint should force neighboring corona blocks to have mutually correlated conformations (thereby leading to the micellar lattice formation). Such correlated corona blocks cannot behave as independent entropic strands. This correlation possibly reduced the effective number density of the entropic strands to give $G_e < G_e^o$.



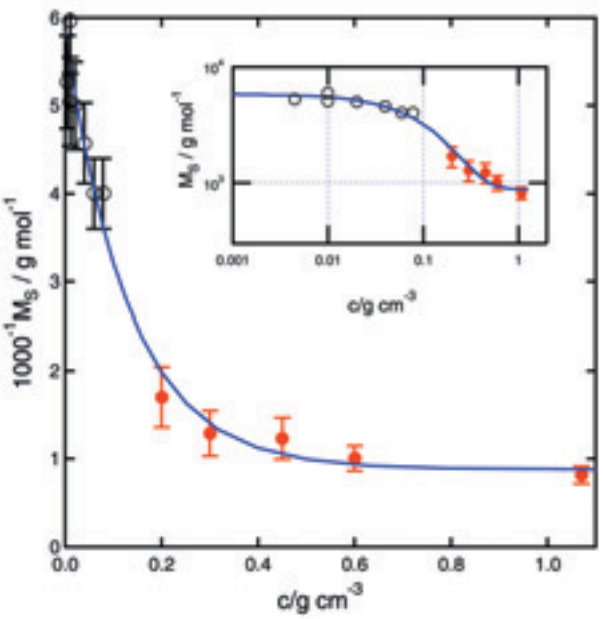

1. H. Watanabe, *Acta Polymerica*, 48, 215(1997).
2. H. Watanabe, Y. Matsumiya, T. Kanaya, and Y. Takahashi, Macromolecules, 34, 6742(2001).

## The significance of the Rouse segment

The Rouse segment is the smallest unit of global motions that are responsible for viscoelastic relaxation. The molecular weight of the Rouse segment, $M_S$, can be estimated with rheo-optical methods using birefringence measurements. Measurements on bulk polystyrene showed that $M_S$ ~ 900. This value agrees with molecular weight of the Kuhn segment size, $M_K$, which is a measure of statistical flexibility of the chain.[1] On the other hand, in dilute solutions, $M_S$ for polystyrene was reported as 5000 although $M_K$ is almost constant.[2]

Recently, we obtained $M_S$ data covering the concentration regime 0.2 ~ 1 gcm$^{-3}$.[3] (See Figure) $M_S$ changes remarkably around c = 0.1gcm$^{-3}$, suggesting that screening of the intermolecular interactions may affect the size of the Rouse segment.

The Rouse segment size is related with the initial orientation of chain induced by instantaneous step deformation. Large $M_S$ in dilute regime implys that deformation of chain in dilute solutions is heterogenous in local scales.




1. T. Inoue and K. Osaki, *Macromolecules*, **29**, 1595(1996).
2. D. J. Massa,J. L. Schrag, and J. D. Ferry, *Macromolecules*, **4**, 210(1971).
3. T. Inoue, Uematsu, and K. Osaki, *Macromolecules*, in press.

# Fundamental Material Properties -Polymer Materials Science-

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## Scope of Research

The structure and molecular motion of polymer substances are studied using mainly scattering methods such as neutron, X-ray and light with intention of solving fundamentally important problems in polymer science. The main projects are: the mechanism of structural development in crystalline polymers from the glassy or molten state to spherulites; the dynamics in disordered polymer materials including low-energy excitation or excess heat capacity at low temperatures, glass transition and local segmental motions; formation processes and structure of polymer gels; the structue and molecular motion of polyelectrolyte solutions; the structure of polymer liquid crystals.

## Research Activities (Year 2001)

### Presentations

*In situ* microscopic observation of crystallization process of PET by a rapid temperature jump method, Nishida K, Matsuba G, Kaji K, Kanaya T, Polymer Symposium (Kobe), Soc. Polym. Sci. Jpn., 6 July.

Microscopic observation of frozen structure of melt-crystallization process of PET, Okuyama T, Nishida K, Kaji K, Kanaya T, Polymer Symposium (Kobe), Soc. Polym. Sci. Jpn., 6 July.

Microscopic observation of glass-crystallization process of PET, Konishi T, Nishida K, Kaji K, Kanaya T, Polymer Symposium (Kobe), Soc. Polym. Sci. Jpn., 6 July.

A novel concept in mechanism of polymer crystallization and its application for the control of higher order structure of polymer materials, Nishida K, Kaji K, Kanaya T, Matsuba G, Okuyama T, Konishi T, Meeting of the POVAL COMMITTEE, 7 July.

Self organization in polymer crystallization - Microphase separation during the induction period and structure control - (invited), Kaji K, the 32nd Joint Autumn Meeting, General Association for Chubu Branches of Chemistry-Related Societies, Jpn., 6 October.

Fast process in glass-forming polymers (invited), Kanaya T, Tsukushi I, Kaji K, The Fourth International Discussion Meeting of Relaxations in Complex Systems, Crete, Greece, 20 June.

Hierarchic structure of polymer gels revealed by WANS, SANS and USANS (invited), Kanaya T, International Symposium on Advanced Utilization of Research Reactor, Kumatori, Japan, 28 February.

Spinodal decomposition and syneresis of gels, Takahashi N, Takeshita H, Kanaya T, Nishida K, Kaji K, Autumn Meeting, Soc. Polym. Sci. Jpn., 13 September.

Phase diagram of polyelectrolyte solutions, Nishida K, Kaji K, Kanaya T, Autumn Meeting, Soc. Polym. Sci. Jpn., 14 September.

Structure and dynamics of polymer micelles as studied by small-angle neutron scattering and neutron spin-echo techniques, Kanaya T, Watanabe H, Nagao M, Kaji K, Monkenbusch M, Richter D, Autumn Meeting, Soc. Polym. Sci. Jpn, 14 September.

### Grants

Kaji K, Kanaya T, Fukao K, Imai M, Preparatory mechanism of polymer crystallization, Grant-in-Aid for Scientific Research (B) (2), 1 April 2000 - 31 March 2002.

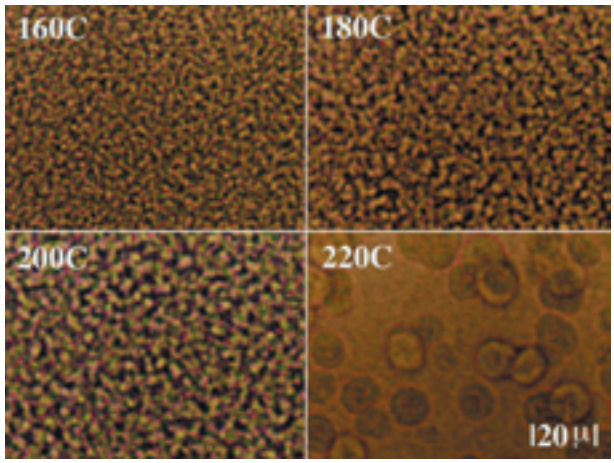
Kanaya T, Ebisawa T, Tasaki S, Glass transition mechanism of polymers, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

Nishida K, Control of higher order structures of polymer materials by a rapid temperature jump method, Industrial Technology Research Grant Program by New Energy and Industrial Technology Development Organization (NEDO) of Japan, 1 April 2001 - 31 March 2003.

Topics

## A finding of spinodal decompositon-assisted crystal nucleation in polymers

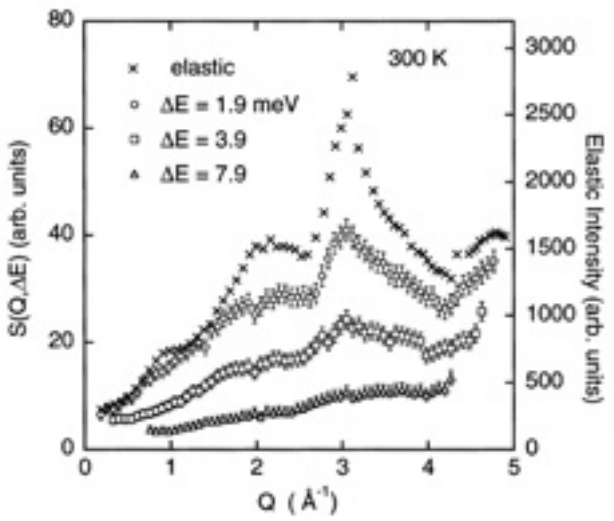
About ten years ago we found a surprising phenomenon that a spinodal decomposition (SD) type phase separation due to the orientation fluctuations of rigid segments occurs prior to crystal nucleation. Recently it has been revealed that this is a new type of crystal nucleation. The well-known homogeneous crystal nucleation occurs at high temperatures above the binodal $T_b$ directly from the melt in the liquid-crystal coexistence domain, while the SD-assisted crystal nucleation does belew spinodal temperature $T_s$. The figure shows the optical micrographs for crystallization of poly(ethylene terephthalate) where a sudden change of morphology from an SD pattern to a spherulitic or nucleation-and-growth pattern is seen above $T_s = 213$°C [1].




1. K. Nishida, K. Kaji, T. Kanaya, G. Matsuba, T. Okuyama and T. Konishi, *Meeting Report of the Poval Committee*, **No.118**, 55 (2001).

## Evidence for localization of the Boson peak in glassy PMMA

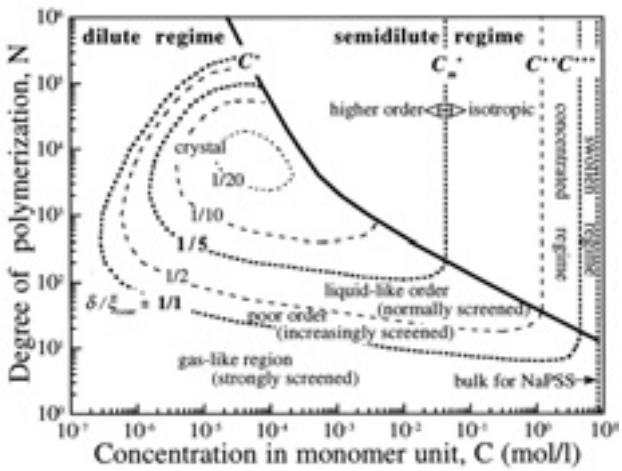
One of the most important but controversial problems in dynamics of glassy materials is the origin of the boson peak and the picosecond fast process observed in many glass-forming materials [1]. In this work [2], we carried out coherent inelastic neutron scattering measurements on glassy poly(methyl methacrylate) (PMMA) to elucidate the spatial scale of the boson peak and the fast process. Comparing the observed $Q$ dependence of the inelastic scattering intensity at various excitation energies $\Delta$E with that of the elastic scattering (see figure), we found that the boson peak and the fast process modes do not move in phase at a length scale of ~7Å, suggesting that they are localized modes on two monomers within a PMMA chain.




1. T. Kanaya, K. Kaji, *Adv. Polym. Sci.*, **154**, 87 (2001).
2. T. Kanaya, I. Tsukushi K. Kaji, B. J. Gabrys, S. M. Bennington, H. Furuya, *Phys. Rev.* **B64**, 144202 (2001).

## Phase diagram of polyelectrolyte solutions

We have presented an improved phase diagram of polyelectrolyte solutions as functions of the degree of polymerization and the concentration [1]. This new phase diagram was drawn for salt-free solutions of vinyl-type polyelectrolytes, and the main improved points are the dilute-semidilute crossover concentrations, which were determined from the recent experimental data on the polyion persistence length. The concentrated regime and the swollen regime were newly introduced according to our findings. Furthermore, the degrees of orderliness in the dilute regime were specified according to the ratio $\delta/\xi_{cent}$ of the amplitude of thermal fluctuations to the mean intermolecular distance. Thus, the new phase diagram considerably well describes the realistic structure of polyelectrolyte solutions.




1. K. Nishida, K. Kaji and T. Kanaya, *J. Chem. Phys.*, **115**, 8217 (2001).

# Fundamental Material Properties - Molecular Dynamic Characteristics -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YAMADA, Shusaku (D1)
NAKAMURA, Hisako (M2)
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TSUJITANI, Kouji (B4)

## Scope of Research

The research activities in this subdivision cover structural studies and molecular motion analyses of polymers and related low molecular weight compounds in the crystalline, glassy, liquid crystalline, solution, and frozen solution states by high-resolution solid-state NMR, dynamic light scattering, electron microscopy, X-ray diffractometry, and so on, in order to obtain basic theories for the development of high-performance polymer materials. The processes of biosynthesis, crystallization, and higher-ordered structure formation are also studied for bacterial cellulose.

## Research Activities (Year 2001)

### Presentations

Molecular Dynamics Simulation of Conformation and Dynamics for Liquid Crystalline Polyether, Ishida H, Maekawa Y, Horii F, et al., Annual Meeting, Soc. Polym. Sci., Jpn., 24 May.

Structural Analysis of Polyether Crystallized from the Liquid Crystalline Glass, Murakami M, Ishida H, Horii F, Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 14 September.

Structure and Optical Properties of σ–π Conjugated Polymers with Different Silylene Chain Lengths [I] Analysis of Conformation by Solid-State NMR Spectroscopy, Yamada S, Kaji H, Horii F, Annual Meeting, Soc. Polym. Sci., Jpn., 23 May.

Dynamic Properties of Cellulose Triacetate in Methyl Acetate in Dilute-Semidilute Solution Region, Tsunashima Y, Mizuno M, Horii F, Annual Meeting, Soc. Polym. Sci., Jpn., 24 May.

Dynamic Clustering of Cellulose Triacetate in Solution as Measured by Dynamic Light Scattering (Prague, Czech), Tsunashima Y, IUPAC Czech Chemical Society, 11 July.

Dynamics and Structure Formation of Cellulose Triacetate in Dilute Solution, Tsunashima Y, Onodera G, Horii F, Soc. Polym. Sci., Jpn., 13 September.

Dissipative Structures and Non-Ergodic Scattering in Solution of Cellulose Acetates in Couette Flow (New York, USA), Tsunashima Y, SUNY Chemical Society, 14 December.

TEM structure analysis of band-like cellulose assemblies produced by *Acetobacter xylinum* at low temperature, Hirai A, Tsuji M, Horii F, Annual Meeting, Soc. Polym. Sci., Jpn., 23 May.

Structure changes of band-like cellulose assemblies produced by *Acetobacter xylinum* during low temperature cultivation, Hirai A, Tsuji M, Horii F, Annual meeting, Cellulose Soc. Jpn, 13 July.

Aggregated state of cellulose molecules produced by *Acetobacter xylinum*, Hirai A, Tsuji M, Horii F, Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 12 September.

Study on the new microbe isolated from reservoir rock. 2. Structures on different levels for cellulose produced, Horii F, Hirai A, Kuwabara K, et al., Annual meeting, Cellulose Soc. Jpn, 13 July.

Conformational Analyses of Poly(ethylene naphthalene-2,6-dicarboxylate) by Two-Dimensional Double-Quantum Solid-State NMR Spectroscopy, Inui N, Kaji H, Horii F, et al., Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 12 September.

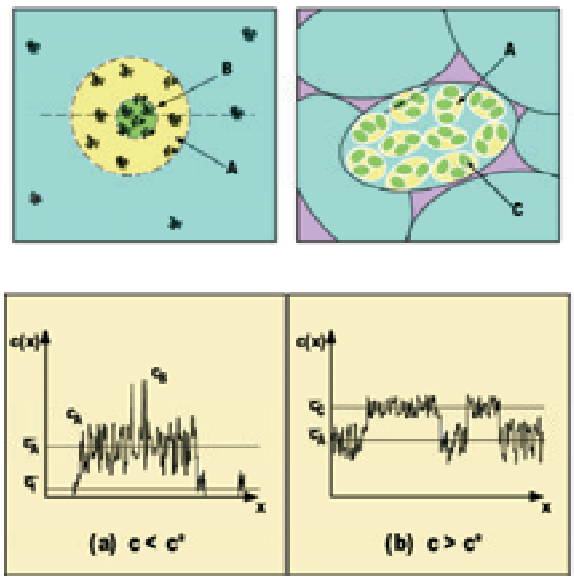
Topics

## Dynamic Self-Assemblies of Cellulose Acetates in Polar Solvents

**Abstract.** Dynamics of cellulose diacetates (CDA, the degree of substitution DS=2.44, Mw = $1.70\times10^5$, Mw/Mn = 1.23) in polar solvents, dimethylacetamide (DMAc), was investigated at 2–60°C through dynamic light scattering (DLS) in quiescent state. CDA formed a few types of structures in polar solvents; a single CDA chain and the dynamical self-assemblies due to concentration fluctuations, which were created temporarily and locally by a solvent-mediated hydrogen bonding between the inter-molecular C-6 position hydroxyl groups. In addition, CDA showed low-temperature solubility; CDA was expected to dissolve molecularly below –20°C, but to take a phase separation above 65°C, and exhibited a chain reorganization in dynamic structures around a middle temperature T* = 34°C. Both the correlation length and the dynamical second virial coefficients of the dynamic structures gave a discontinuity, maximum, or minimum at T*. These dynamic features could correspond to the critical fluctuations and the LCST behavior provided that T* were regarded as the critical temperature.

**Discussion.** CDA took three translational modes in DMAc, i.e., the single chain diffusion (Mode I) and two dynamical fluctuations (Modes II and III). The former gave the hydrodynamic radius $R_H$ and the latter the correlation lengths $\xi_{II}$ and $\xi_{III}$. The temperature dependence of these sizes in the temperature range of 2–62°C shows a unique feature. In contrast to the monotonic increase of $R_H$ with decreasing temperature (Mode I), $\xi_{II}$ and $\xi_{III}$ seem to show a singularity around T* = 33.8 °C in the way that they rise sharply toward a maximum or an infinity from both sides of T*. In addition, $\xi_{II}$ and $\xi_{III}$ disappear below −12 °C, and come to join into a small value above 65°C. These two features indicate that the molecular dispersion of the single chain can be achieved below −12°C and two phase separation occurs above 65°C. Thus, CDA is in the low temperature solubility system, i.e., stable at lower temperature. The extreme increase of $\xi_{II}$ and $\xi_{III}$ at T* means that Modes II and III would amplify their concentration fluctuations excessively and critically as T approaches to T*.

In accordance with the change in $\xi$, the dynamical second virial coefficients $k_{D,I}$ for the single chain changes its sign from positive (repulsive) to negative (attractive) at T*, while $k_{D,II}$ and $k_{D,III}$ for the assemblies are always negative but take zero or discontinuity at T*. The state that $k_{D,I} = k_{D,II} = 0$ would mean that the chains are unstable and that a variety of cluster formation would be amplified at T* because the intermolecular interactions are apparently cancelled out under a delicate balance between multi-order interactions acting on the chains. We could thus have an image that T* is a critical temperature in the LCST system. The peculiarity in $\xi_{II}$ and $\xi_{III}$ around T* could be recognized as the dynamic critical fluctuation. This image can be verified by double-logarithmically plotting $\xi$ and $R_H$ against $|T - T^*|$, as is the case for the usual critical phenomena. The critical exponent $\nu$ in the expression that $\xi \propto |T - T^*|^{-\nu}$ was given as 0.15, 0.68, and 1.5 for $\xi_{III}$, $\xi_{II}$, and $R_H$ at $T > T^*$, respectively. The value $\nu = 0.68$ is close to the theoretical one, 0.625. The self-assemblies discussed above are formed in a nest of structures as illustrated by Figure below, where the temporarily created excess-concentration-fluctuations c(x) at a given time spot are plotted against the local space x.




Precise Conformational Analyses of Poly(acrylonitrile) by Two-Dimensional Multiple-Quantum Solid-State NMR Methods, Kaji H, Schmidt-Rohr K (Iowa State Univ.), Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 12 September.

The analysis of $O^2H$-$\pi$ interaction in phenoxy resins by a MAS NMR method without irradiating $^2H$ nuclei, Kaji H, Horii F, Schmidt-Rohr K (Iowa State Univ.), NMR Conf. Jpn., 14 November.

The analysis of dynamics in polymers by a two-dimensional solid-state $^{13}C$ MAT technique, Fuke K, Kaji H, Isomura T, et al., NMR Conf. Jpn., 16 November.

## Grants

Horii F, Studies on effects of dynamics factors and hydrogen bonding on structure formation for main-chain thermotropic liquid crystalline polymers, Grant-in Aid for Scientific Research (B)(2), 1 April 2000 -31 March 2002.

Hirai A, Molecularly aggregated state of bacteria-produced cellulose made through nano-spinning, Grant-in Aid for Scientific Research (C)(2), 1 April 2001 -31 March 2003.

Kaji H, Precise analyses of polyamorphous structure and dynamics by advanced solid-state NMR, Grant-in Aid for Young Scientists (A), 1 April 2001 -31 March 2003.

# Organic Materials Chemistry -Polymeric Materials-

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KOH, Kyoung-moo (D1) HIROSE, Yuichi (M2) YOSHIKAWA, Chiaki (M2) MARUTANI, Eizo (M1)
KWAK, Yungwan (M1) NISHIDA, Shinya (UG) SUGIYAMA, Satoshi (UG)

## Scope of Research

Kinetic and mechanistic analyses are made for better understandings of the chemical and physicochemical reactions occurring in polymerization systems and for better routes to the synthesis of well-defined polymers. By various polymerization techniques, in particular, living polymerizations, new well-defined polymers or polymer assemblies are prepared, and their structure/properties relationships are precisely analyzed. Projects in progress include: (1) kinetics and mechanisms of living radical polymerization (LRP). (2) Synthesis of new polymeric materials by living polymerizations and their structure/properties studies. (3) Synthesis, properties, and applications of high density polymer brushes.

## Research Activities (Year 2001)

### Presentations

Kinetics of Free Radical Copolymerization, Fukuda T, IUPAC International Symposium on Free Radical Polymerization, Italy, 3-9 Jun.

Kinetics of LRP, Fukuda T, European Polymer Congress, The Netherland, 15-20 Jul.

Polymer Gels and Brushes Synthesized by LRP, Fukuda T, Gordon Research Conference on Elastomers, USA, 5-10 Aug.

LRP, Fukuda T, Summer Seminar, Soc Fiber Sci. Tech. Jpn., 5-7 Sep.

Surface Modification by LRP, Fukuda T, Controlled Polymer Synthesis, USA, 3-4 Dec.

6 Presentations, Spring Meeting, Soc. Polym. Sci, Jpn., 23-25 May. 1 Presentation, Annual Meeting, Cellulose Soc. Jpn., 12-13 Jul. 7 Presentations, Autumn Meeting, Soc. Polym. Sci, Jpn., 12-14 Sep.

### Grants

Fukuda T, Structure and Properties of High-Density Polymer Brushes, Grant-in-Aid for Scientific Research. (B)(2), 1 Apr 2000 – 31 Mar 2002.

Fukuda T, Development of Living Radical Emulsion Polymerization, Grant-in-Aid for Scientific Research. (B)(2), 1 Apr 2000 – 31 Mar 2003.

Tsujii Y, Development of New Surface-Modifying Technology by LRP Method, Ind. Tech. Research Grant Program in 2000 from NEDO, 1 Nov 2000 – 31 Mar 2003.

Kaya K, Collaboratory on Electron Correlations, Grant-in-Aid for Creative Scientific Research., 1 Apr 2001, 31 Mar 2006

Topics

## Well-Defined, High-Density Polymer Brushes Synthesized by Living Radical Polymerization

In recent years, surface modifications by polymers have been increasingly important for various applications ranging from biotechnology to advanced microelectronics. We were the first to succeed in applying atom transfer radical polymerization (ATRP), a variant of living radical polymerization (LRP), to the graft polymerization of methyl methacrylate, styrene, and functional monomers on a solid surface and yielding a graft layer of low-polydispersity polymer with the highest graft density reported to date. Atomic force microscopic and ellipsometric studies revealed that in such a graft layer, polymer chains are highly extended in a good solvent, nearly to their full lengths, and that the properties of these high-density polymer brushes are quite different and unpredictable from those of the "moderately dense" polymer brushes previously studied. In addition to such parameters as graft density, chain length, chain length distribution of the graft polymer, the morphology of the grafted surface was successfully controlled by the combination of surface-initiated LRP with a lithographic technique. These techniques and findings will open up a new route to "precision" modification of surfaces.

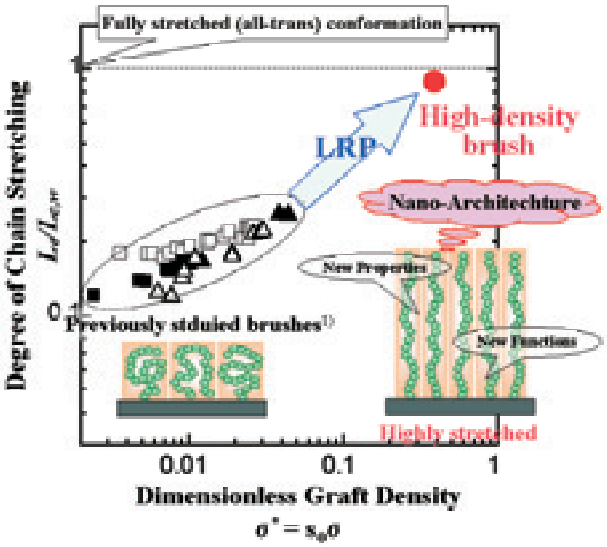


**Figure 1.** Relationship between graft-chain conformation and graft density in a good solvent. The vertical axis represents $L_e/L_{c,w}$, where $L_e$ is the equilibrium thickness of the swollen brush and $L_{c,w}$ is the weight-average full length of the graft chain in the all-trans conformation. [1)] For example, see Kent et al., *J. Chem. Phys.* **1995**, *103*, 2320 & Bijsterbosch et al., *Langmuir* **1995**, *11*, 4467.

## A Kinetic Study on Dithioester-Mediated Living Radical Polymerization of Styrene

In order to find a clear explanation for the rate retardation in RAFT polymerization, an on-going issue of debate, the polymerization of styrene mediated by a polystyryl dithiobenzoate was studied. Electron spin resonance spectroscopy was used to determine the concentration of the intermediate radical produced by the addition of polystyryl radical to the dithiobenzoate. The polymerization was also followed by dilatometry to estimate the concentration of the growing radical. The results showed that the fragmentation of the intermediate radical is a fast process with a relevant rate constant on the order of $10^4$ $s^{-1}$ (at 60 °C) and that the intermediate radical undergoes the cross-termination with polystyryl radical to form a 3-arm star chain, thus causing a retardation in the rate of polymerization. The rate constant of cross-termination was estimated to be similar to (somewhat smaller than) that of the termination between polystyryl radicals. The formation of the star was evidenced by a model experiment, as shown in Figure 2. The star was fairly stable at 60 °C (without decomposition for 24 h).

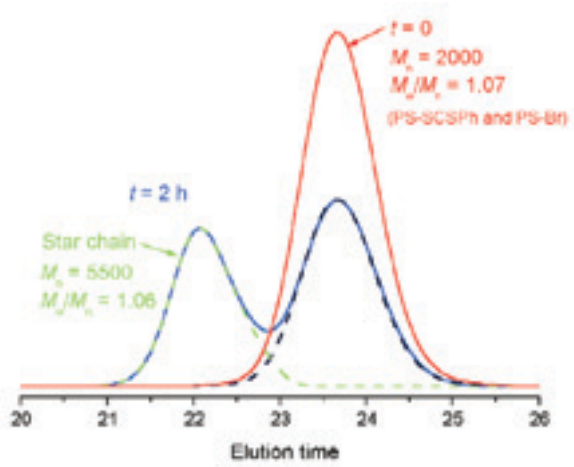


**Figure 2.** The GPC chromatogram for the mixture of *t*-butyl benzene, polystyryl dithiobenzoate (PS-SCSPh: $M_n$ = 1990, $M_w/M_n$ = 1.07), polystyryl bromide (PS-Br: $M_n$ = 2000, $M_w/M_n$ = 1.05), and CuBr complex heated for 2 h (60 °C). PS-Br is activated by the CuBr complex to give the polystyryl radical PS·. PS· will add to PS-SCSPh to form the intermediate radical, which subsequently will be attacked by another PS· and give a star chain. This system mimics the RAFT polymerization without propagation.

# Organic Materials Chemistry -High-Pressure Organic Chemistry-

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CHENG, Fuyong
(D Sc)

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KONNO, Hirofumi (M2)
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WAKAMIYA, Atsushi (D2)
INOUE, Ryota (M2)
SUZUKI, Mitsuharu (M2)
MIYATA, Yasuo (M1)
MASAOKA, Naoki (UG)

## Visitor

Prof WANG, Guan-Wu University of Science and Technology of China, 1 July 2001 - 31 August 2001

## Scope of Research

Fundamental studies are being conducted for creation of new functional materials with novel structures and properties. The major subjects are: synthetic and structural studies on novel cyclic π-conjugated systems, particularly the positively charged species stabilized by σ-π interaction; synthesis of new redox-active and supramolecular π-systems; organo-chemical transformation of fullerene $C_{60}$, specifically the synthesis of fullerene dimers and trimers by the use of mechanochemical solid-state reactions; synthesis and reactions of open-cage fullerene derivatives; generation of alkylated $C_{60}$ cation and its application for synthesis of functional materials.

## Research Activities (Year 2001)

### Presentations

Synthesis of the first planar COT annelated with bicyclo[2.1.1]hexene, Komatsu K, Matsuura A, International Symposium on Novel Aromatics, 5 August.

Generation and properties of the first alkylated $C_{60}$ cations, Kitagawa T, Takeuchi K, Komatsu K, et al., International Symposium on Novel Aromatics, 5 August; International Symposium on Reactive Intermediates and Unusual Molecules, 13 September.

Synthesis of the fullerene trimer $C_{180}$ and its STM observation, Komatsu K, Kunitake M (Kumamoto), Ito O (Tohoku), et al., Japan-Israel Binational Symposium on the Functional Supramolecular Materials, 16 October.

Synthesis and σ-π interaction of cyclic π-conjugated molecules annelated with bicyclic frameworks, Komatsu K, Nishinaga T, et al., Kyushu International Symposium on Physical Organic Chemistry, 28 November.

### Grants

Komatsu K, Design and synthesis of π-electronic and related cationic systems having σ-π interaction, Grant-in-Aid for Scientific Research on Priority Areas (A) (2), 1 April 2000 - 31 March 2002.

Kitagawa T, Development of the method of alkylating $C_{60}$ by way of alkylfullerenyl cation, Grant-in-Aid for Scientific Research (C) (2), 1 April 2000 - 31 March 2002.

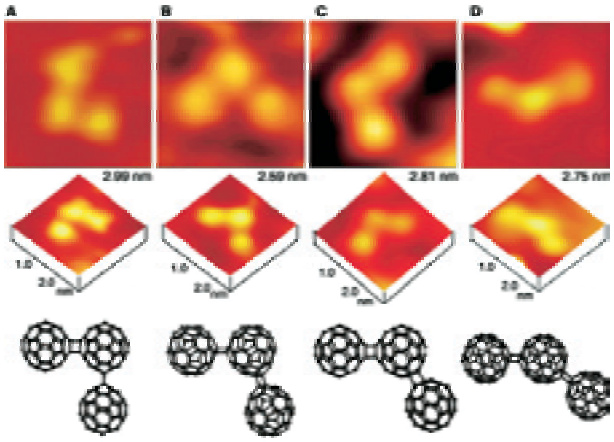
Nishinaga T, Synthesis and properties of sulfur-containing cyclic π-electronic systems annelated with bicyclic frameworks, Grant-in-Aid for Encouragement of Young Scientists (A), 1 April 2000 - 31 March 2002.

Murata Y, Transformation of fullerene $C_{60}$ using mechanochemical high-speed vibration-milling technique, Grant-in-Aid for Encouragement of Young Scientists (A), 1 April 2000 - 31 March 2002.

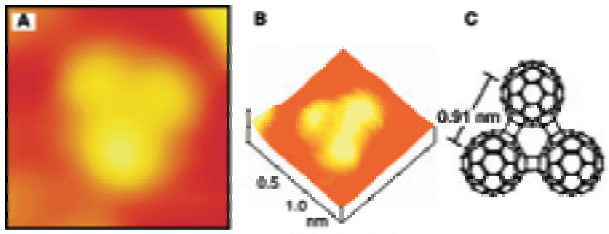
Topics

## First synthesis of fullerene trimer $C_{180}$ and its structural identification by scanning tunnelling microscopy (STM)

The fullerene dimer and trimer are the most essential subnits of the all-carbon fullerene polymers. The mechanochemical solid-state reaction of fullerene $C_{60}$ catalyzed by 4-aminopyridine was found to give not only the dimer $C_{120}$ but also the trimer $C_{180}$ albeit in a low yield (4%). The HPLC analysis indicated that $C_{180}$ consists of several structural isomers. These isomers were separated into two fractions, I and II, which were supposed to have the extended / folded structures and a cyclic structure, respectively, based on the HPLC absorption behavior and theoretical calculations. This supposition was proved by the first direct STM observation of actual images of individual isomers as shown in the figure.[1]




STM images of fraction I




STM images of fraction II

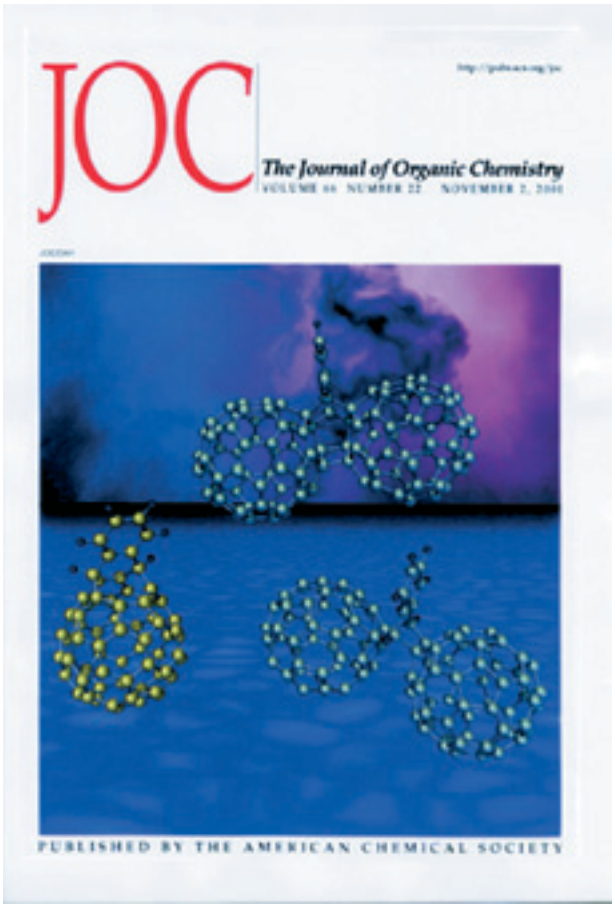
1. Kunitake M, Uemura S, Ito O, Murata Y, Fujiwara K, Komatsu K, *Angew. Chem. Int. Ed.*, in press.

## Synthesis of novel derivatives of fullerene dimers and an open-cage fullerene

The solid-state and the liquid-phase thermal reactions of fullerene $C_{60}$ with 2, 3-diazanaphthalene afforded, respectively, the $C_{60}$ dimers incorporated in a bicyclic framework (shown in silver) and a benzo-derivative of an open-cage fullerene (shown in gold) in the figure.[1] The orifice of the latter was further enlarged to a 12-membered ring by the photochemical oxidation with singlet oxygen, thus suggesting the possibility of organic synthesis of endohedral fullerenes.[2]

On the other hand, the directly connected fullerene dimer $C_{120}$ containing $^3He$ in one of the cages was synthesized by solid-state reaction, and its cyclopropanation reaction was examined. Based on the $^1H$, $^{13}C$, and $^3He$ NMR analysis on the products carefully separated by HPLC, the isomer distribution of the two types of products (A and B, shown below) was clarified. It was proved that the reactivity of the $C_{60}$ cage is not affected by incorporation of the He atom and there is appreciable magnetic interaction between the two cages.[3]


1. Murata Y, Kato N., Komatsu K, *J. Org. Chem.*, **66**, 7235 (2001).
2. Murata Y, Komatsu K, *Chem. Lett.*, **2001**, 896.
3. Fujiwara K, Komatsu K, Wang G-W, Tanaka T, Hirata K, Yamamoto K, Saunders, M., *J. Am. Chem. Soc.*, **123**, 10715 (2001).



# Synthetic Organic Chemistry - Synthetic Design -

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Assoc Prof
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(D Eng)

Res
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(D Sc)

PD (JSPS)
MAEDA, Hirofumi
(D Eng)

### Students

ITAMI, Yujiro (D3)
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KANETA, Yasuhiro (M2)
FUJIMURA, Hirokazu (M1)
FUKAZAWA, Aiko (U4)
SHIRASAKA, Toshiaki (D3)
MINAMIMOTO, Takashi (D1)
MIKI, Takashi (M2)
KATAOKA, Takeshi (M1)
UMEHARA, Teruhiko (U4)

### Visitor

FORSSIER, Kareen Ecole Polytechnique, France, 3 July 2001–23 August 2001

## Scope of Research

Our research is concerned with some new aspects in the elemento-organic chemistry, including (1) the design and synthesis of novel π-conjugated systems containing main group elements such as boron and silicon for electronic and photonic applications, (2) the synthesis, structural studies, and synthetic applications of organosilicon compounds, such as pentacoordinate silicon compounds and functionalized silyl anions, (3) the elucidation of the σ-conjugation in the polysilane framework using the configuration-constrained oligosilane model systems, (4) the old but new chemistry of the disilapropellane and related compounds, and (5) the development of new efficient reactions using main group element reagents and transition metal complex catalysts.

## Research Activities (Year 2001)

### Presentations

Main Group Organic Chemistry Directed towards Materials Science: Photophysical Properties Control by Coordination Number Change, Tamao K, Yamaguchi S, JOM Symposium on New Frontiers in Organometallic Chemistry, 27–28 August, Chicago, USA.

Chemistry of 1,6-Disila[4.4.4]propellane and Related Compounds, Toshimitsu A, Katkevics M, Sano A, Asahara M, Miki T, Fujimura H, Tsuji H, Yamaguchi S, Tamao K, 18th International Congress of Heterocyclic Chemistry, 31 July, Yokohama, Japan.

Preparation and Reactions of Sulfur-Substituted Silyllithiums, Kawachi A, Oishi Y, Kataoka T, Tamao K, International Symposium on Reactive Intermediates and Unusual Molecules, 8–13 September, Nara, Japan.

### Grants

Tamao K, Elements Scienece towards Construction of Organic and Inorganic Frameworks Focusing on Quality of Elements, Grant-in-Aid for Scientific Research on COE, April 2000–March 2005.

Toshimitsu A, Chemistry of Propeller-Shaped Cyclic Compounds Bearing Disilane as an Axis, Grant-in-Aid for Scientific Research on Priority Areas (A) "Exploitation of Multi-Element Cyclic Molecules", April 2000–March 2001.

Kawachi A, Intramolecular Reactions of Functionalized Silyllithiums with Olefins: Development and Application to Stereoselective Synthesis, Grant-in-Aid for Scientific Research No. 12750763, April 2000–March 2002.

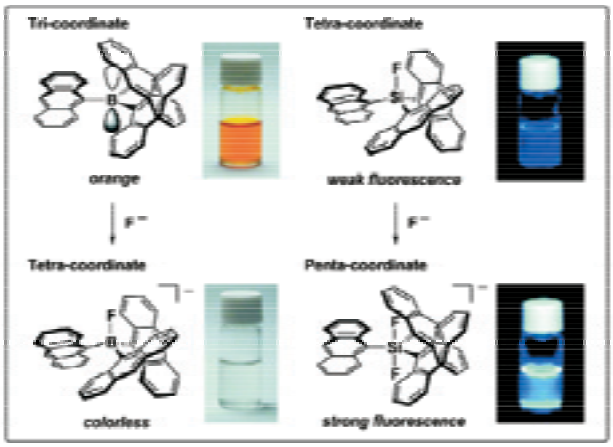
Kawachi A, New Reactions and Reactivity Control of Heteroatom-Substituted Silyl Anions, Grant-in-Aid for Scientific Research on "Molecular Physical Chemistry", No. 12042241, April 2000–March 2002.

Yamaguchi S, Elemento-Organic π-Electron Systems

Topics

## Properties Control of Main Group Element π-Electron Systems Based on Coordination Number Change

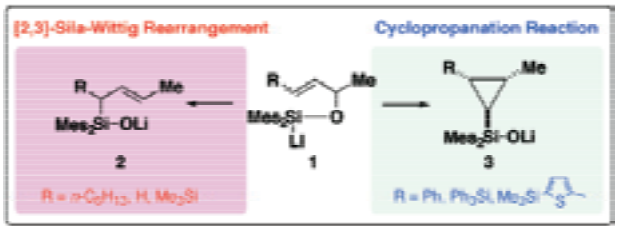
The incorporation of main group elements into π-conjugated framework enables access to new π-electron systems with intriguing photophysical and electronic properties and functions. We have explored a new possibility of controlling the properties of the π-electron systems based on a change in the coordination states of the elements. In a series of trianthryl derivatives of boron, silicon, and phosphorus, the control of the photophysical properties by changing the coordination number of the element has been achieved in various modes dependent on the element. In particular, the silicon and boron derivatives have new functions as the fluorescent and colorimetric fluoride sensors, respectively [1].




1. S. Yamaguchi, S. Akiyama, and K. Tamao, *J. Am. Chem. Soc.*, **123**, 11372 (2001).

## Substituent Effect on the Intramolecular Reactions of the [(Allyloxy)silyl]lithiums

Whereas intramolecular reactions of organolithium reagents with olefins have been extensively studied in organic synthesis, less attention has been paid to the intramolecular reactions of silyllithium reagents with olefins despite the potential utility for the regio- and stereoselective Si–C bond formation. We have investigated the substituent effect on the intramolecular reaction of the [(allyloxy)silyl]lithiums and found that the reaction modes are strongly influenced by a substituent on the terminus of the olefins [2]. In the [(allyloxy)silyl]lithiums **1**, the trimethylsilyl group and non-substituent as well as the

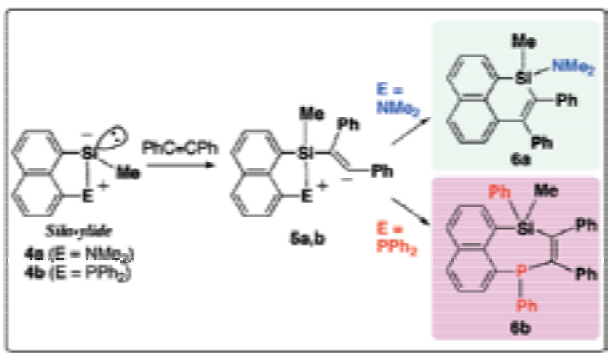



*n*-hexyl group cause the [2,3]-sila-Wittig rearrangement to afford **2** whereas the phenyl, triphenylsilyl, and thienyl groups cause the cyclopropanation reaction to yield **3**. Ab initio molecular orbital calculations revealed that the electronic effect of the substituents on the LUMO determines the reaction modes.

2. A. Kawachi, H. Maeda, H. Nakamura, N. Doi, and K. Tamao, *J. Am. Chem. Soc.*, **123**, 3143 (2001).

## Phosphonium Sila-Ylide: Reaction Pathway Different from Ammonium Sila-Ylide

While a divalent silicon species, silylene, generally has an electrophilic character, we have recently clarified that intramolecularly amine-coordinated silylene **4a** behave as a nucleophilic sila-ylide. Thus, **4a** reacts with a trapping agent such as diphenylacetylene to afford a silaphenalene derivative **6a** via a zwitterionic intermediate **5**. In contrast to this, we have now disclosed that its phosphonium analog **4b** undergoes a reaction course completely different from that of **4a** [3]. Thus, **4b** affords a seven-memberd cyclic product **6b**, through the incorporation of the acetylene between the silicon atom and the phosphorus atom accompanied by the migration of one phenyl group from phosphorus to silicon. This reaction seems to proceed through a pentavalent phosphorane intermediate or transition state structure.




3. A. Toshimitsu, T. Saeki, and K. Tamao, *J. Am. Chem. Soc.*, **123**, 9210 (2001).

for the Materials Science, PRESTO, Japan Science and Technology Corporation, December 2001–November 2004.

## Award

Kawachi A, The Chemical Society of Japan Award for Distinguished Young Chemists, 29 March.

# Synthetic Organic Chemistry - Fine Organic Synthesis -

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BAGUL, D. Trusar
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Guest Res Assoc
OZTURK, Orhan
(Ph D)

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OHTSUBO, Tadamune (D2)
TANAKA, Hiroyuki (D1)
FUKAYA, Takayuki (M2)
KUSUMOTO, Tomokazu (M2)
KAWAKAMI, Shin-pei (M2)
MORIMOTO, Tatsuya (M2)
HIRASE, Keizo (M1)
MORIKAWA, Hiroshi (M1)
NAGAOKA, Yoshie (M1)

## Scope of Research

The research interests of the laboratory include the development of new synthetic methodology, molecular recognition, and total synthesis of natural products. Programs are active in the areas of use of chiral leaving groups for an asymmetric induction, asymmetric alkylation of carbonyl compounds based on "memory of chirality", development of new type of chiral nucleophilic catalysts, utilization of 8,8'-disubstituted 1,1'-binaphthyls as a chiral controller, visualization of molecular length by functionalized phenolphthalein, use of homooxacalixarene for molecular recognition, syntheses of molecular switch, structural and functional investigation of homo- and heterochiral oligomers.

## Research Activities (Year 2001)

### Presentations

Dynamic chirality of enolates: Memory of chirality in alkylation reactions, Kawabata T, Symposium on Chiral Molecular Science of 21st Century, 7 March.

Design and preparation of a new generation of chiral nucleophilic catalysts derived from 4-hydroxyproline, Kawabata T, Stragies R, et al., The 15st French-Japanese Synposium on Medicinal and Fine Chemistry, 8 May.

Sequence-selective visual recognition of non-protected dipeptides, Tsubaki K, Fuji K, et al., 26th International Symposium on Macrocyclic Chemistry, 15 July.

Asymmetric induction based on the dynamic chirality of enolates, Fuji K, 18th International Congress of Heterocyclic Chemistry, 30 July.

Enantioselective acceleration in kinetic resolution with a chiral nucleophilic catalyst, Kawabata T, Momose Y, Fuji K, et al., 18th International Congress of Heterocyclic Chemistry, 2 August.

Memory of chirality: A new principle in enolate chemistry, Fuji K, The First NIAF-Merinos- Joint Meeting on Basic and Applied Organic Synthesis, 1 October.

Asymmetric induction based on dynamic chirality of enolates: Direct asymmetric alkylation of α-amino acids, Kawabata, T, 32th Annual Meeting of Union of Chemistry, 5 October.

### Grants

Kawabata T, Aymmetric synthesis through nucleophilic catalysis, Grant-in-Aid for Scientific Research (B) (2), 1 April 1999 - 31 March 2002.

Kawabata T, Dynamic control of stereochemistry, Grant-in-Aid for Scientific Research on Priority Areas No.706, 1 April 1998 - 31 March 2001.

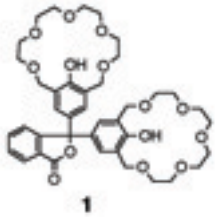
Fuji K, Construction of asymmetric environment by axially chiral molecules, Grant-in-Aid for Scientific Research (B) (2), 1 April 1998 - 31 March 2001.

Tsubaki K, Recognition and visualization of chirality by functionalized cyclic polyethers, Grant-in-Aid for Scientific Research Shorei A, 1 April 1999 - 31 March 2001.

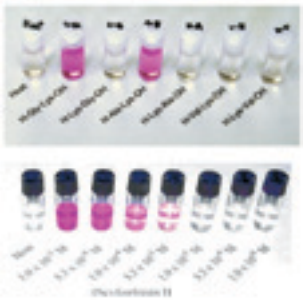
Topics

## Sequence-specific coloration of dipeptides by functionalized phenolphthalein in aqueous media

Tracing the binding of host molecules with the guests by color change attracts scientists of many disciplines and is of great fun. We have found that a receptor **1** with phenolphthalein and two crown ethers in a molecule develops brilliant purple color in the presence of dipeptides with a specific amino acid-sequence containing lysine as a *C*-terminal. This type of color development could be extended to the detection of oligopeptides of a specific sequence at the *N*-terminal (Scyliorhinin I = H-Ala-Lys-Phe-Asp-Lys-Phe-Tyr-Gly-Leu-Met-$NH_2$). Advantage of this method includes that 1) the non-protected peptides can be used as a guest molecule and 2) detection leading to color development can be performed in the aqueous solution.




1

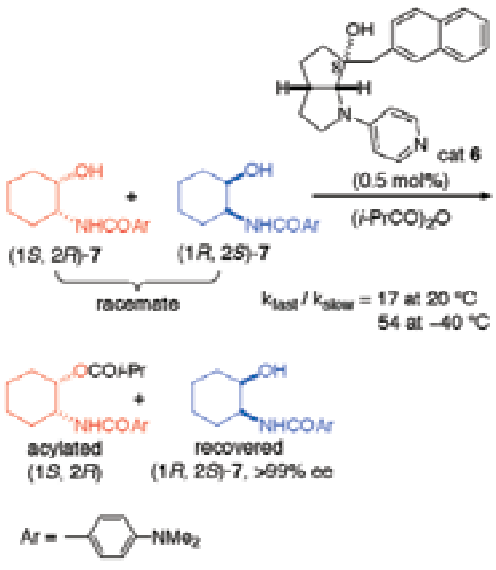


## Total synthesis of a cell cycle regulator, spirotryprostatin B

Spirotryprostatin B (**2**), a potent antimitotic agent that was isolated from the fermentation broth of *Aspergillus fumigatus* has been shown to inhibit progression of the mammalian cell cycle in the G2/M phase at micromolar concentrations. Total synthesis of **2** was performed *via* asymmetric nitroolefination. Treatment of oxindole **3** with *n*-BuLi followed by **4** gave (*S*)-**5** in 97% ee, which was successfully transformed to **2**.


## Enantioselective acceleration in kinetic resolution of racemic alcohols with a chiral nucleophilic catalyst

Development of an artificial low molecular-weight catalyst with enzymatic functions is a long-standing challenge of organic chemistry. A chiral nucleophilic catalyst **6** was developed to mimic the enantioselective acylating properties of enzyme such as lipase. Kinetic resolution of *racemic*-**7** was performed through acylation in the presence of 0.5 mol% of **6**. Enantiopure (1*R*, 2*S*)-**7** was recovered at 66% conversion. The selectivity factor {*s* = k(fast-reacting enantiomer / k(slow-reacting enantiomer)} is 17 at 20 °C and 54 at –40 °C. Kinetic study of the acylation and analysis of the reactive intermediate indicated that the discrimination of enantiomers by **6** is due to the specific acceleration of one enatiomer's reaction pathway, rather than the specific deceleration of the others'. This is in contrast to typical non-enzymatic catalysis. The observed enantioselective acceleration could be ascribed to the transition state hydrogen bonding between C(8)-OH of **6** and the carbonyl group of the fast-reacting enantiomer, (1*S*, 2*R*)-**7**.



# Bioorganic Chemistry - Organoelement Chemistry -

Prof
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NAKATA, Norio (DC2)
YAMANAKA, Rio (DC2)
HORI, Mariko (MC2)
KAJIWARA, Takashi (MC2)
SHINOHARA, Akihiro (MC2)
KIMURA, Satoshi (MC1)
MIZUHATA, Yoshiyuki (MC1)

## Scope of Research

Organic chemistry has been developed as that of second-row elements such as carbon, oxygen, and nitrogen so far, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds have been one of "dreams" for organic chemists. Our main research interest is the elucidation of the resemblance and difference in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting from the standpoints of not only fundamental chemistry but also opening the way to more extensive application of main group chemistry. Organic synthesis mediated by biocatalysts are also studied.

## Research Activities (Year 2001)

### Presentations

Synthesis and properties of compounds having novel structures containing heavier group 14 elements, Tokitoh N, Sasaki T, Sasamori T, Takeda N, 6th Int. Conference on Heteroatom Chem., 25 Jun. Nakata N, Takeda N, Tokitoh N, Xth Int. Conference on the Coord. and Organomet. Chem. of Germanium, Tin and Lead, 10 Jul. Other 21 papers were presented.

Synthesis and reactivity of low-coordinated compounds containing group 15 elements, Sasamori T, Takeda N, Tokitoh N, XVth Int. Conference on Phosphorus Chem., 31 Jul. Other 4 papers were presented.

Synthesis and reactivity of platinum-dichalcogenido complexes, Nagata K, Takeda N, Tokitoh N, XVth Int. Conference on Phosphorus Chem., 2 Aug. Other 3 papers were presented.

Organic synthesis mediated by biocatalysts, Kawai Y, Hayashi M, Tokitoh N, Molecular Chirality 2001, 8 Jun. Yamanaka R, Nakamura K, Hori M, *et al*, Biotrans'01, 4 Sep. Other 14 papers were presented.

Others, 16 papers were presented.

### Grants

Tokitoh N, Systematic studies on the synthesis, structures, and properties of aromatic compounds containing heavier group 14 elements, Grant-in-Aid for Scientific Research (A) (2), 1 Apr 1999 - 31 Mar 2002.

Tokitoh N, Development of synthetic methods for novel species on the basis of the concept of steric protection, Grant-in-Aid for Scientific Research on Priority Areas (A) (2), 1 Apr 1999 - 31 Mar 2002.

Kawai Y, Studies on the novel enzymatic reaction mechanisms taking into account the enzyme fluctuations, Grant-in-Aid for Scientific Research (C) (2), 1 Apr 2000 - 31 Mar 2002.

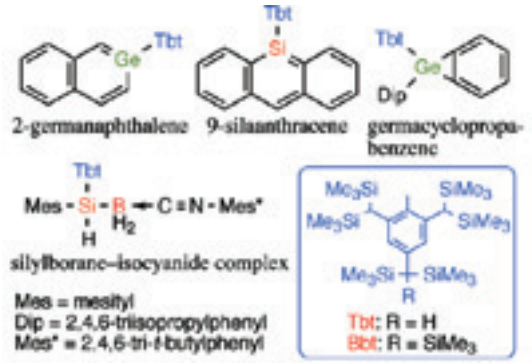
Takeda N, Synthesis of novel multiple-bond species of silicon by taking advantage of silylene-isocyanide complexes and their properties, Grant-in-Aid for Encouragement of Young Scientists, 1 Apr 2001 - 31 Mar 2003.

# Topics

## Synthesis and properties of compounds having novel structure containing heavier group 14 elements

In recent decades, the chemistry of compounds having novel structure containing heavier group 14 elements has been extensively studied. We have developed novel steric protection groups, 2,4,6-tris[bis(trimethylsilyl)methyl]phenyl (Tbt) and 2,6-bis[bis(trimethylsilyl)methyl]-4-[tris(trimethylsilyl)methyl]phenyl (Bbt), which are very useful for the kinetic stabilization of various highly reactive species of main group elements.

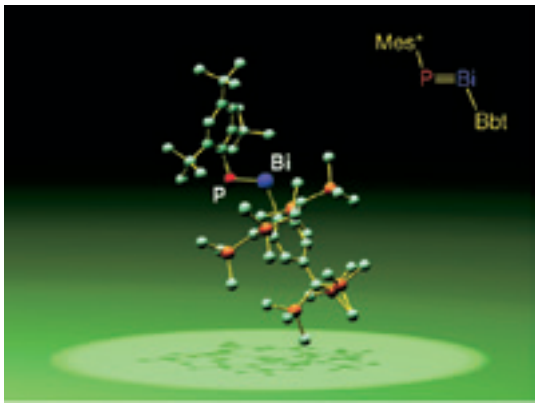
We succeeded in the synthesis of the first stable 2-germanaphthalene, 9-silaanthracene, germacyclopropabenzene, and silylborane-isocyanide complexes by taking adventage of Tbt group, and elucidated their interesting properties. Especially, it is noteworthy that the 2-germanaphthalene is the first neutral germaaromatic compound.




## Synthesis of the first stable phosphorus-bismuth double-bond compound

In recent years there has been much interest in compounds with a double bond between heavier group 15 elements. However, there is no heteronuclear doubly bonded system between phosphorus and bismuth, *i. e.*, phosphabismuthene. We now report the synthesis of the first stable phosphabismuthene by taking advantage of the Bbt group, which is also effective for the synthesis of distibene, dibismuthene, and stibabismuthene.

Condensation of Mes*$PH_2$ with BbtBi$Br_2$ using 1,8-diazabicyclo[5.4.0]undec-7-ene as a base afforded the first stable phosphabismuthene Mes*P=BiBbt, which is also the first stable double-bond compound between the third and sixth row main group elements.

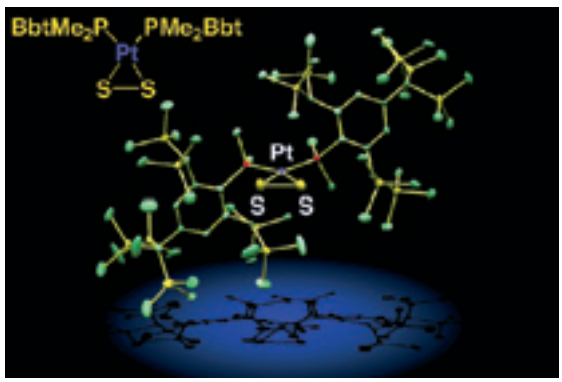



Molecular structure of Mes*P=BiBbt.

## Synthesis and properties of the first platinum-dichalcogenido complexes

Much attention has been paid to transition metal complexes with a disulfur or diselenium ligand, which are heavier congeners of well-studied dioxygen complexes. However, the platinum complexes with disulfur and diselenium (*i. e.*, $PtE_2$ ring systems) remain unknown.

The first platinum disulfur and diselenium complexes have been synthesized by taking advantage of new bulky phosphine ligands $ArMe_2P$ (Ar = Tbt or Bbt). These complexes have a square planar geometry and a three-membered $PtE_2$ (E = S, Se) ring.




Molecular structure of $(BbtMe_2P)_2PtS_2$.

## Awards

Nakata N, Symposium Poster Award, 6th Symposium of the Soc. of Silicon Chem., Jpn., Reactivity of kinetically stabilized 2-germanaphthalene, the Soc. of Silicon Chem., Jpn., 16 Nov.

Nagata K, Symposium Lecture Award, 80th Annual Meeting of the Chem. Soc. Jpn., Syntheses and properties of novel three-membered cyclic platinum complexes having a dichalcogenido ligand, the Chem. Soc. Jpn., Dec.

Kawai Y, 5th Japanese Symposium on the Chem. of Biocat., Best Poster Award, Characterization of nitroalkene reductases, The Committee of 5th Japanese Symposium on the Chem. of Biocat., 14 Dec.

Yamanaka R, 5th Japanese Symposium on the Chem. of Biocat., Best Poster Award, Asymmetric reduction of ketones by cyanobacteria, The Committee of 5th Japanese Symposium on the Chem. of Biocat., 13 Dec.

Yamaguchi H, 5th Japanese Symposium on the Chem. of Biocat., Best Poster Award, Purification and characterization of α-keto ester reductase from streptomyces coelicolor A3(2), The Committee of 5th Japanese Symposium on the Chem. of Biocat., 14 Dec.

# Bioorganic Chemistry - Bioactive Chemistry -

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NIWA, Miki (RS)
WAKAKO, Naoya (U4)
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KIWADA, Tatsuto (M2)
KONDO, Yumi (M1)
ITAZU, Masako (U4)
SUZUKI, Tomoki (D2)
DOI, Yoshihide (M2)
SHIRAISHI, Yasuhisa (M1)
HAJI, Akiko (U4)
NOMURA, Akiko (D2)
NAKASE, Ikuhiko (M2)
HADA, Shintaro (M1)
YOSHIMOTO, Rei (U4)

## Scope of Research

The major goal of our laboratory is to elucidate the molecular basis of the activity of various bioactive substances by biochemical, physicochemical, and synthetic approaches. These include studies on the mechanism of sequence-specific DNA cleavage by antitumor or carcinogenic molecules, studies on the DNA recognition of zinc-finger proteins, and model studies on the action of ion channels. In addition, artificial designed peptides have also been developed as useful tools in molecular biology and potentially in human medicine.

## Research Activities (Year 2001)

### Presentations

Multiconnection of identical zinc finger: implication for unit modulation of the three zinc finger domain, Nagaoka M, Kaji T, Imanishi M, Hori Y, Nomura W, Sugiura Y, Annual meeting, Pharm. Soc. Jpn., 28 March.

Design of artificial novel zinc finger peptides, Nagaoka M, Sugiura Y, 10th international conference on bioinorganic chemistry, 30 August.

Design of artificial multi zinc finger protein: regulation of DNA binding mode by alteration of linker sequence, Nomura W, Shiraishi Y, Nagaoka M, Sugiura Y, 11th symposium on the role of metals in bilogical reaction, biology and medicine, 25 May.

Translocation of various arginine-rich peptides and the potential of these peptides as carriers for intracellular protein delivery, Futaki S, Suzuki T, Ohashi W, Yagami T, Tanaka S, Ueda K, Sugiura Y, 2nd international peptide symposium, 10 June.

Argnine-rich peptides that translocate through cell membranes, Futaki S, Suzuki T, Nakase I, Niwa M, Ohashi W, Sugiura Y, 16th symposium on biofunctional chemistry, 20 September.

### Grants

Sugiura Y, Architecture of transcription regulation: creation and functional analysis of multi-zinc finger, Grant-in-Aid for Scientific Research (B) (2), 1 April 2000 - 31 March 2002.

Sugiura Y, Regulation of cellular gene function by novel DNA bending finger, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2004.

Futaki S, Creation and intracellular delivery of novel peptides for the regulation of transcription, Grant-in-Aid for Scientific Research (B) (2), 1 April 2000 - 31 March 2003.

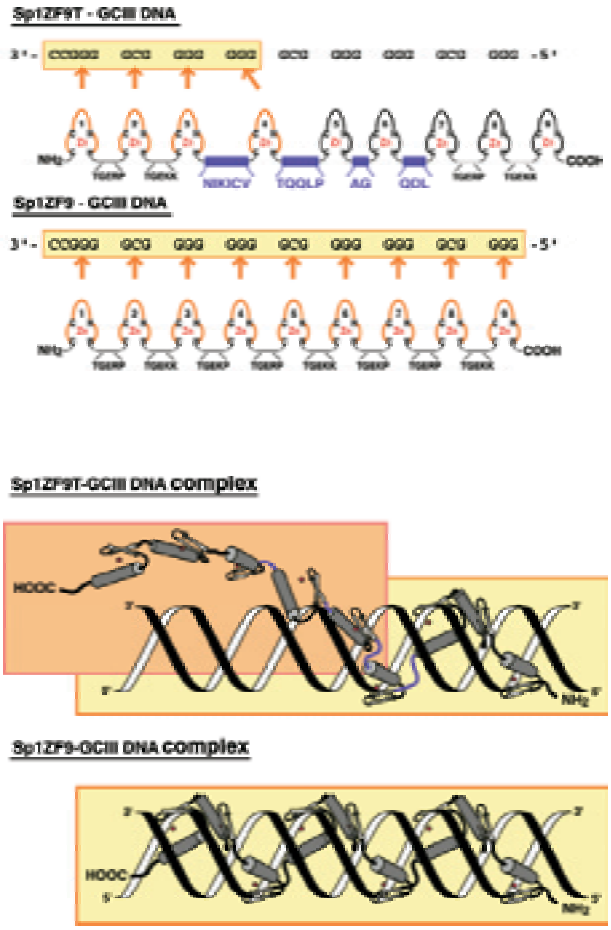
Futaki S, Design of membrane-current regulatory systems using assembly modulation of transmembrane peptides by extramembrane signals,Grant-in-Aid for Scientific Research on the Priority Area of Molecular Synchronization for the Design of New Materials, 1 April 2001 - 31 March 2003.

Nagaoka M, Design of metallofinger with novel functions: transcription regulation based on the metal substitution in zinc finger, Grant-in-Aid for Encouragement of Young Scientists (A), 1 April 2001 - 31 March 2003.

Topics

## Effect of linker sequence on DNA recognition by multi-zinc finger protein

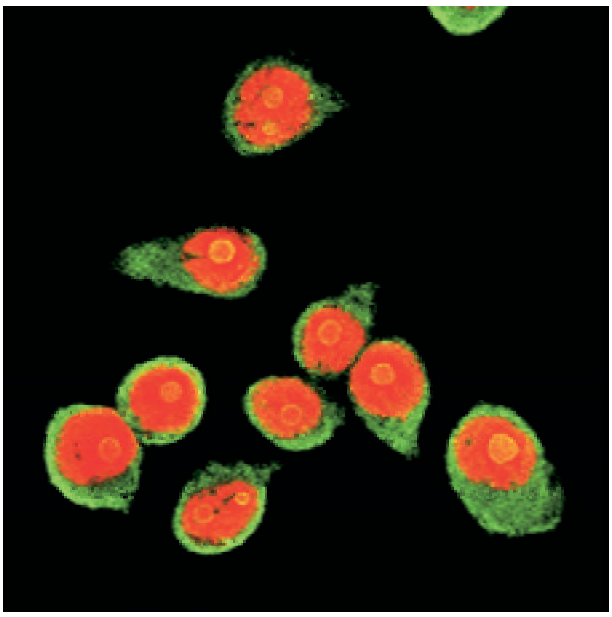
The unique linker sequence of the native nine zinc finger transcription factor IIIA (TFIIIA) appears to significantly affect its novel DNA recognition mode. An artificial new nine zinc finger peptide Sp1ZF9T has been created by connecting three units of the three zinc finger domains of Sp1 with the TFIIIA-type linker [1]. The DNA binding characteristics of Sp1ZF9T were evaluated and compared with those of the previous Sp1ZF9 with a Krüppel-type linker [2]. Sp1ZF9T forms two complex species, a short-lived species (B-2) and a long-lived species (B-1), with GCIII DNA (5'-GGG GCG GGG GGG GCG GGG GGG GCG GGGCC-3'). The B-2 complex dissociated into the free peptide and DNA, whereas the B-1 complex was stable even after 72 h. In the B-1 complex, 3'- and central portions of GCIII DNA are recognized by Sp1ZF9T. The present DNA binding mode of Sp1ZF9T is evidently different from that of Sp1ZF9. Namely, fingers 1-5 participate in the DNA contact of Sp1ZF9T, and fingers 1-9 in that of Sp1ZF9. Therefore, the linker sequence among the zinc finger domains has a significant effect on the specific DNA recognition by the multi-zinc finger proteins. To estimate the DNA contacts of the natural multi-zinc finger proteins and to design artificial zinc finger peptides with desired sequence specificity, the present results will provide useful information.




1. M. Nagaoka, W. Nomura, Y. Shiraishi, Y. Sugiura, *Biochem. Biophys. Res. Commun.*, **282**, 1001-1007 (2001).
2. T. Kamiuchi, E. Abe, M. Imanishi, T. Kaji, M. Nagaoka, Y. Sugiura, *Biochemistry*, **37**, 13827-13834 (1998).

## Intracellular protein delivery using arginine-rich basic peptides

Basic peptides derived from the HIV1-1 Tat protein and Drosophila Antennapedia protein have been reported to have the ability to translocate through the cell membranes and to carry exogenous molecules into cells. We have demonstrated that various arginine-rich RNA or DNA-binding peptides such as HIV-1 Rev-(34-50) and flock house virus (FHV) coat-(35-49) were also membrane permeable and have the ability to bring proteins into cells [1]. These results suggested that there seems to be new types of ubiquitous transmembrane mechanisms for the arginine-rich peptides. Using these peptides as carrier, establishment of novel concepts for the intracellular protein and drug delivery is expected.



1. S. Futaki, T. Suzuki, W. Ohashi, T. Yagami, S. Tanaka, K. Ueda, Y. Sugiura, *J. Biol. Chem.*, **276**, 5836-5840 (2001).

# Bioorganic Chemistry -Molecular Clinical Chemistry-

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### Guest Scholar
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CHEN, Liping (D2)
TAKANO, Emiko (RF)
BAHK, Songchul (D3)
OYANAGI, Hiroki (D2)
IIDA, Shinya (RS)

### Guest Res Assoc
STEDEFORD, Todd (D Sci)

### Visitors
Dr SUCHECKI Tomasz — Institute of Environmental Engineering of the Polish Academy of Sciences, Poland, 29 October 2001 - 8 November 2001

Mr CHAN Robert — Stanford Universiry, U.S.A., 9 July 2001 - 29 August 2001

## Scope of Research

This laboratory was founded in 1994 with the aim of linking (bio)chemical research and clinical medicine. Thus, the scope of our research encompasses the structure, function and regulation of various biomolecules, the pathophysiological significance of bioreactions in relation to human diseases, and the application of molecular techniques to clinical diagnosis and therapy. Our current interest is focused on poly(ADP-ribosyl)ation, nuclear localization of proteins in association with apoptosis, and the molecular etiology of cancer and neurodegenerative disorders including Alzheimer's disease.

## Research Activities (Year 2001)

### Presentations

A possible role of poly(ADP-ribose) synthetase in neuronal degeneration.

Ueda K. and Tanaka S. 21st Annual Meeting of the Australian Neuroscience Society in conjunction with the Asian Pacific Society for Neurochemistry, Brisbane, 28-31 January, 2001.

The effect of organic solvents on poly(ADP-ribose) synthetase activity: Implications for risk assessment.

Banasik M., Stedeford T. and Ueda K. SEPATEC/ Asia-Pacific Symposium 2001. Kanazawa, 1-2 November, 2001.

### Grants

Ueda K. Special Coordination Funds for Promoting Science and Technology from the ministry of Education, Culture, Sports, Science and Technology. 1 April 1998 - 31 March 2003.

Ueda K. A role of poly(ADP-ribose) synthetase in recovery from DNA damage. Japan Foundation for Applied Enzymology. 1 April 2001 - 31 March 2002.

Topics

## Poly(ADP-ribosyl)ation and ischemia in brain

Nitric oxide from neuronal cells plays detrimental roles in glutamate neurotoxicity and focal brain ischemia. Nitric oxide directly damages DNA, and breaks in the DNA strands activate poly(ADP-ribosyl)ation of nuclear proteins. The excessive activation of poly(ADP-ribose) synthetase (PARS) is thought to cause depletion of ATP and the energy failure leading to cell death. To clarify the involvement of poly(ADP-ribosyl)ation in ischemic insult, we examined poly(ADP-ribosyl)ation by immunohistochemical methods and tested the protective effect of 3-aminobenzamide, which is a PARS inhibitor, on focal brain ischemia using a rat model of permanent middle cerebral artery occlusion. Poly(ADP-ribosyl)ation was widely and markedly detected 2 hours after the ischemic insult in the cerebral cortex and striatum where infarction developed 24 hours later. The enhanced immunoreactivity of poly(ADP-ribose) gradually decreased, and 16 hours later, no immunoreactivity was detected. Intraventricular administration of 3-aminobenzamide 30 min before the ischemic insult decreased infaction volume in a dose-dependent manner along with the immunohistochemical reduction of poly(ADP-ribosyl)ation. Pretreatment with 7-nitroindazole, a selective neuronal nitric oxide synthetase inhibitor, partially reduced poly(ADP-ribosyl)ation. These data suggest the involvement of poly(ADP-ribosyl)ation in the development of cerebral infarction.

Ref. Tokime, T., *et al.* J. Cerebral Blood Flow Metab. 18(9), 911-997 (1998)

## Cloning and characterization of LUN, a novel RING finger protein

We isolated cDNAs encoding a novel RING finger protein (LUN), the mRNAs of which were expressed at high levels in the lung. *In situ* hybridization revealed that LUN mRNAs were expressed in the alveolar epithelium of the lung. The *LUN* gene locus was assigned to chromosome 9p21, which contains candidate tumor suppressor genes associated with loss of heterozygosity in more than 86% of small cell lung cancers. We clarified that LUN is localized to the nucleus and has a $Zn^{2+}$-dependent DNA binding activity. The amino acid 51 - 374 region of LUN is responsible for the DNA binding. Furthermore, we identified a novel palindromic binding consensus (5'-TCCCAGCACTTTGGGA-3') for the LUN binding. Interestingly, this LUN binding palindromic sequence is found in the upstream transcriptional regulatory region of the E-cadherin gene and two intervening regions of the *talin* gene. Our results suggested that LUN might be an important *trans*-acting transcriptional regulator for lung cancer-associated genes including E-cadherin and *talin* genes.

Ref. Chu, D., *et al.* J. Biol. Chem. 276 (17), 14004-14013 (2001).

## Induction of neuronal apoptosis and generation of reactive oxygen species by NAC amyloid

Amyloid deposition in senile plaque cores is one of the histopathological changes characteristic of Alzheimer's disease (AD). The AD amyloid consists of Aβ protein and many minor substances, including the non-Aβ component (NAC) of AD amyloid. NAC is a very hydrophobic peptide consisting of at least 35 amino acids derived from a precursor protein, NACP (α-synuclein). While NAC has been demonstrated to bind to Aβ and stimulate its aggregation *in vitro*, NAC displays a β-sheet structure and is amyloidogenic by itself. The exposure of cortical neurons to NAC fibrils induced apoptosis by generation of reactive oxygen species (ROS) in mitochondria. It also increased the nuclear translocation of NF-κB, and enhanced its DNA-binding activity. NF-κB is known to be activated by oxidative stress. We propose a working hypothesis that NAC interacts with Aβ protein to form amyloid fibrils and then the fibrils cause neuronal cell injury via ROS generation in mitochondria in AD brain.

Ref. Tanaka, S., *et al.* α-Synuclein/NACP and neurodegeneration. In "*Neuroscientific Basis of Dementia*" (*C. Tanaka, et al. eds.*), *Birkhäuser Verlag, Basel,* 137-141 (2001).

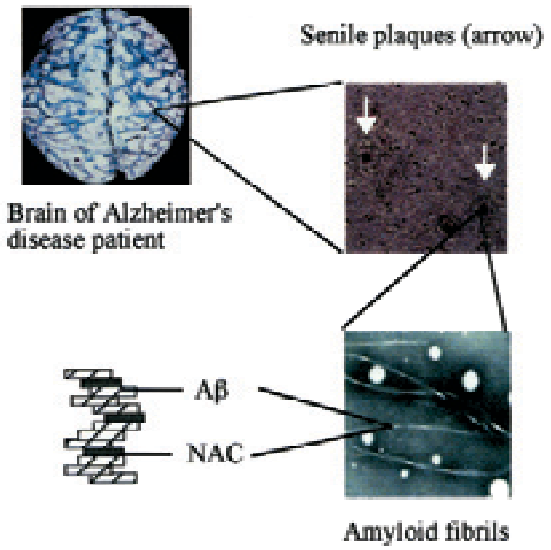


Fig. 1. NAC / Aβ amyloid in Alzheimer's disease brain

# Molecular Biofunction -Chemistry of Molecular Biocatalysts-

Prof
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(D Agr)

Assoc Prof
HIRATAKE, Jun
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MIZUTANI, Masaharu
(D Agr)

Instr
SHIMIZU, Bun-ichi
(D Agr)

Guest Res Assoc
SINGH, Inder Pal
(Ph D and D Agr)

Lecturer (Part-time) KATO, Hiroaki (D Agr) SPring8, RIKEN

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NAKANISHI, Tsugumi (D1)
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OHNISHI, Toshiyuki (M1)
NOGUCHI, Etsuko (M1)
MAEKAWA, Mika (UG)
MA, Seung-Jin (D3)
INOUE, Kazuko (M2)
SAITO, Shigeki (M2)
OKUTSU, Reiko (M1)
TACHI, Norihito (M1)
AHN, Young Ock (D1)
INOUE, Toshiki (M2)
UTSUNOMIYA, Yuji (M2)
KAI, Kosuke (M1)
YAMAGUCHI, Ayako (M1)

## Visitors

Dr ZHANG Zhengzhu Anhui Agricultural University, China, 1 October 2001 - 30 September 2002
Dr LUO Shaojun Hanzhou Tea Research Institute, China, 2 October 2001 14 October 2001

## Scope of Research

Using various techniques of Natural Product Chemistry, Organic Synthetic Chemistry, Biochemistry as well as Molecular Biology, we are trying to clarify, on molecular basis, various biological events during life cycles where many kinds of biocatalysts (enzymes) are concerned. Our research covers the comprehensive understanding of the physiological roles of various kinds of biocatalysts and receptors as well as the reaction mechanism and specificity of each enzymatic reaction. **1)** Chemical, biochemical and molecular biological studies on β-primeverosidase (EC 3.2.1.149), a diglycosidase deeply concerned with tea aroma formation. **2)** Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ-glutamyltranspeptidase and γ-glutamylcysteine synthetase. **3)** Design and synthesis of glycosyl amidines as new glycosidase inhibitors and their application for affinity chromatography. **4)** X-Ray crystallographic analysis of pyruvate phosphate dikinase from maize. **5)** Directed evolutional studies of *Pseudomonas* lipase. **6)** Molecular mechanism of the activation/inactivation process of plant hormones (brassinosteroides, gibberellins, cytokinins, *etc.*) by cytochrome P450. **7)** Molecular mechanism of plant resistance against disease infection specially interested in non-pathogenic *Fusarium* (NPF)-induced-resistance in sweet potato *(Ipomoea batatas* L.).

## Research Activities (Year 2001)

### Presentations

Presentations of each project (**1 - 7** ) are as follows:

**1)** β -Primeverosidase deeply concerned with floral tea aroma formation in oolong tea and black tea manufacturing, Sakata, K, Mizutani, M, Ma, S-J, Nakanishi, H, 11th World Congress of Food Science and Technology, Seoul, Korea, April 22-27, 2001 and **9 papers** in other meetings and symposia.

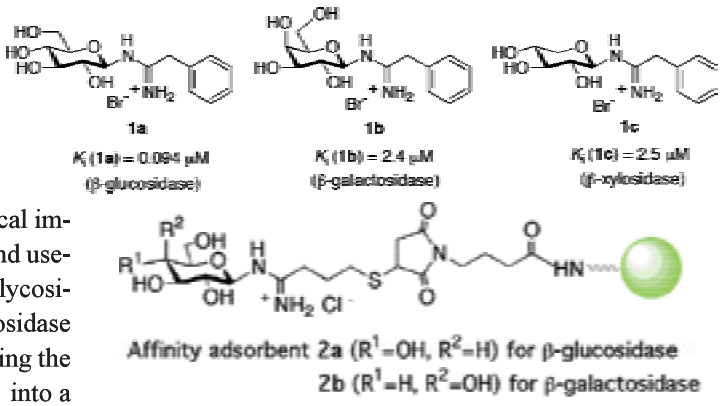
**3)** β-Glycosylamidine as Òtailor-madeÓ β- glycosidase inhibitors with high potency and selectivity, Hiratake J, Kato M, Takada M (Nihon Shokuhin Kako Co., Ltd.), Inoue K, Yamamoto M (Nihon Shokuhin Kako Co., Ltd.), Sakata K, BioTrans 2001, Darmstadt, Germany, September 2-7, 2001 and **5 papers** in other meetings and symposia.

**4)** X-Ray crystallographic study on PPDK from maize, Nakanishi, T, Nakatsu, T (RIKEN), Matsumoto, T (RIKEN) , Sakata, K, *et al.*, The 2001 Annual Meeting of

Topics

## Design, Synthesis and Applications of Selective β-Glycosidase Inhibitors, β-Glycosylamidines

Selective inhibitors of glycosidases are of critical importance in developing chemotherapeutic agents and useful probes or tools to understand the function of glycosidases. We have developed highly selective β-glycosidase inhibitors, β-glycosylamidines **1a-c**, by incorporating the property of the transition state (a positive charge) into a chair-form sugar pyranose ring. The β-glycosylamidines were synthesized readily from the corresponding glycopyranoses in two steps without using protecting groups. The β-glycosylamidines **1a-c** inhibited the corresponding β-glycosidase with an inhibition constant (*Ki*) of μM level, while they did not inhibit other glycosidases with different glycon- and stereospecificities; for example, no inhibition of α-glucosidases, α- and β-galactosidases and β-xylosidase by **1a**. The nature of the β-glycosylamidines as a "tailor-made" glycosidase inhibitor has been successfully used for affinity purification of glycosidases. Thus, the affinity adsorbents **2a** and **2b** were prepared with the β-glucosyl- and β-galactosylamidine as a ligand, respectively. A β-glucosidase from tea leaves was purified to almost homogeneity in one step from a crude enzyme extract by affinity chromatography using **2a** (Figure 1 and 2). Similarly, one-pot purification of a fungal β-galactosidase from crude enzyme preparation was also achieved by affinity chromatography on **2b**. The glycosylamidines thus promise "custom-made" preparation of glycosidase inhibitors and a useful tool for glycosidase study.



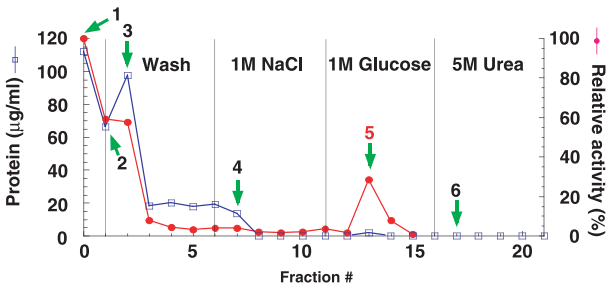




Figure 1. One Step Affinity Purification of β-Glucosidase from Tea Leaves.

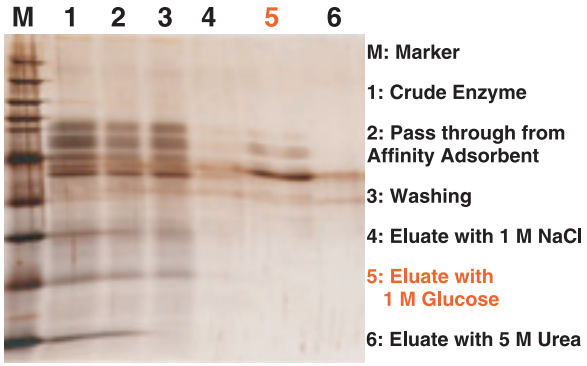



Figure 2. SDS-PAGE of Fractions Obtained by Affinity Chromatography.

Japanese Society for Bioscience, Biotechnology, and Agrochemistry, 24-27 March, Kyoto, 2001.

**5)** Random mutagenesis of lipase for amide hydrolyzing catalyst, Fujii R, Utunomiya Y, Atsushi S (Toyobo Co., Ltd.), *et al.*, BioTrans 2001, Darmstadt, Germany, September 2-7, 2001 and **3 papers** in other meetings and symposium.

**6)** Biochemical characterization of cytochrome P450s involved in brassinosteroid metabolism, Mizutani M, Ohta, D (Osaka Pref. Univ), Sakata K, 17th International Conference on Plant Growth Substances, Bruno, Czech Republic, July 4-5, 2001 and **11 papers** in other meetings and symposia.

And **5 presentations** on other reseach projects.

## Grants

Sakata K, Clarification of a new group of plant diglycosidase family, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2004.

Sakata K, A new combinatorial method to determine substrate specificities of glycosidases, Grant-in-Aid for Exploratory Research, 1 April 2001 - 31 March 2003.

Hiratake J, Bio- and organic chemical studies on glycosidases by using transition-state and substrate analogue inhibitors as a tool, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2004.

Mizutani M, Molecular mechanisms of the activation /inactivation of a plant hormone,Grant-in-Aid for Scientific Research Priority Areas [(A) 13024243] , 1 April 2001 - 31 March 2003.

Mizutani M, Investigation of the regulation mechanisms by which phytohormones control plant growth and development, Grant-in-Aid for Scientific Research from Kyoto University, 1 April 2001 - 31 March 2001.

# Molecular Biofunction -Molecular Microbial Science-

Prof
ESAKI, Nobuyoshi
(D Agr)

Assoc Prof
YOSHIMURA, Tohru
(D Agr)

Instr
KURIHARA, Tatsuo
(D Eng)

Instr
MIHARA, Hisaaki
(D Agr)

**Technicians (pt)** TANAKA, Yumi UTSUNOMIYA, Machiko
**Guest Res Assoc** Deligeer (D Sc)

## Students

| | | | |
|---|---|---|---|
| KATO, Shin-ichiro (D3) | NAKAYAMA, Daisuke (D2) | WEI, Yun-Lin (D2) | YOW, Geok-Yong (D2) |
| KWAK, Mi-sun (D1) | HIZUKURI, Yoshiyuki (M2) | IGARASHI, Motoki (M2) | KURATA, Atsushi (M2) |
| OKUBO, Fumi (M2) | AKABORI, Manami (M1) | KAKUTANI, Ryo (M1) | KOZAKI, Maiko (M1) |
| KUWANA, Eriko (M1) | MARUOKA, Naruyuki (M1) | OGAWA, Shin-ichiro (M1) | WATANABE, Shingo (RS) |

## Visitors

| | |
|---|---|
| Dr Marinus Pilon | Colorad State University, USA, 20 May 2001 - 15 Jun 2001 |
| Dr Erizabeth Pilon-Smits | Colorad State University, USA, 20 May 2001 - 15 Jun 2001 |
| Mr Valdez Michael Corpus | University of Santo Tomas, Phillippines, 7 November 2001 - 30 November 2001 |

## Scope of Research

Structure and function of biocatalysts, in particular, pyridoxal enzymes and enzymes acting on xenobiotic compounds, are studied to elucidate the dynamic aspects of the fine mechanism for their catalysis in the light of recent advances in gene technology, protein engineering and crystallography. In addition, the metabolism and biofunction of sulfur, selenium, and some other trace elements are investigated. Development and application of new biomolecular functions of microorganisms are also studied to open the door to new fields of biotechnology. For example, molecular structures and functions of psychrophilic enzymes and their application are under investigation.

## Research Activities (Year 2001)

### Presentations

Purification and characterization of glycine dehydrogenase from *Bacillus megaterium* MN223, Nakano M, Kurihara T, Esaki N, 2001 Annual Meeting, Jpn. Soc. Biosci, Biotech, and Agrochem., 24 March.

D-Amino acid metabolism of Yeasts, Yow GY, Ohkubo F, Yoshimura T, Esaki N. Annual Meeting, Jpn. Soc. Biosci, Biotech, and Agrochem., 24 March. 2001 Annual Meeting, Jpn. Biochem. Soc., 27 October.

Structural analysis of fluoroacetate dehalogenase from *Burkholderia* sp., Takahata M, Kurihara T, Esaki N, Annual Meeting, Jpn. Soc. Biosci, Biotech, and Agrochem., 24 March.

Enzymes involved in the formation of active sulfur and selenium, Mihara H, Kato S, Kurihara T, HataY, Esaki N, 2001 Annual Meeting, Jpn. Biochem.Soc., 25 and 27 October.

### Grants

Esaki N, Development and application of new psychrophilic enzymes, Grant-in-Aid for Scientific Research on Priority Areas (B), 1 April 2000 - 31 March 2001.

Kurihara T, Structures, functions and physiological roles of enzymes catalyzing formation of sulfur- and selenium-containing biofactors, Grant-in-Aid for Encouragement of Young Scientists, 1 April 2000 - 31 March 2002.

Yoshimura T, Development of new methods for recovery and elimination of trace amount of substances in water by phage display system, Grant-in-Aid for Exploratory Research, 1 April 2000 - 31 March 2002.

Esaki N, Structural biology and biosynthesis of selenium-containing proteins, Grant-in-Aid for Scientific Research (B), 1 April 2001 - 31 March 2002.

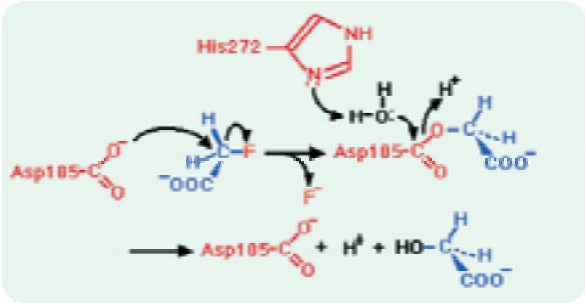
Esaki N, Construction and functional analysis of composite biocatalysts, Grant-in-Aid for Scientific Reseach on Priority Areas (B), 1 April 2001 - 31 March 2003.

Esaki N, Determination of whole genome sequence of psychrophilic bacteria, analysis of genes involved in their adaptation to cold environments, and exploitation of cold-active enzymes, Grant-in-Aid for Scientific Re-

Topics

## Probing Active-site Environment of Fluoroacetate Dehalogenase by Catalysis-Linked Inactivation with Ammonia

Fluoroacetate dehalogenase(FAc-DEX; EC 3.8.1.3) from *Moraxella* sp. B catalyzes the hydrolytic dehalogenation of fluoroacetate and other haloacetates to produce glycolate. FAc-DEX is the only enzyme that catalyzes the degradation of an aliphatic fluorinated compound by cleaving the carbon-fluorine bond, whose dissociation energy is among the highest in natural compounds. Asp105 of the enzyme acts as a nucleophile to attack the α-carbon of haloacetate to form an ester intermediate, which is subsequently hydrolyzed by a water molecule activated by His272 (Scheme 1). We found that FAc-DEX is inactivated concomitantly with defluorination of fluoroacetate by incubation with ammonia. Mass spectrometric analyses revealed that the inactivation of FAc-DEX was caused by nucleophilic attack of ammonia on the ester intermediate to convert the catalytic residue, Asp105, into an asparagine residue. The results indicates that ammonia reacted the active site of FAc-DEX without losing its nucleophilicity.

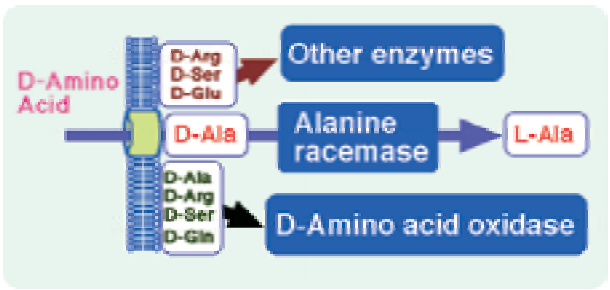



**Scheme 1**

Analysis of the three-dimensional structure of the enzyme by homology modeling showed that the active site of the enzyme is mainly composed of hydrophobic (Phe35, Tyr148, Trp151, Tyr213, and Phe273) and basic (His104, Arg106, Arg109, and His272) residues, which are considered to be essential for an ammonia molecule to retain its nucleophilicity. In a normal enzyme reaction, the hydrophobic environment is supposed to prevent hydration of the highly electronegative florine atom of the substrate and contribute to fluorine recognition by the enzyme. Basic residues probably play a role in counterbalancing the electronegativity of the substrate.

## Functional characterization of Alanine racemase from *Schizosaccharomyces pombe*

Recent discovery of the physiological importance of D-amino acids has attracted much interest in the study of metabolism of D-amino acids in eucaryotic cells. We found that fission yeast, *Schizosaccharomyces pombe,* has several enzymes acting on D-amino acids (Scheme 2). We here describe one of these enzymes, alanine racemase, encoded by the *alr1*$^+$ gene. We cloned the *alr1*$^+$ gene in *E. coli* and purified the gene product (Alr1p) with an *Mr* of 41,590 to homogeneity. Arl1p contains pyridoxal 5'-phosphate as a coenzyme and catalyzes racemization of alanine. The enzyme is almost specific to alanine, but L-serine are racemized slowly at rate of 3.7 % of that of L-alanine. *S. pombe* uses D-alanine as a sole nitrogen source, but deletion of the *alr1*$^+$ gene resulted in retarded growth on the same medium. *Saccharomyces cerevisiae* differes markedly from *S. pombe*: *S. cerevisiae*




**Scheme 2.** **D**-Amino acid metabolism in *S.pombe*

uses L-alanine but not D-alanine as a sole nitrogen source.

Moreover, D-alanine is toxic to *S. cerevisiae*. However, heterologous expression of the *alr1*$^+$ gene enabled *S. cerevisiae* to grow efficiently on D-alanine as a sole nitrogen source. The recombinant yeast was relieved from the toxicity of D-alanine.

search (B)1 April 2001 - 31 March 2002.

Mihara H, Analyses of *suf* gene cluster and Suf proteins involved in iron transport, Grant-in-Aid for Encouragement of Young Scientists, 1 April 2001 - 31 March2002.

Kurihara T, Production of useful compounds and bioremediation of environments by cryobiotechnology using cold-adapted microorganisms, (NEDO), 1 April 2001 - 31 March 2003.

Kurihara T, *In vivo* and *in vitro* analysis of selenium metabolism – a multidisciplinary approach, Cooperative Research under the Japan-U.S. Cooperative Science Program(JSPS) 1 April 2001 - 31 March 2003.

# Molecular Biology and Information - Biopolymer Structure -

Assoc Prof
HATA, Yasuo
(D Sc)

Instr
HIRAGI, Yuzuru
(D Sc)

Instr
FUJII, Tomomi
(D Sc)

### Student

HAYASHIDA, Minoru (D1)

### Assistant Researcher

AKUTAGAWA, Tohru

### Visitors

| | |
|---|---|
| Prof JOHNSON John E. | Scripps Research Institute, USA, 16 January 2001 |
| Prof VELMURUGAN Devadasan | University of Madras, India, 4 October 2001 |
| Dr RAJ S. Shanmuga Sundara | Nagoya University, India, 4 October 2001 |

## Scope of Research

Our research aims are to elucidate structure-function relationships of biological macromolecules, mainly proteins, by using X-ray diffraction method and other physicochemical methods . The following attempts have been mainly made in our laboratory for that purpose. (1) X-ray diffraction studies on protein structures in crystal and in solution are carried out by crystallographic and/or small-angle X-ray scattering techniques to elucidate structure-function relationships of proteins. (2) Molecular mechanism for myosin assembly is studied by proteolytic method, electron microscopy, and computer analysis of the amino acid sequence.

## Research Activities (Year 2001)

### Presentations

Structure-based analysis of functional sites of thermostable aspartase, Hata Y, Fujii T, Sakai H, Kawata Y (Tottori), Annual Meeting, Jpn. Soc. Biosci. Biotech. AgroChem., 25 March, Annual Meeting, Prot. Sci. Soc. Jpn., 2 June, Kyushu Symp. on Struct. Funct. Prot. Enzy., 12 July, Annual Meeting, Crystallogrr. Soc. Jpn., 3 October, Annual Meeting, Jpn. Biochem. Soc., 25 October, AsCA'01, 21 November.

Direct detection of change in protein quaternary structure by scattering method, Hiragi Y, Ichimura K (Dokkyo), Seki Y (Nagoya), et al., Annual Meeting, Prot. Sci. Soc. Jpn., 2 June, ICMSB2001, 7 September.

Analyses of enzymes involved in biogenesis of iron-sulfur cluster, Fujii T, Hata Y, Esaki N, et al., Annual Meeting, Prot. Sci. Soc. Jpn., 2 June, Annual Meeting, Jpn. Biochem. Soc., 25 October.

Differences in structural change between acid-denaturation state and urea-denaturation state of apomyoglobin, Seki Y (Nagoya), Tomizawa T (Nagaoka), Ichimura K (Dokkyo), Hiragi Y, et al., Annual Meeting, Prot. Sci. Soc. Jpn., 3 June.

Elucidation of functional regions and molecular mechanism in formation of musclemyosin fiber, Akutagawa T, Hata Y, Ooi T and Katayama E (Tokyo), Annual Meeting, Bophys. Soc. Jpn., 6 October.

Kinetics of recognition mechanism of target molecules by calmodulin, Matsufuji T (Yamagata), Jinbo Y (Yamagata), Izumi Y (Yamagata), et al., Annual Meeting, Bophys. Soc. Jpn., 7 October.

### Grants

Hata Y, Structural investigations of 2-oxo acid: ferredoxin oxidoreductases from archaea, Grant-in-Aid for Scientific Research on Priority Areas (A) (2), 1 April 2001 - 31 March 2003.

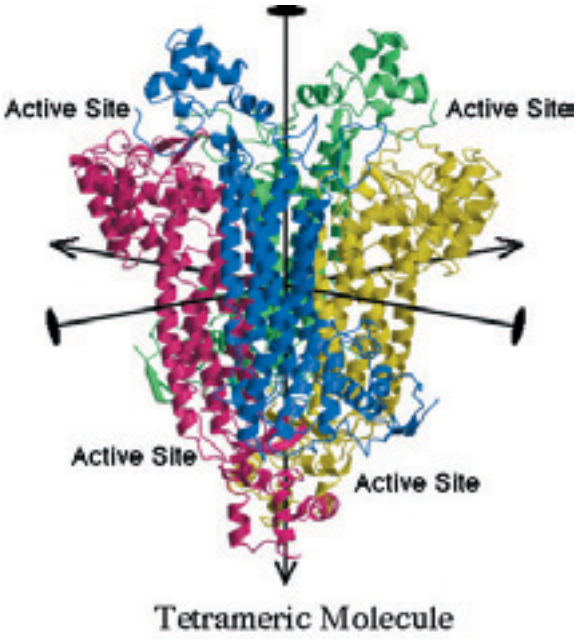
Fujii T, Elucidation of reaction mechanism of high-active-thermostable aspartase by crystallographic analyses of complexes, Grant-in-Aid for Encouragement of Young Scientists, 1 April 2000 - 31 March 2003.

Hata Y, X-Ray crystal structure analyses of functional proteins, Grant of Rice Genome Project PR-2202, MAFF, JAPAN, 1 April 2000 - 31 Mach 2002.

Topics

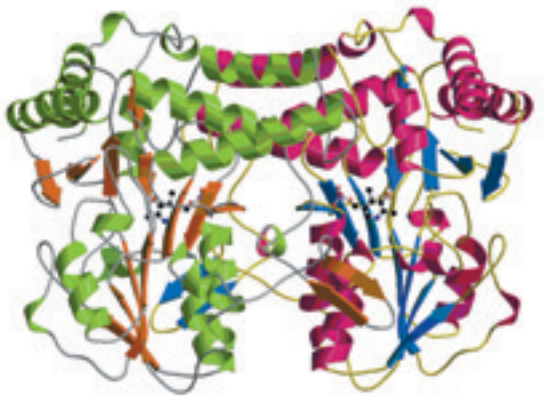
## Structure-based analysis of functional sites of thermostable aspartase

Aspartase catalyzes the reversible conversion of L-aspartate to fumarate and ammonium ion, and plays an important role in the bacterial nitrogen metabolism. The structure of the thermostable enzyme from *Bacillus* sp. YM55-1 was determined by X-ray diffraction method and compared with those of *E. coli* aspartase and fumarase C, which belong to the same family. The results revealed four conformationally different regions which were located around putative functional sites, suggesting the involvement of these regions into functions characteristic of the indivisual enzymes. Moreover, the increase in the number of intersubunit hydrogen-bonds and salt-bridges explains the thermostability of the present aspartase.



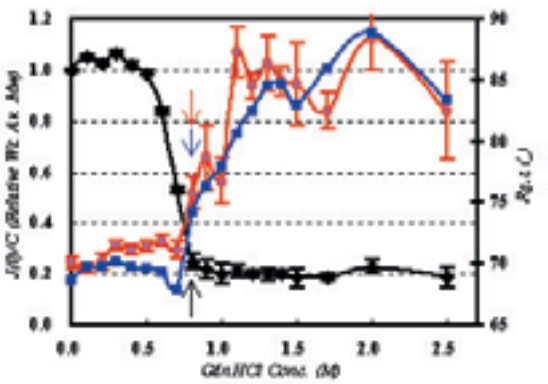

## Analyses of enzymes involved in biogenesis of iron-sulfur cluster

*E. coli* CsdB is a dimeric PLP-dependent NifS-homologue and catalyzes the decomposition of L-selenocysteine into selenium and L-alanine with specificity higher than that for cysteine. The structure of the enzyme has been determined by X-ray crystallographic method. The subunit of CsdB comprises a large domain, a small domain, and an N-terminal segment. A remarkable structural feature of CsdB is that an α-helix in the lobe extending from the small domain to the large domain in one subunit of the dimer interacts with a β-hairpin loop protruding from the large domain of the other subunit. Cys364, which is essential for the activity toward cysteine but not toward selenocysteine, is clearly seen on the loop of the extended lobe (Thr362-Arg375).



## Direct detection of protein quaternary structure and denatured entity by SAXS

A change in the quaternary structure of the oligomeric protein is directly detectable by a small-angle scattering method. Denaturation process of the chaperonin protein GroEL showed that the disappearance of the quaternary structure can be monitored by the Kratky plot of the scattered intensities, demonstrating the advantage of the SAXS method over other indirect methods. The quaternary structure collapsed at a GdnHCl concentration of 0.8 M. The pair wise plots of the change in J(0)/C and the Rg,z enabled us to estimate the stability and nature of the denatured protein. The GroEL tetradecamer was dissociated directly to unfolded coils. The denatured ensemble is some mixture of entangled aggregates and monomeric coil molecules.



# Molecular Biology and Information - Molecular Biology -

Prof
OKA, Atsuhiro
(D Sc)

Assoc Prof
AOYAMA, Takashi
(D Sc)

Instr
KAWASHIMA, Shuichi

Instr
SAKAI, Hiroe
(D Sc)

Assoc Instr
HONMA, Takashi
(Deceased 14 July 2001)

Techn
YASUDA, Keiko

PD (BRAIN)
MURAMOTO, Takuya
(D Sc)

### Students

LIANG, Yajie (D3, left)
OHGISHI, Maki (D3, left)
OHASHI, Yohei (D3)
IWAKOSHI, Shintaro (M1)
IMAI, Kumiko (M1)

## Scope of Research

The major subjects are mechanisms involved in signal transduction and regulation of gene expression responsive to environmental stimuli, differentiation and development of plant organs, and plant-microbe interaction. As of December 2001, study is being concentrated on the roles of two-component response regulators and homeodomain proteins of higher plants in signal transduction and developmental processes.

## Research Activities (Year 2001)

### Presentations

Transcriptional networks regulated by *Arabidopsis* HD-Zip proteins, Aoyama T, Muramoto T, Ohgishi M, Morelli G, Ruberti I, Oka A; Target gene analysis of *Arabidopsis* ATHB-1, Muramoto T, Tukuda M, Oka A, Tabata S, Ruberti I, Morelli G, Aoyama T; Characterization of the homeobox gene, *ATHB-10/GL2*, Ohashi Y, Oka A, Ruberti I, Morelli G, Aoyama T, Ann Meeting of Jpn. Soc. Plant Physiol., 24-26 March (Fukuoka).

Function of GL2/ATHB-10 in epidermal cellular differentiation, Ohashi Y, Oka A, Ruberti I, Morelli G, Aoyama T, 29-30 November (Tsukuba), International Symposium "New era of transcription factor research in plants" organized by Takatsuji H and Aoyama T.

The *Arabidopsis* ARR1 response regulator is a transcription factor for genes immediately responsive to cytokinins, Sakai H, Honma T, Aoyama T, Oka A; Entopically additive expression of ATHB-10/GL2 alters the frequency and spacing of trichome initiation, Ohashi Y, Oka A, Ruberti I, Morelli G, Aoyama T, Ann Meeting of Mol. Biol. Soc. Jpn., 9-12 December (Yokohama).

### Grants

Oka A, Research project for network mutually controlling plant responses to environmental stimuli with morphogenesis: Hierarchy of transcriptional controls in plant signal transduction, Special Coordination Fund of the Ministry of Education, Culture, Sports, Science, and Technology of Japan, 1 April 1997 - 31 March 2003

Aoyama T, Functional analysis of homeodomain proteins controlling the flexibility of plant morphogenesis, Grant from the Bio-oriented Technology Research Advancement Institution (BRAIN), 1 April 1998 - 31 March 2003

Aoyama T and Oka A, Molecular mechanism of adaptive responses controlled by *Arabidopsis* His-Asp phosphorelay signal transduction, Grant-in-Aid for Scientific Research on Priority Areas (B), 1 April 2000 - 31 March 2003

### Award

Honma T, Complexes of MADS-box proteins are sufficient to convert leaves into floral organs, The ICR Special Award for Young Scientists.

Topics

## Negative autoregulation of the *Arabidopsis* homeobox gene *ATHB-2* [1]

ATHB-2 is a transcription factor belonging to the *Arabidopsis* homeodomain-leucine zipper (HD-Zip) protein family. The *ATHB-2* gene is tightly regulated by light signals, and thought to direct morphological changes during shade avoidance responses. To understand how ATHB-2 mediates light signals in plant morphogenesis, we investigated its transcriptional network. We constructed a gene encoding a chimeric transcription factor (HD-Zip-2-V-G) that is expected to activate target genes of ATHB-2 in a glucocorticoid-dependent manner. In transgenic *Arabidopsis* plants expressing HD-Zip-2-V-G, glucocorticoid treatment activates the *ATHB-2* gene itself independently of *de novo* protein synthesis. An *in vitro* DNase I-footprinting experiment showed that the recombinant ATHB-2 protein specifically binds to an *ATHB-2* promoter region. These complementary results indicate that ATHB-2 recognizes its own promoter. Consistent with the fact that ATHB-2 itself has been shown to act as a repressor, expression of the endogenous *ATHB-2* gene was repressed in transgenic plants overexpressing an *ATHB-2* transgene. Moreover, target-gene analyses using the HD-Zip-2-V-G suggested that ATHB-2 recognizes other HD-Zip II subfamily genes. Thus, ATHB-2 has a negative autoregulatory loop and may be involved in a complicated transcriptional network including paralogous genes, like that of animal homeobox genes.

1. M. Ohgishi1, A. Oka, G. Morelli, I. Ruberti, and T. Aoyama1, *Plant J.*, **25**, 389-398 (2001) .

## Complexes of MADS-box proteins are sufficient to convert leaves into floral organs [2]

Genetic studies, using floral homeotic mutants, have led to the ABC model of flower development. This model proposes that the combinatorial action of three sets of genes, the A, B and C function genes, specify the four floral organs (sepals, petals, stamens and carpels) in the concentric floral whorls. However, attempts to convert vegetative organs into floral organs by altering the expression of ABC genes have been unsuccessful. Here we show that the class B proteins of *Arabidopsis*, PISTILLATA (PI) and APETALA3 (AP3), interact with APETALA1 (AP1, a class A protein) and SEPALLATA3 (SEP3, previously AGL9), and with AGAMOUS (AG, a class C protein) through SEP3. We also show that vegetative leaves of triply transgenic plants, *35S::PI*; *35S::AP3*; *35S::AP1* or *35S::PI*; *35S::AP3*; *35S::SEP3*, are transformed into petaloid organs and that those of *35S::PI*; *35S::AP3*; *35S::SEP3*; *35S::AG* are transformed into staminoid organs. Our findings indicate that the formation of ternary and quaternary complexes of ABC proteins may be the molecular basis of the ABC model, and that the flower-specific expression of SEP3 restricts the action of the ABC genes to the flower.

2. T. Honma and K. Goto, *Nature*, **409**, 525-529 (2001).

## An upstream region of the *CDC2aAt* gene directs transcription during trichome development [3]

Proliferation of eukaryotic cells proceeds according to a common cell cycle program. The cell cycle is regulated at two checkpoints at least (i.e., the G1-to-S phase transition and entry into mitosis) through a particular class of protein kinase activity. Since these kinases require an associating protein, cyclin, for their activity, they are called cyclin-dependent kinases (CDKs). The *Arabidopsis CDC2aAt* gene is thought to encode such a protein kinase, since it is actively transcribed in proliferating tissues and can complement defects in the *Schizosaccharomyces pombe cdc2* gene. We analyzed the functional structure of the *CDC2aAt* promoter, using fusion genes between various upstream regions of *CDC2aAt* and the *Escherichia coli* β-glucuronidase (GUS) gene. A 595-base pair (bp) DNA fragment upstream from the transcription start site conferred GUS activity on developing trichomes, but not on proliferating tissues. On the other hand, another upstream fragment extending to the 5' non-coding transcribed region gave GUS activity to both proliferating tissues and developing trichomes (Figure 1). Under the *gl2* mutant background, GUS activity directed by the 595-bp fragment was detected in single-stalk cells, but not in giant cells without obvious polar extension growth. These results revealed that the 595-bp fragment lacks *cis* element(s) essential for proliferating-cell-specific promoter activity, but can direct transcription in a specific period during trichome development, which doesn't include cell division. These results suggests that CDC2aAt functions during cell morphogenesis as well as cell proliferation.

3. Y. Imajuku, Y. Ohashi, T. Aoyama, K. Goto, and A. Oka, *Plant Mol. Biol.* **46**, 205-213 (2001).

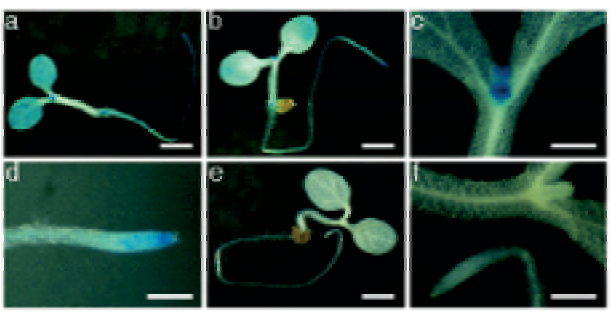



**Figure 1.** Histochemical analysis of *CDC2aAt* promoter activity in seedlings. Transgenic *Arabidopsis* 5 days after germination carrying *P(-1299/+677)::GUS* (a), *P(-591/+677)::GUS* (b-d), or *P(-591/+4)::GUS* (e and f) were examined histochemically. Close-up pictures of apical and root meristems are shown for *P(-591/+677)::GUS* (c and d, respectively) and *P(-591/+4)::GUS* (f). The bars in a, b, and e = 1 mm, and the bars in c, d and f = 0.2 mm. Quoted from ref 3.

# Bioinformatics Center -Bioknowledge Systems-

Prof
KANEHISA, Minoru
(D Sc)

Assoc Prof
GOTO, Susumu
(D Eng)

Instr
NAKAYA, Akihiro
(D Sc)

PD
OKUNO, Yasushi
(D Pharm Sci)

PD
VERT, Jean-Phillipe
(D Sc)

PD
BICHET, Adeline
(D Sc)

### Assoc Instr (pt)

HATTORI, Masahiro
IGARASHI, Yoshinobu
KATAYAMA, Toshiaki

### Res

HIRAKAWA, Mika
PARK, Keun-joon

### Research Student

LEVCHENKO, Maria

### Students

NAKAO, Mitsuteru (D3)
YOSHIZAWA, Akiyasu (D3)
OKUJI, Yoshinori (D2)
KOTERA, Masaaki (D1)
LIMVIPHUVADH, V (D1)
MINOWA, Yosuke (D1)
ITOH, Masumi (M2)
FUJITA, Masashi (M1)
MORIYA, Yuki (M1)
OKUDA, Shujiro (M1)
YAMADA, Rikuhiro (M1)
YAMADA, Takuji (M1)

### Visitors

| | |
|---|---|
| ROLOFF, Tim | Louis Pasteur University, January 2001 - August 2001 |
| PALMER, Andrew | University of Wisconsin-Madison, July 2001 - August 2001 |
| SELINGER, Douglas | Harvard Medical School, July 2001 - August 2001 |

## Scope of Research

Owing to continuous developments of high throughput experimental technologies, ever increasing amounts of data are being generated in genomics and proteomics. We have been developing bioinformatics technologies for analyzing a large number of genes or proteins at a time, toward the understanding and utilization of higher order functional information of the cell or the organism. The suite of databases and associated software that we develop is called KEGG and is made publicly available as part of the GenomeNet service (http://www.genome.jp).

## Research Activities (Year 2001)

### Grants

Kanehisa M, Deciphering genetic and molecular networks by comparative genomics and systematic interaction experiments. Genome Frontier Project, MEXT.

Kanehisa M, Biological systems database and genome information science. Research for the Future Program, JSPS.

Kanehisa M, BRITE: deductive database of the genome and the biological system based on binary relations. Bioinformatics Research and Development, JST.

Goto S, Construction and retrieval of highly integrated biological databases. Grant-in-Aid for Scientific Research on Priority Areas (C) "Genome Information Science", MEXT.

Nakaya A, Extraction of correlated gene clusters by parallel data mining, Grant-in-Aid for Scientific Research on Priority Areas (C) "Genome Information Science", MEXT.

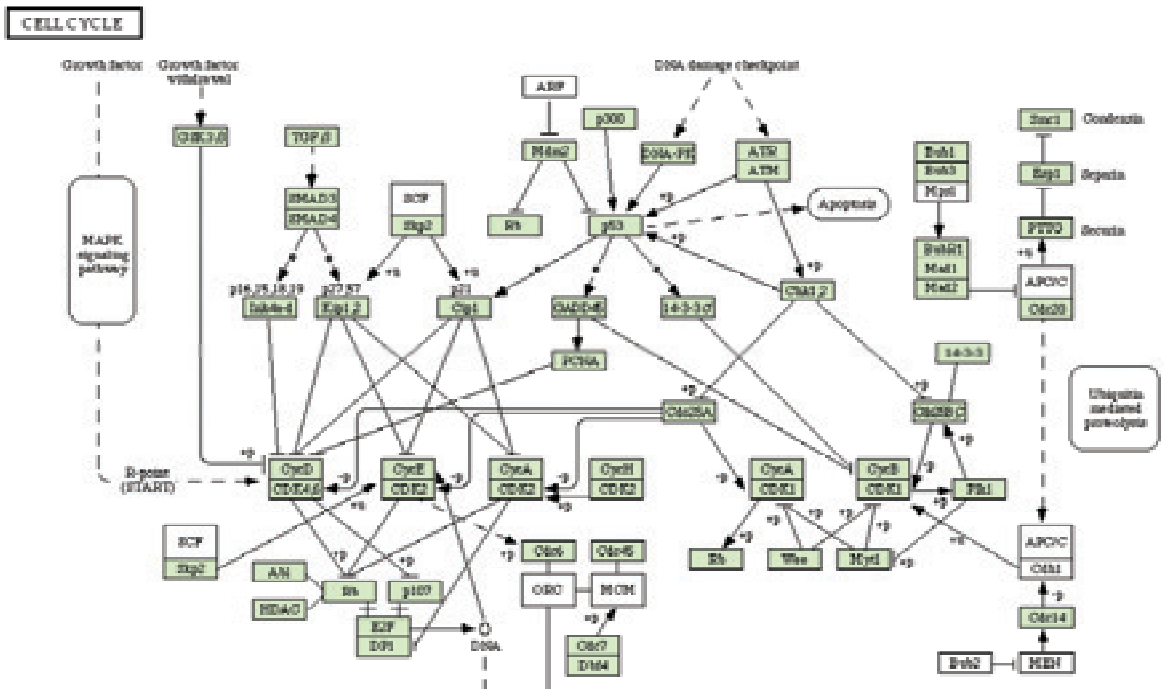
### Award

Kanehisa M, Okawa Publications Prize, *Invitation to Post-genome Informatics*, Okawa Foundation for Information and Telecommunications, 29 November 2001

Topics

## KEGG/SSDB is a new database for exploring the protein universe

SSDB (Sequence Similarity Database) is a new addition to the KEGG suite of databases. It contains the information about amino acid sequence similarities among all protein coding genes in all known genomes. The parallel supercomputer has been used to compute sequence similarities of 5 x $10^{10}$ pairs of genes, as well as continuous updates resulting from newly determined genomes. The data in SSDB can be considered as a huge graph consisting of protein-coding genes as nodes and similarity relations as edges. The graph alorithms that we have developed are used to perform extensive analyses of this graph, such as the gene clustering of orthologs and paralogs, genome comparisons and functional predictions.




## Human cell cycle pathway and its comparison to viral genomes

Molecular mechanisms of the eukaryotic cell cycle regulation have been studied extensively in the past decade. We have assembled current knowledge from published literature and constructed yeast and human cell cycle regulatory pathway diagrams under the KEGG project. Compared to other works, our presentation provides an overall picture on the control flows involving various molecular interactions in the eukaryotic cell division. The pathway diagrams can be used for gene function assignment in other organisms, comparative network analysis of complex biological pathways, visualization and correlation analysis of microarray gene expression data, among others.

Here we show the result of mapping homologous viral genes onto the pathway diagrams by sequence similarity searches. We have constructed a database of viral genes from a set of complete viral genomes, called vGENES. As a result of homology searches of vGENES entries against pathway components, it is shown that many viruses have counterparts of the cell cycle regulatory genes. For example, viruses have G1 Cyclin/CDK and its regulators or G1 transcription initiators, but do not have any subunit of a large protein complex. Such a tendency suggests that viruses carry only those genes that can critically affect initiation of the host cell's proliferative activities.

# Bioinformatics Center -Biological Information Network-

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(D Eng)

Assoc Prof
SUGISAKI, Hiroyuki
(D Sc)

### Students

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FUKAGAWA, Daiji (M1)
SAIGO, Hiroto (M1)
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YAMAMURA, Masaki (M1)

## Scope of Research

Due to rapid progress of the genome projects, whole genome sequences of many organisms and a draft of human genome sequence have been already determined. But, the determination of the whole genome sequence does not mean the end of analysis of genetic code. In order to understand the meaning behind the genetic code, we have been developing algorithms for analyzing proteomics data and genomics data. Recently, we focus on the following topics: protein structure prediction, classification of protein structures, motif extraction, inference of metabolic pathways and genetic networks, and analysis of two-dimensional electrophoresis gel images. We also conduct experimental studies on 4-Hydroxy-4-methyl-2-oxoglutarate (HMG) aldolase.

## Research Activities (Year 2001)

### Presentations

Selecting informative genes for cancer classification using gene expression data, Akutsu T, Miyano S, 2001 IEEE-EURASIP Wokshop on Nonlinear Signal and Image Processing, 5 June.

A local search algorithm for local multiple alignment: special case analysis and application to cancer classification, Akutsu T, Int. Conf. Parallel and Distributed Processing Tech. and Appl., 26 June.

A Gibbs sampiling algorithm for numerical sequences: detection of subtle motifs from protein sequence and structures, Asian Workshop on Protein Informatics, Akutsu T, Horimoto K (Saga Med. ), 14 December.

Local multiple alignment of numerical sequences: detection of subtle motifs from protein sequences and structures, Akutsu T, Horimoto K (Saga Med. ), Int. Conf. Genome Informatics, 18 December.

### Grants

Akutsu T, Miyano S, Algorithms for finding common patterns in bioinformatics, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2005.

Akutsu T, Genome Informatin Science (a member of the project), Grant-in-Aid for Scientific Research Priority Areas (C) , 1 April 2000 - 31 March 2005.

Topics

## Local multiple alignment of numerical sequences: detection of subtle motifs from protein sequences and structures

Motif extraction is one of the well studied problems in Bioinformatics. We developed a new mehod to find motifs from multiple protein sequences and multiple protein structures (see Fig.1). The method consists of two parts: quantification and local multiple alignment. In the former part, protein sequences and protein structures are transformed into sequences of real numbers and real vectors respectively. In the latter part, fixed length regions having similar shapes are located. A variant of the Gibbs sampling algorithm [1], which can be applied to sequences of real numbers/vectors, is newly developed for finding common regions.

We also study a related problem: given positive and negative examples (sequences), find a PSSM (Position Specific Score Matrix)[1] which correctly discriminates between positive and negaive examples (see Fig. 2). We proved some theoretical results on the computational complexity of this problem.

1. R. Durbin et al., Biological Sequence Analysis. Probabilistic Models of Protein Structures and Nucleic Acids, Cambridge University Press (1998).

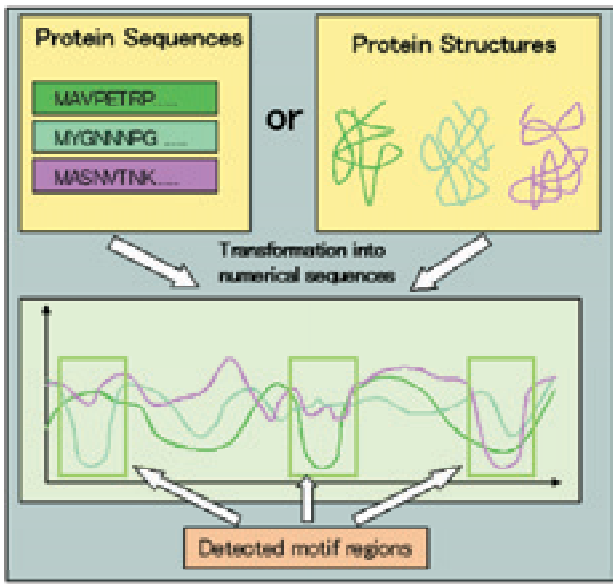


**Figure 1.** Motif detection using local multiple alignment of numerical sequences.

## Cloning, sequencing, and expression of the gene encoding 4-hydroxy-4-methyl-2-oxoglutarate aldolase from Pseudomonas ochraceae NGJ1

4-Hydroxy-4-methyl-2-oxoglutarate (HMG) aldolase is involved in the a-keto acid pathway for degradation of meta-fission products of protocatechuate in bacteria. A DNA fragment that carried the proA gene encoding HMG aldolase was cloned from the chromosomal DNA of Pseudomonas ochraceae, and the coding region was assigned to the nucleotide sequence based on the N-terminal amino acid sequence of the purified from the organism. The proT and proH genes encoding putative transporter and 4-oxalomesaconate hydratase, respectively, were upstream, and the 3'truncated proL gene encoding 2-pyrone-4, 6-dicarboxylate lactonase was downstream from the proA gene in the same orientation on the DNA fragment. These enzymes are also members of the enzymes responsible for the a-keto acid pathway for protocatechuate degradation.

1. K. Maruyama et al., Cloning, sequencing, and expression of the gene encoding 4-hydroxy-4-methyl-2-oxoglutarate aldolase from Pseudomonas ochraceae NGJ1, *Bioscience, Biotechnology, and Biochemistry*, **65**, 2701-2709 (2001).

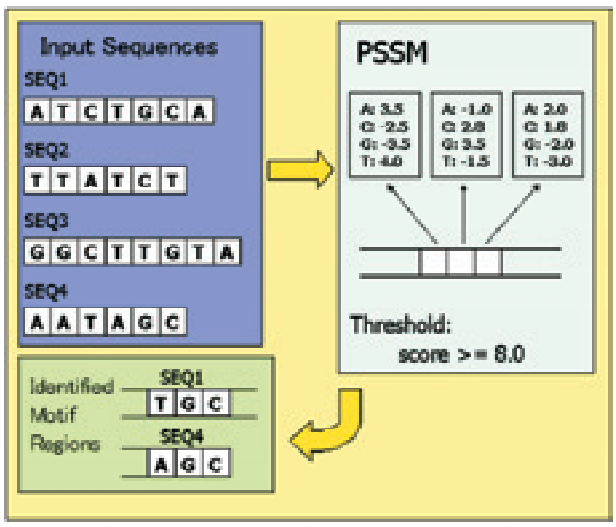


**Figure 2.** Motif detection using a position specific score matrix.

# Biointormatics Center - Pathway Engineering -

Prof
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[adjunct prof]

## Scope of Research

This laborabory develops research on computational knowledge discovery, e.g. inference of pathway information from gene expression profile data, and simulation system for cells and organisms through the biopathway simulation of gene regulatory networks, signaling pathways, metabolic pathways, and physical simulations, etc. With this approach, the functions of genes and systems of genes will be analyzed and predicted.

## Research Activities (Year 2001)

### Presentations

Views: fundamental building blocks in the process of knowledge discovery, Bannai H, Tamada Y, Maruyama O, Miyano S, The 14th International FLAIRS Conference, Florida, 21-23 May.

Selecting informative genes for cancer classification using gene expression data, Akutsu, T, Miyano, S, IEEE-EURASIP Workshop on Non-linear Signal and Image Processing - NSIP-01, Baltimore, 1-3 June.

VML: a view modeling language for computational knowledge discovery, Bannai H (U Tokyo), Tamada Y (Tokai U), Maruyama O (Kyushu U), Miyano S, The Fourth Internatinal Conference on Discovery Science, Washington DC, 26-28 November.

Learning conformation rules, Maruyama O, Shoudai T, Furuichi E, Kuhara S, Miyano S, The Fourth Internatinal Conference on Discovery Science, Washington DC, 26-28 November.

XML documentation of biopathways and their simulations in Genomic Object Net, Matsuno H (Yamaguchi U), Doi A (Yamaguchi U), Hirata Y, Miyano S, The Twelfth International Conference on Genome Informatics, Tokyo, 17-19 December.

Genomic Object Net: Hybrid Object Net Architecture and XML Visualization for Biopathway Simulation, Third Biopathway Consortium Meeting, Copenhagen, 19-20 July.

HypothesisCreator: concepts for accelerating the computational knowledge discovery process, Bannai H, Tamada Y, Maruyama O, Miyano S, The 18th Machine Intelligence Conference, York, England, 19-21 September.

### Grants

Miyano S, Genome-Wide Analysis of Genes Related to Disease Susceptibility and Drug Responsiveness, Research for Future Programs by Japan Society for the Promotion of Science, 1 April 2000 - 31 March 2004.

Miyano S, Mathematical Foundations of Computational Knowledge Discovery from cDNA Microarray Data, Grant-in-Aid for Scientific Research (B)(1), 1 April 2000 -31 March 2003.

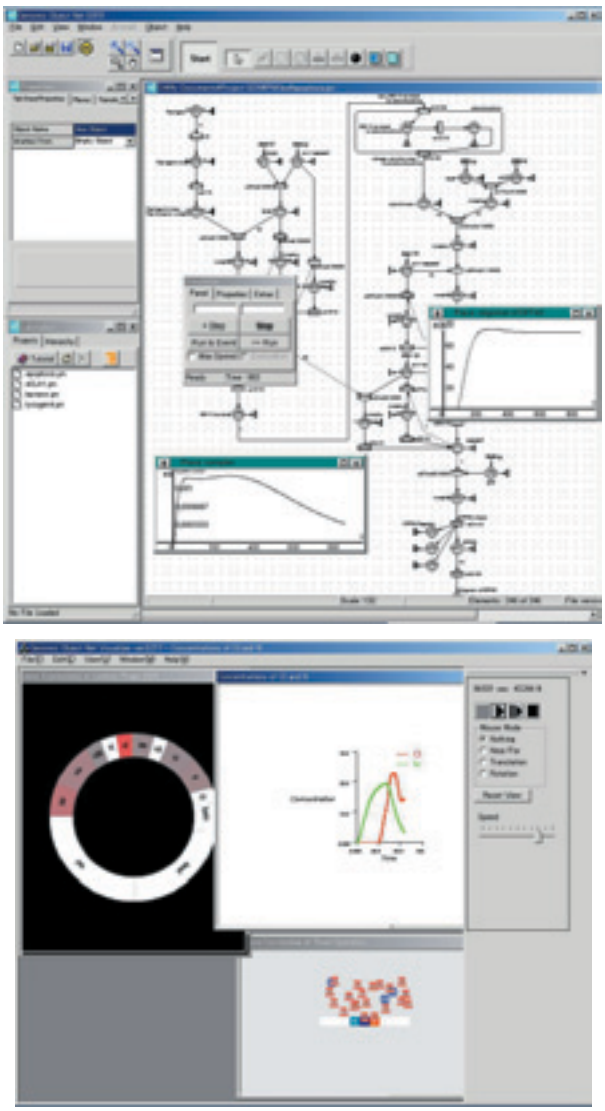
Topics

## Genomic Object Net: Towards Biopathway Modeling and Simulation

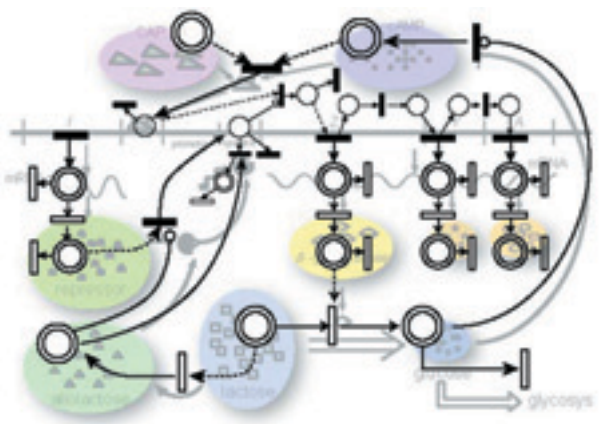
Like in high-energy physics, if events in biological organisms could be simulated and predictions could be made on computers, such system would contribute to drug discovery and therapy in a drastically efficient way, and biology would be driven to a new era with a new methodology for discovery. This idea is not yet fully realized but some portions are being realized.

Biological knowledge in molecular and cellular biology has been typically represented as a series of natural language narratives together with schemes/pictures which would describe the processes of interactions and effects of various entities, e.g. molecules, stimuli, locations, etc. True understanding and interpretation of such knowledge often lie only in the human minds, i.e. experimental biologists.

We have been developing Genomic Object Net for modeling and simulating biopathways. Two key techniques are employed; hybrid functional Petri net (HFPN) for basic architecture, and XML for biopathway representation and simulation visualization. With Genomic Object Net, users can model biopathways as HFPNs based on their intuitive understanding and can result in confidence that the models designed with this software coincides with the understanding and knowledge in their minds. Our target pathways are structurally complex dynamic causal interactions and processes of various biological objects such as genomic DNA, mRNA, proteins, functional proteins, molecular transactions occurring at specific locations and time. For example, metabolic pathways, gene regulatory networks, and signal transduction cascades are counted as typical biopathways. With Genomic Object Net, we can observe in silico how these objects interact and behave quantitatively and qualitatively in biopathways.Genomic Object Net enables investigations which are usually impossible in experimental systems, such as searching for multiple small perturbations that produce large effects when they are combined. Differencies between observed system behavior by simulation and observations in laboratory may suggest a change of model and will invoke new experiments for discovery. The large-scale modeling, such as the whole yeast biopathway modeling, is also feasible with the forthcoming version of this software if we combine various information from many difference sources, e.g. cDNA microarray data, protein interaction data, etc. The modeling process should go along with experimental activity in laboratory and Genomic Object Net will do so. The approach with such predictive simulations has obviously a big possibility to create a tremendous value in drug discovery and therapeutic development.



Genomic Object Net Snapshot



1. http://www.GenomicObject.Net/

# Nuclear Science Research Facility -Particle and Photon Beams-

Prof
NODA, Akira
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Assoc Prof
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Instr
SHIRAI, Toshiyuki

Techn
TONGUU, Hiromu

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FADIL, Hicham (M2) YAMAZAKI, Atsushi (M1) FUJIMOTO, Shinji (M1)

## Visitors

| | |
|---|---|
| Dr BISOFFI, Giovanni | Legnaro National Laboratory, Italy, 11-12, September 2001 |
| Dr GRIESER, Manfred | Max-Planck-Institut für KernPhysik, Germany, 9-22, November 2001 |
| Dr HASSE, Reiner | Gesellschaft für Schwerionenforschung, Germany, 11-14, November 2001 |
| Dr DANARED, Hakan | Manne Siegbahn Laboratory, Sweden, 11-14, November, 2001 |
| Dr HANGST, Jeffrey | Institute of Physics and Astoronomy, Aarhus University, Denmark, 11-14, 2001 |
| Dr SIDORIN, Anatoly | Joint Institute for Nuclear Research, Dubna, Russia, 11-14, November 2001 |
| Mr SCHAETZ, Tobias | Ludwig-Maximilians-University München, Germany, 8-16, November 2001 |

## Scope of Research

Particle and photon beams generated with accelerators and their instrumentations both for fundamental research and practical applications are studied. The following subjects are being studied: Beam dynamics related to space charge force in accelerators: Beam handling during the injection and extraction processes of the accelerator ring: Radiation mechanism of photons by electrons in the magnetic field: R&D to realize a compact synchrotron dedicated for cancer therapy; and Irradiation of materials with particle and photon beams.

## Research Activities (Year 2001)

### Presentations

Slow Beam Extraction of Electron with Combination of Third Order Resonance and RFKO, SugimuraT, Shirai T, Tongu H, Noda A et al., Annual Meeting, Phys. Soc. Jpn., 28 March, 2001 Particle Accelerator Conference, 21 June

Field Measurement and Analysis of Combined Function Magnet, Morita M, Iwashita Y, Noda A et al., Annual Meeting, Phys. Soc. Jpn., 28 March

Electron Beam Cooling of Hot Ion Beam, Noda A, Fadil H, Grieser M (MPI, Heidelberg) et al., Annual Meeting, Phys. Soc. Jpn., 28 March

High Gradient Cavities for Long Bunch Muon Beam, Iwashita Y and Morita A, 2001 Particle Accelerator Conference, 18 June

Very High-Field Short-Pulse Dipole Magnet for Compact Proton Synchrotron, Tokura S (IHI), Miyauchi Y (IHI), Noda A et al., 2001 Particle Accelerator Conference, 21 June

High Gradient RF Cavities for Phase Space Manipulation of Muons, Iwashita Y, The Second Asian Particle Accelerator Conference, 20 September

Collection and Cooling Scheme of Laser Produced Ion Beam, Noda A, Nakamura S, Daido H (JAERI), et al., The Second Asian Particle Accelerator Conference, 21 September

### Grants

Shirai T, Coherent X-ray production and beam cooling of electron with use of laser undulator, Grant-in-Aid for Scientific Research, Syourei (A) (2), 1 April 2000 - 31 March 2002.

Noda A, Beam Accumulation and Cooler Ring, Advanced Compact Accelerator Development, 25 June 2001-31 March 2002.

Iwashita Y, High gradient acceleration with standing-wave structure for linear collider, KEK joint research and development program, 1 April 2001 - 31 March 2002.

Topics

## Pulse stretcher of electron beam with use of a storage ring, KSR

The duty factor of the S-band disc-loaded type electron linac at NSRF has been limited below $2\times10^{-5}$ because of its maximum pulse width(1μsec) and repetiotion rate(20Hz). The electron storage ring, KSR is utilized as a stretcher of the output electron beam to increase the duty factor up to ~90 % for avoiding the pile up of the signals from the particle detector. A slow beam extraction using the third order resonance in combination with the RF knockout is utilized in order to spread out the beam spill, which can be changed in the range between 0.2 sec and 40 sec by adjustment of the transverse RF power from 0.55W to 0.09 W as shown in Figure 1. Beam extraction efficiency has been also measured with use of a Faraday cup and DCCT in the ring (Fig. 2). The extraction efficiency now exceeds 50 % [1].

1. Sugimura T. et al., to be printed in JJAP.

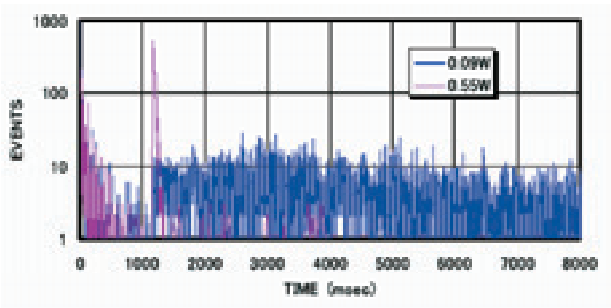


**Figure 1.** Beam spill of the electron beam stretched by KSR.

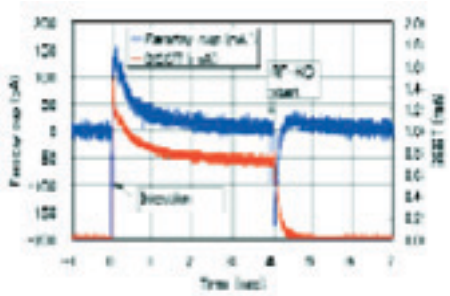

**Figure 2.** Electron beam intensity circulating in KSR(Orange) and extracted (Blue)

## Research and development to realize a compact accelerators for cancer therapy

Recently cancer therapy with use of charged particles has been paid attention from the point of view of "quality of life" of the patient because of its merit of preserving function and shape of human body. Carbon beam irradiated with synchronization to the breathing of the patients at National Institute of Radiological Sciences(NIRS) has attained a good clinical results for liver and lung cancers. For the purpose of downsizing of such a cancer therapy facility, we have studied a combined-function proton synchrotron. This year, the evaluation of the fabricated model combined-function magnet has been completed by making particle tracking with use of the measured magnetic field, which showed the operating points of the synchrotron is well in the stable region free from major lower order resonances (Figure 3)[2].

In parallel, development of a scheme consisting of a laser ion soure followed by a compact cooler ring and a pulse high-magnetic field synchrotron has been started for the purpose of downsizing the needed cost and size of the facility to realize more wide-spread use of the charged particle therapy. Quantitative study of high energy ion production with a high power short pulse laser has been started in collaboration with Advanced Photon Research Center, JAERI, Kansai Research Establishmen, University of Tokyo and Hiroshima University. Feasibility of the electron beam cooling of hot ion beam has also been studied in collaboration with Max-Planck-Institut für Kernphysik, Heidelberg Germany and NIRS.

2. Morita A et al., Phys. Rev. ST-AB, Dec. 2001, 122401

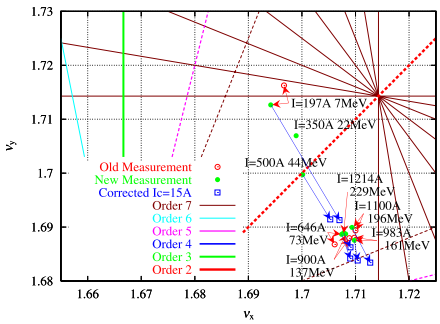


**Figure 3.** Operating points evaluated for the combined-function synchrotron.

## Ion beam cooling --toward the crystalline beam

Recent electron beam cooling experiments of highly charged heavy ions at ESR of GSI in Darmstadt, Germany and CRYRING at Manne Siegbahn Laboratory in Stockholm, Sweden have shown the indication of one dimensional ordering effect. Three dimensional laser cooling is expected to realize much lower temperature although the applicable ion is limited due to the restriction of available lasers. A workshop was organized at Large Seminor Room of Joint Research Laboratory of ICR from the 12th to 14th in November with financial support from ICR and NIRS so as to obtain the common understanding among the participants of the presently attained results and desirable future approach . More than 40 participants including 6 from abroad joined. Many enthusiastic talks were presented as shown in Figure 4.

**Figure 4.** Invited talk on electron beam cooling by Dr. M. Grieser given at the workshop.

# Nuclear Science Research Facility - Beams and Fundamental Reaction-

Assoc Prof.
MATSUKI, Seishi
(D Sc)

PD (JSPS)
HASEYAMA, Tomohito
(D Sc)

### Researcher (pt)

TADA, Masaru (D Sc)

### Students

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KOMINATO, Kentaro (D3)
SHIBATA, Masahiro (D3)

## Scope of Research

Atoms, nuclei, and dark matter particles in the Universe are studied with quantum electronic methods: Current research subjects are 1) search for a cosmological dark-matter candidate particle, axion, in the Universe with the Rydberg-atom cavity detector, 2) highly excited Rydberg atoms in an electric field and their applications to fundamental physics research, and 3) nuclear magnetism in 3-5 semiconductors with laser-assisted Overhauser process and optical pumping.

## Research Activities (Year 2001)

### Presentations

Coherent time evolution of highly excited Rydberg states in pulsed electric field, Tada M, Kishimoto Y, Kominato K, Shibata M, Ooishi C, Yamada S, Saida T, Funahashi H, Yamamoto K, and Matsuki S, Spring Meeting, Phys. Soc. Jpn., Tokyo, 24 March.

Radiative transitions in highly excited Rydberg states detected with the field ionization method, Kishimoto Y, Tada M, Shibata M, Kominato K, Funahashi H, Yamamoto K, and Matsuki S, Spring Meeting, Phys. Soc. Jpn, 24 March.

### Grant

Matsuki S, Search for Dark Matter Axions, Grant-in-Aid for Specially Promoted Research(2), 1 April 1997 - 31 March 2003.

Topics

## Stark structure and field ionization characteristics of highly excited Rydberg states

Rydberg atoms have been widely utilized for fundamental physics research [1,2]. Highly excited Rydberg states with the principal quantum number $n$ larger than 80, however, have not been investigated in detail, partly because it is more difficult to detect selectively a particular state. We developed a quite sensitive method to detect selectively a low-angular momentum state with a newly developed field ionization method in a pulsed electric field [3]. With the new detection method, we investigated systematically the characteristics of the pulsed field ionizations in the highly excited Rydberg states. It was found that in these highly excited Rydberg states, the ionization processes proceed in two ways, that is, via 1) tunneling, and 2) autoionization-like processes. Indeed as shown in Fig.1, field ionization spectrum shows, in general, two peaks which are due to the two processes mentioned above. Lower peak is due to the autoionization-like process, while the higher peak corresponds to the ionization due to the tunneling process. The relative strength of these peaks depends on the related $n$ and the slew rate and detailed pulse shape of the applied electric field. The tunneling process dominates with increasing $n$ because the interactions of the bound blue state with the unbound red states coming from the higher excited $n$ states, are responsible for the autoionization-like process of the bound blue state and these interactions become weaker as $n$ increases.

Along with these investigations, we have developed a quantum theoretical method to calculate the Stark map of the highly excited Rydberg states based on the Hamiltonian diagonalization. Various experimental parameters then have been numerically calculated with the obtained eigenstates . Quantum theoretical predictions for the ionization field values from both processes together with the experimental results are shown in Fig.2. Here the Rydberg states in the n=117 manifold were excited with two-step laser excitation scheme and the field ionization values corresponding to each peak are plotted in the figure. Agreement between the experimental and the calculated results are good, indicating that the present theoretical method is quite satisfactory to predict various experimental observations even for such highly excited Rydberg states in alkali atoms.

Adiabatic and non-adiabatic transition probabilities at the first avoided crossing of $113p_{3/2}$ state with the 110 manifold states were also measured with the new selective field ionization method. To compare the experimental results with theoretical predictions, we have developed a new formalism to calculate the time evolution of the multi-level Rydberg system in the pulsed electric field. The theoretical results are in good agreement with the experimental results, thus indicating also the present theoretical method is quite satisfactory for predicting the time evolution of such highly excited Rydberg system in the time varying electric field and also for calculating the various experimental parameters such as an energy gap bewteen the relevant states in avoided crossings.

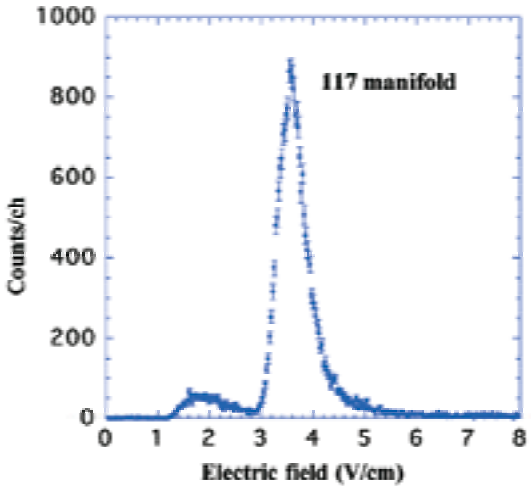


**Figure 1.** Typical field ionization spectrum of 117 manifold states observed with the present selective ionization scheme in the pulsed electric field.

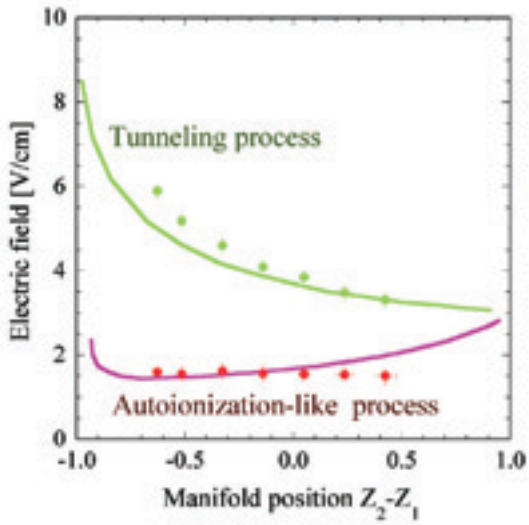


**Figure 2.** Field ionization values of 117 manifold states which correspond to the two peaks observed in the spectra: Z2-Z1=-1 for the bluest state, =+1for the reddest state. The higher peak is due to the tunneling process, while the lower peak corresponds to the ionization from the autoionization-like process. Solid and dashed lines are the predictions from the present theoretical calculations.

1. T. F. Gallagher, *Rydberg atoms* (Cambridge University Press, Cambridge, 1994).
2. I. Ogawa, S. Matsuki and K. Yamamoto, Phys. Rev. **D53** (1996) R1740, and references cited therein.
3. M. Tada, Memoirs of the Faculty of Science, Kyoto University, Series of Physics, Astrophysics, Geophysics and Chemistry, Vol.**43**, in press; M. Tada et al., LANL Preprint archive, Physics/0010071.

# LABORATORIES OF VISITING PROFESSORS

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**Lectures at *ICR***
Advanced nitride

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**Lectures at *ICR***
Raman scattering study of solids

## FUNDAMENTAL MATERIAL PROPERTIES — Composite Material Properties—

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**Professor**
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**Lectures at *ICR***
Micro-structure study and development of liquid crystal polymer film
Basic theory of microwave measurement for polymer segment orientation
Computer simulations of glossy filament fiber and gel permeation chromatography.
Theory and development of pervaporization separation membrane
Efficient development using a Taguchi-method for quality control

Vis Assoc Prof
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**Associate Professor**
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**Lectures at *ICR***
Bonding and electronic states of organic molecules on Si surfaces studied by synchrotron-radiation photoelectron spectroscopy and STM
Dynamical processes of adsorbed molecules on transition metal surfaces

## SYNTHETIC ORGANIC CHEMISTRY — Synthetic Theory —

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**Lectures at *ICR***
Acyl Nitroso Diels-Alder Reactions: Application to Synthesis of Antitumor Marine Alkaloids
Total Synthesis of Pumiliotoxin

Vis Assoc Prof
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**Associate Professor**
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**Lectures at *ICR***
Development of Catalytic Asymmetric Baylis Hillman Reaction and its Application to Natural Product Synthesis

# PERSONAL

# Retirement

## Professor OSAKI Kunihiro
## (Molecular Rheology, Fundamental Material Properties)

On the 31st of March 2002, Dr. Kunihiro Osaki retired from Kyoto University after his 35 years of service at Kyoto University. The title of Emeritus Professor was granted to him by the University on the following day.

Dr. Osaki was born in Matsuyama, Ehime on the 29th of October, 1938. After graduation from the Department of Industrial Chemistry, Faculty of Engineering, Kyoto University in 1961, he continued his study on polymer rheology as a graduate student for 5 years. He finished his course in 1966 and was granted a degree of Doctor of Engineering from Kyoto University for this study in 1968. In 1966, he was appointed to be Instructor of the Department of Industrial Chemistry, Faculty of Engineering, Kyoto University.

In 1967, he moved to the laboratory directed by Professor Michio Kurata, Institute for Chemical Research, Kyoto University. On a leave of absence in the year 1970 to 1971, he stayed at the Department of Chemistry, University of Wisconsin, USA, as a visiting scientist that was a concurrent post of Instructor of Institute for Chemical Research, Kyoto University. During his stay, he collaborated with Professor John D. Ferry to investigate viscoelastic properties of dilute polymer solutions. In 1972, he returned to Institute for Chemical Research, Kyoto University. On a leave of absence in the year 1982, he stayed at Center of Nuclear Energy, Sacley, France, as a visiting scientist that was a concurrent post of Instructor of Institute for Chemical Research, Kyoto University. During his stay, he utilized neutron scattering technique to investigate the chain conformation in bulk polymeric materials under deformation. He returned to Institute for Chemical Research, Kyoto University in 1983, and was promoted to Associate Professor in 1987. In 1988, he was appointed to be Full Professor of Institute for Chemical Research, Kyoto University and directed the Laboratory of Rheology (presently Molecular Rheology, Division of Fundamental Material Properties). At the Graduate School of Engineering, Kyoto University, he gave lectures on rheology and physical properties of macromolecules, and supervised the dissertation studies of graduate students.

During the past three decades, he has been extensively investigating the molecular dynamics and rheology of polymeric materials. His early work on the dilute solution rheology has been highly appreciated as a land mark of the first experimental resolution of the isolated polymer chain dynamics. Through his extensive research of nonlinear viscoelasticity of entangled polymeric liquids, he discovered beautiful universality in the nonlinear damping of the relaxation modulus and offered its molecular interpretation. His discovery and interpretation stimulated a development of a later molecular theory of entanglement, which is currently known as the tube theory. On the basis of this discovery, he also established a phenomenological framework of nonlinear viscoelasticity that has been serving as a world-widely accepted fundamental framework connecting various kinds of nonlinear viscoelastic functions under various deformation histories. Furthermore, he applied rheo-optical methods that he developed in his early work to polymeric glasses and revealed molecular origins of the stress in these glasses and detailed features of the glass-to-rubber transition.

He has been driving progress of polymer rheology through these excellent researches. Furthermore, he has been serving as a representative delegate of the International Committee of Rheology as well as the editors of prestigious international journals such as Journal of Polymer Science, Rheological Acta, and Journal of Non-Newtonian Fluid Mechanics to enhance the rheological research in the world. He also served as the President of the Society of Rheology, Japan (SORJ), and the Vise-President of the Material Research Society, Japan (MRSJ), to guide and enhance the rheological research of various materials in Japan. For these extraordinary research as well as social contributions, he won the SORJ Research Award in 1983 and the SORJ Award in 2001.

His contribution to Institute for Chemical Research, Kyoto University, through his scientific, social, and administrative activities is hereby gratefully acknowledged.

# Retirement

## Professor KAJI Keisuke
## (Polymer Materials Science, Fundamental Material Properties)

On the 31st of March, 2002, Dr. Keisuke Kaji retired from Kyoto University after 35 years of service to the University and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Kaji was born in Kobe on 14th of February, 1939. After graduation from the Department of Industrial Chemistry, Faculty of Engineering, Kobe University in 1963, he continued his studies on polymer chemistry at the Graduate School of Engineering, Kyoto University for five years. Under the supervision of Professor Emeritus Ichiro Sakurada, he was granted a doctoral degree from Kyoto University in 1970 for his studies on the determination of elastic moduli of polymer crystals by an X-ray diffraction method. In 1968, he was appointed an instructor of Department of Polymer Chemistry, Faculty of Engineering, Kyoto University. On leave from the University, in the years 1976 to 1977, he stayed in the Institut für Physikalische Chemie, Johannes-Gutenberg-Universität Mainz (the University of Mainz, West Germany) as Wissenschaftlicher Mitarbeiter to work on neutron scattering of polymers in collaboration with Professor Dr. Erhard W. Fischer. Dr. Kaji was promoted to an Associate Professor in 1981, and to a full Professor of Kyoto University in 1988 and directed the Division of Polymer Materials Science, Laboratory of Fundamental Material Properties, Institute for Chemical Research.

During the past 40 years, Dr. Kaji's research interest encompassed a wide area in polymer science including fiber science. He is known as a pioneer of neutron scattering researches of polymers in Japan, and he applied this method as well as X-ray and light scattering methods for elucidating structure, dynamics and phase behavior of polymer materials to relate their microscopic and macroscopic behaviors. His scientific life started mainly with determining crystalline elastic moduli of various polymers by an X-ray scattering technique, which give the limiting values for super-high modulus fibers. In this connection he solved several problems of abnormal scattering from small polymer crystallites in the amorphous matrix as well. After Mainz, he applied inelastic neutron scattering techniques to elucidate the origins of the glass transition and excess heat capacities in amorphous polymers. He is the first to perform systematic experiments on the structure of polyelectrolyte solutions, establishing the phase diagram as functions of the degree of polymerization and the concentration in their wide ranges and revealing the cause for the well-known anomalous behavior in reduced viscosity at very dilute concentrations. He also investigated the structure and its formation processes of poly(vinyl alcohol) gels, showing that the structure is controlled by a competition between the rates of the gelation and the phase separation. His researches on polymer crystallization are prominent. He discovered for the first time a completely new type of primary crystal nucleation, called spinodal decomposition (SD)-assisted crystal nucleation, which is greatly different from the usual homogeneous crystal nucleation. This distinct research has inspired many international investigations in this field. To promote this finding, he organized a project team on polymer crystallization as a coordinator of NEDO International Joint Research Project supported by New Energy and Industrial Technology Development Organization.

For his excellent achievements, he was frequently invited to international conferences such as Conference of American Physical Society, Gordon Research Conference, and Congress of European Physical Society. For his prominent studies on static and dynamic structure of polymers by neutron and X-ray scattering, he was awarded the Prize of the Society of Polymer Science, Japan in 1985.

Dr. Kaji devoted himself to the Society of Fiber Science and Technology, Japan. He served as the Head of Kansai Branch in 1994, as the Chairperson of the Advanced Fiber Materials Research Committee in the years 1994 to 1995, and as the vice-President of the Society in the years1999 to 2002. He has also devoted to the Society of Polymer Science, Japan as the Regional Manager of Kansai Branch since 1984 and as the Associate Editor of Polymer Journal since 1999.

Dr. Kaji gave lectures on Polymer Spectroscopy since 1988 at the Graduate School of Engineering, Kyoto University, and was charged with supervising dissertation works of many graduate students. He was a visiting lecturer at many universities such as Kyoto Institute of Technology, Kyushu University, Okayama University, Kobe University, Osaka University, Nagoya University and so on.

His contribution to the University through both academic and administrative activities is gratefully acknowledged.

# Retirement

## Professor SHINJO Teruya
## (Artificial Lattice Alloys, Solid State Chemistry)

On the 31st of March, 2002, Dr. Teruya Shinjo retired from Kyoto University and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Teruya Shinjo was born in Kyoto Prefecture on August 18, 1938. He graduated from Faculty of Science, Kyoto University in 1961. He studied the magnetic properties of iron oxide particles by Mössbauer spectroscopy in the Graduate School of Science, Kyoto University under the supervision of the Professor H.Takaki. He finished the Doctor Course of Chemistry and received the Doctor Degree of Science in 1966.

He started his academic carrier as an instructor of Institute for Chemical Research, Kyoto University in 1966 with the late Professor T.Takada. In 1976, he was promoted to an associate professor and since 1982, he has directed the Laboratory of Solid State Chemistry, Institute for Chemical Research as a full professor. During 1996-1998, he served as the Director of Institute for Chemical Research. At the Graduate School of Science, Kyoto University, he gave lectures on the properties of magnetic materials and supervised the dissertation works of many graduate students.

During his academic carrier, Prof. Shinjo has extensively investigated the properties of magnetic thin films. The keywords of his investigation may be "Mössbauer spectroscopy" and "giant magnetoresistance effect". He investigated the surface/interface magnetic properties of ferromagnetic metals such as iron and cobalt with 57Co and 57Fe Mössbauer probes. These studies are now recognized as pioneering works in the field of magnetic thin films. The studies on surface/interface magnetism were developed to the production of metallic multilayer films with artificial stacking structures of nanometer scale. The artificially structured metallic multilayers are novel alloy systems which may potentially have various useful properties. He discovered a non-coupling type giant magnetoresistance (GMR) effect in NiFe/Cu/Co/Cu multilayer systems. His discovery stimulated the development of read head devices of the magnetic recordings. Nowadays the GMR heads are widely used in the hard disks of computers. Recently he started new researches of nano-scale magnetism. The GMR effect is utilized to detect the magnetization reversal of narrow magnetic wires. In the submicron-size magnetic dots, he successfully observed the turned-up magnetization spot in the center of the magnetic vortex structure by magnetic force microscope. Such a magnetic structure was theoretically predicted long time ago, but has never been observed by experiments. For his long-term studies on the properties of magnetic films including the discovery of the non-coupling type GMR effect, he was awarded the Prize of the Magnetic Society of Japan in 1991 and 1998, the Prize of the Japan Society of the Applied Physics in 1993 and a Purple Ribbon Medal (Shijuhosho) in November 2000. From 1992 to 2000, he has served as a science advisor of Monbusho.

It is worth referring to his international activities in the academic society. He is one of the Japanese representatives of International Board on the Application of the Mössbauer Effect for many years, and an international committee member of the International Colloquium on Magnetic Films and Surfaces and served as the chair. He is serving as an editorial member of international journals: Journal of Physics D, Applied Physics and Journal of Magnetism and Magnetic Materials.

# Retirement

## Professor FUJI Kaoru
## (Fine Organic Synthesis, Synthetic Organic Chemistry)

On the 31st of March 2002, Dr. Kaoru Fuji retired from Kyoto University after his 34 years' service at Kyoto University, and was honored with the title of Emeritus Professor of Kyoto University on the following day.

Dr. Fuji was born in Osaka on February 13, 1939. He graduated from Faculty of Pharmaceutical Sciences, Kyoto University in 1961. After one year of service to Shionogi Co. Ltd., he entered the Graduate School of Pharmaceutical Sciences, Kyoto University and started his study on alkaloids, Lythranine, Lythranidine and Lythramine under the supervision of Professor Eiichi Fujita. He was granted a doctoral degree from Kyoto University in 1970.

He was appointed an instructor of Institute for Chemical Research, Kyoto University in 1967 and an associate professor in 1973. On leave from Kyoto University, he stayed at the University of British Columbia, Canada and worked on synthesis of an antitumor alkaloid, Vincristine with Professor James P. Kutney during 1971 and 1973. He also stayed at the University of Minnesota as a visiting research fellow with Professor Paul G. Gassman during 1981 and 1982. He was promoted to a full professor of Institute for Chemical Research, Kyoto University in 1983. At the Graduate School of Pharmaceutical Sciences, Kyoto University, he gave lectures in bioorganic chemistry. He was invited as a visiting professor by Universite Louis Pasteur, Universite Paris-Sud, Technical University of Vienna, and other institutions.

During these years, he made many distinguished studies on organic chemistry, especially on asymmetric synthesis, natural product synthesis, and molecular recognition. He has developed asymmetric nitroolefination via addition-elimination process, 8,8'-disubstituted 1,1'-binaphthyls as a chiral controller, chiral nucleophilic catalysts, and especially, a new principle of enolate chemistry, memory of chirality. He has completed total syntheses of natural products, including Lythranidine, Aspidospermidine, Eburnamonine, Quebrachamine, Podocarpic acid, Gibberellin A12, Pysostigmine, Pseudophrynaminol, Horsfiline, and recently Spirotryprostatin B. He also focused on molecular recognition by functional phenolphthaleins. Visualization of molecular length and chirality of α, ω-diamines and sequence-specific coloration of dipeptide have been achieved. For his brilliant achievements, he was awarded The Pharmaceutical Society of Japan Award for Young Scientists in 1980 and The Pharmaceutical Society of Japan Award in 1998.

Dr. Fuji devoted himself to various scientific societies and international journals. He served as the president of Kansai-branch of Synthetic Organic Chemistry, Japan in 1996 and as a vice president of The Pharmaceutical Society of Japan in 2000. He also served as an editor of Chemical and Pharmaceutical Bulletin during 1997 and 1999 and serves as an Asian editor of Chirality since 1998.

His contribution to the Institute through both academic and administrative activities is greatly acknowledged. His sincere and warmhearted personality has been admired by his friends, colleagues, and especially by his students.

# Awards

**KAWACHI, Atsushi**
The Chemical Society of Japan
Award for Distinguished Young Chemists
Development of the Chemistry of Nitrogen, Oxygen, and Sulfur-Functionalized Silyl Anions
The Chemical Society of Japan
29 March 2001

**MURAKAMI, Syozo**
The Chemical Society of Japan
Award for Technical Achievements
29 March 2001

**MATUBAYASI, Nobuyuki**
Helmholtz Award
NMR and computer-simulation studies of supercritical water
International Association for the Properties of Water and Steam
9 May 2001

Promotion Award
Structure, dynamics, and reactions of supercritical water
Japan Society of High-pressure Science and Technology
21 November 2001

**OSAKI, Kunihiro**
SROJ Award for 2001
Nonlinear rheology of polymeric systems
Society of Rheology, Japan
17 May 2001

**TAKAHASHI, Masahide**
Award for young scientists
Studies on the optical properties and structure of photonic glasses
The Ceramics Society of Japan
17 May 2001

**UCHINO, Takashi**
Vittorio Gottardi Prize
Studies on the structure and properties of glasses
International Commission on Glass
2 July 2001

**KANEHISA, Minoru**
The Okawa Publications Prize
Invitation to post-genome informatics
The Okawa Foundation for Information and Telecommunications
29 November 2001

**OKAMURA, Kei**
The ICR Award for Young Scientists
Development of deep-sea *in situ* automated analytical system using highly sensitive chemiluminescence and its application for hydrothermal plume observation
ICR
7 December 2001

# Poster Awards

**NIIDA, Haruki**

A E Owen Student Poster Award
First Prize
Preparation, properties and structure of organic-inorganic hybrid low-melting glasses
Society of Glass Technology
6 July 2001

**KAWAI, Yasushi**

5th Japanese Symposium on the Chemistry of Biocatalysis
Best Poster Award
Characterization of Nitroalkene Reductases
The Committee of 5th Japanese Symposium on the Chemistry of Biocatalysis
14 December 2001

**NAKATA, Norio**

Symposium Poster Award
6th Symposium of the Society of Silicon Chemistry, Japan
Reactivity of Kinetically Stabilized 2-Germanaphthalene
The Society of Silicon Chemistry, Japan
16 November 2001

**YAMANAKA, Rio**

5th Japanese Symposium on the Chemistry of Biocatalysis
Best Poster Award
Asymmetric Reduction of Ketones by Cyanobacteria
The Committee of 5th Japanese Symposium on the Chemistry of Biocatalysis
13 December 2001

**NAGATA, Kazuto**

Symposium Lecture Award
80th Annual Meeting of the Chemical Society of Japan
Syntheses and Properties of Novel Three-membered Cyclic Platinum Complexes Having a Dichalcogenido Ligand
The Chemical Society of Japan
14 December 2001

**YAMAGUCHI, Hitomi**

5th Japanese Simposium on the Chemistry of Biocatalysis
Best Poster Award
Purification and Characterization of α-Keto Ester Reductase from Streptomyces coelicolor A3(2)
The Committee of 5th Japanese Symposium on the Chemistry of Biocatalysis
14 December 2001

**[The news of their death]**

Honma, Takashi (Associate Instructor): Deceased 14 July 2001 with the age of 30.

Former Associate Professor of Nuclear Science Research Facility, Dr. FUKUNAGA, Kiyoji who moved to Yamagata University as a Professor in 1991, regretfully passed away on the 8th November, 2001 with the age of 69.

# PUBLICATIONS

## STATES AND STRUCTURES

### I. Atomic and Molecular Physics

A. M. Vlaicu (NIRM), Y. Ito, T. Mukoyama (Kansai Gaigo-Daigaku): *M*-shell satellite structure of W x-ray emission lines, *Rad. Phys. & Chem.*, **61**, 401 (2001)

Y. Ito, T. Tochio, H. OoHashi, N. Shigeoka: Double-electron excitation above Xe *K*-edge, *Rad. Phys. & Chem.*, **61**, 405 (2001)

K. Aoki (Himeji Institute of Technology), Y. Ito, A. M. Vlaicu (NIRM): Probability of nuclear excitation by electron transition in Os atoms, *Phys. Rev. C*, **64**, 044609 (2001)

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S. Emura (Osaka Univ.), K. Mutaguchi, Y. Ito, Y. Takabayashi (Okayama Univ.) and Y. Kubozono (Okayama Univ.): Local Lattice Instability of Cuprous Ions in NaBr and NaCl, *CP554, Physics in Local Lattice Distortions, edited by H. Oyanagi and A. Bianconi*, 309-14 (2001)

N. Shigeoka, H. OoHashi, T. Tochio, Y. Ito, A. M. Vlaicu (NIRM) and S. Emura (Osaka Univ.): *K*a x-ray spectra on $L_{III}$ and $L_{II}$ shell in $Cr_2O_3$, *Spring-8 User Experiment Report No.6 (2000B)* (2001)

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## MOLECULAR BIOFUNCTION

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MASUDA, Kenji
D Eng, Kyoto University
"Studies on Structure and Hydrogen Bonding of Poly(vinyl alcohol) and Its Related Polymer by Solid-State $^{13}C$ and $^{1}H$ NMR Spectroscopy"
Supervisor: Prof HORII, Fumitaka
23 March 2001

MATSUO, Takashi
D Sc, Kyoto University
"A Kinetic Study on Reaction Mechanism of Serine Proteases from the Viewpoint of Fluctuation of Enzyme"
Supervisor: Assoc Prof NAKAMURA Kaoru
23 March 2001

MATSUURA, Akira
D. Eng, Kyoto University
"Synthesis and Properties of Novel Cyclic π-Conjugated Hydrocarbons with σ-π Interaction"
Supervisor: Prof KOMATSU, Koichi
23 March 2001

ODA, Seiji
D Sc, Kyoto University
"Stereoselectivity in the Redox Reaction and the Alkylation of NAD(P)(H) Model Compounds"
Supervisor: Prof TOKITOH Norihiro
23 March 2001

OHGISHI, Maki
D Sc, Kyoto University
"Functional Analysis of the Transcription Factor ATHB-2 , a Regulator of Photomorphogenesis"
Supervisor: Prof OKA, Atsuhiro
23 March 2001

RYU, Deug-Soo
D Eng, Kyoto University
"Rheo-Optical Studies in Elongation Process"
Supervisor: Prof OSAKI, Kunihiro
23 March 2001

SAKAI, Hiroe
D Sc, Kyoto University
"Studies on the Response Regulators of Two-component Regulatory System Involved in *Arabidopsis* Cytokinin Signal Transduction"
Supervisor: Prof OKA, Atsuhiro
23 March 2001

SHINTANI (URAKABE), Eriko
D Sci, Kyoto University
"Spot Scanning Using Rafdioactive $^{11}C$ Beams for Heavy-Ion Radiotherapy"

Supervisor. Prof NODA, Akira
23 March, 2001

TOKUDA, Yomei
D Eng, Kyoto University
"Studies on the structure and properties of glasses as photonics materiars"
Supervisor: Prof YOKO, Toshinobu
23 March 2001

TSUJI, Hayato
D Eng, Kyoto University
"Synthesis and Photophysical Properties of Oligosilanes Conformationally Constrained by Methylene Tethers"
Supervisor: Prof TAMAO, Kohei
23 March 2001

UO, Takuma
D Agr, Kyoto University
"Enzymological Studies of D-Amino Acid Metabolism in Eucaryotes"
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2001

YOSHIDA, Kaname
D Sci, Kyoto University
"Structure and Multilayer Formation of Oriented Organic Thin Films with One-dimensional Electronic System"
Supervisor: Prof KOBAYASHI, Takashi
23 March 2001

TADA, Masaru
D Sci, Kyoto University
"Coherent Time Evolution of Highly Excited Rydberg States in Pulsed Electric Field: Opening a Stringent Way to Selectively Field-ionize the Highly Excited States"
Supervisor: Prof MATSUKI, Seishi
24 March 2001

FURUBAYASHI, Yutaka
D Sc, Kyoto University
"Preparation of single-crystal thin films of spin-ladder compounds"
Supervisor: Prof TAKANO, Mikio
May 23, 2001

MAEDA, Hirofumi
D Eng, Kyoto University
"Novel Intramolecular Rearrangements of Functionalized Silyllithiums"
Supervisor: Prof TAMAO, Kohei
23 May 2001

MATSUBA, Go
D Eng, Kyoto University
Structure Formation Prior to Crystallization of Polymers
Supervisor: Prof KAJI, Keisuke
23 May 2001

TAKESHITA, Hiroki
D Eng, Kyoto University
Hierarchic Structure of Poly(vinyl alcohol) Gels As Revealed by Scattering Techniques
Supervisor: Prof KAJI, Keisuke
23 May 2001

CHU, Dong
D Med Sc, Kyoto University
"Cloning and characterization of LUN, a novel RING-finger protein that is highly expressed in lung and specifically binds to a palindromic sequence"
Supervisor: Prof UEDA, Kunihiro
23 May 2001

FUJIWARA, Eiichi
D Sci, Kyoto University
"Two-dimensional Packing Efficiency and Epitaxial Modes of Organic Molecular Layers"
Supervisor: Prof ISODA, Seiji
23 July 2001

INABA, Yoshikazu
D Sc, Kyoto University
"Reduction of Nitroalkenes with Biocatalyst"
Supervisor: Assoc Prof NAKAMURA Kaoru
23 July 2001

McNamee, Cathy Elizabeth
D. Sc., Kyoto University
"Atomic Force Microscopy and Electrokinetics Studies for Silica Surfaces Modified with a Polyelectrolyte and Surfactants in Water and in Ethanol"
Supervisor: Dr MATSUMOTO, Mutsuo and Prof NAKAHARA, Masaru
25 September 2001

HAYASHI, Naoaki
D Sc, Kyoto University
"Preparation and Properties of thin films of perovskite-type oxides containing iron in an unusually high valence state of $Fe^{4+}$"
Supervisor: Prof TAKANO, Mikio
25 September 2001

MINAKUCHI, Masayoshi
D Med Sc, Kyoto University
"Molecular cloning and initial characterization of SEB, a novel protein that binds to the acute undifferentiated leukemia-associated protein SET"
Supervisor: Prof UEDA, Kunihiro
23 July 2001

NISHIDA, Koji
D Eng, Kyoto University
Structure of Polyelectrolyte Solutions
Supervisor: Prof KAJI, Keisuke
25 September 2001

KAGAYAMA, Akifumi
D. Eng, Kyoto University
"Studies on Pinacol and Aldol Reactions Promoted by Low-Valent Titanium Reagents and on Haloalkylation Reactions of Esters"
Supervisor: Prof KOMATSU, Koichi
26 November 2001

# SEMINARS

Prof DAVIES, Geoff
Department of Physics and Astronomy, The University of Leeds, Leeds, United Kingdom
"Electrostriction in Polar Elastomers for Artificial Muscles"
Friday 12 January 2001

Prof SIEGEL, Jay8989 S.
Department of Chemistry, University of California, San Diego, U.S.A.
"Topological Motivations in Metal Coordination Chemistry"
Monday 15 January 2001

Prof JOHNSON, John E.
Department of Molecular Biology, The Scripps Research Institute, La Jolla CA, USA
"Structure and Dynamics of RNA and DNA Viruses"
Tuesday 16 January 2001

Prof KAWAKAMI, Yusuke
Graduate School of Materials Science, Japan Advanced Institute of Science and Technology, Japan
"Molecular Design of Si-Containing Polymers"
Tuesday 16 January 2001

Prof BEKAROGLU, Ozer
Technical University of Istanbul, Turkey
"Phthalocyanines Containing Macrocycles"
Firday 19 January 2001

Prof ZHAO, Kongshuang
Department of Chemistry, South China Normal University, Guangzhou, P. R. China
"Dielectric Studies on Molecular Organized Assemblies and Dispersion Systems"
Firday 19 January 2001

Dr CHERNOGUHOVSKY, Michael A.
RCNP, Osaka University, Japan
"Optimal RF Control at Transient Beamloading"
Thurseday 1 February 2001

Dr Per Bo Zetterlund
Faculty of Engineering, Osaka City University, Osaka, Japan
"The Use of Radical Concentrations in the Study of High Conversion and Copolymerization Systems"
Friday 2 February 2001

Prof TORRES, Tomas
Department of Organic Chemistry, The Autonoma Unversity of Madrid, Spain
"Towards Metallophthalocyanine-Based Molecular Materials"
Wednesday 2 February 2001

Prof YAMADA, Bunichiro
Faculty of Engineering, Osaka City University, Osaka, Japan
"Common Sense and New Development of Radical Polymerization"
Friday 2 February 2001

Prof KISO, Makoto
Department of Applied Bioorganic Chemistry, Gifu University, Gifu, Japan
Investigating the function of sugar chain by using ganglioside as a probe
Monday 5 February 2001

Assoc Prof KIMURA, Tsunehisa
Department of Industrial Chemistry, Tokyo Metropolitan University, Japan
"Orientation of Polymers under a High Magnetic Field"
Friday 9 February 2001

Prof TYKWINSKI, Rik
Department of Chemistry, University of Alberta, Canada
"Migrating Alkynes: A New Route to Carbon-rich Rings, Rods, and Spheres"
Wednesday 21 February 2001

Assoc Prof ARIE, Tsutomu
Tokyo University of Agriculture and Technology
Control of the soil disease with non-fungicidal agent and mechanism of the pathogen development
Wednesday 28 February 2001

Dr HASHIM, Azanam
University Sains Malaysis, Malaysia
"Natural Rubber Latex and Its Modifications"
Thursday 1 March 2001

Prof NAKAJIMA, Kazuhisa
High Energy Accelerator Research Organization (KEK), Japan
"Recent Topics of the laser plasma accelerator"
"High Energy Particle Physics by Super Strong Field Interactions"
Thursday 1 March 2001

Dr SMETANIN, Igor
P.N. Lebedev Physics Institute, Russia
"FEL-like interactions in semiconductors, superconductors, X-ray Compton scattering"
Friday 2 March 2001

Dr COLLIER, John M.
Massachusetts General Hospital, USA
"Review of Heavy Ion Radiation Therapy at the Lawrence Berkeley Laboratory"
Tueseday 13 March 2001

Dr BOLSHAKOVA, Inessa
Lviv Polytechnical State University, Ukraine
"Developement of the Micro Hall Sensor and the Status of Micoro Sensor Laboratory"
Monday 19 March 2001

Dr KUMADA, Masayuki
National Institute of Radiological Sciences, Japan
"Developement of 4 T Permanent Magnet"
Monday 19 March 2001

Prof KIKUTANI, Eiji
High Energy Accelerator Research Organization (KEK), Japan
"Recent results of the luminosity upgrade in KEK B-factory"
Thurseday 22 March 2001

Prof EISCH, John J.
Department of Chemistry, State University of New York, USA
"New Aspects of Early Transition Metal Carbenoid Chemistry"
Wednesday 28 March 2001

Dr HAYASHI, Naoto
Graduate School of Human and Environmental Studies, Kyoto

University, Kyoto, Japan
"Studies on Crystal Engineering of Twisted Molecules"
Friday 6 April 2001

Prof KIKKAWA, Shinichi
Graduate School of Engineering, Hokkaido University, Sapporo, Japan
"Advanced nitride"
Monday 16 April 2001

Prof Em SHIOJIRI, Makoto
Kyoto Institute of Technology, Kyoto, Japan
"Structure Analysis of Materials by HAADF and STEM"
Monday 16 April 2001

Prof TAKEDA, Shunichi
Graduate School of Medicine, Kyoto University, Kyoto, Japan
"Reverse Genetic Study of DNA Recombination in the Chicken B Lymphocyte Line, DT40"
Wednesday 18 April 2001

Dr SUFFERT, Jean
CNRS, France
"Recent Results in the Reactivities of Acyclic Eneynes and Synthesis of Highly Unsaturated Polycyclic Systems"
Monday 23 April 2001

Prof BLECHERT, Siegfried
Technische Universität Berlin, Germany
"Olefin Metathesis – Recent Developments"
Friday 27 April 2001

Assoc Prof YAMANAKA, Akio
Chitose Institute of Science and Technology
"Raman scattering study of high-$T_c$ superconductors"
4 May 2001

Dr BACZEWSKI, Lech Tomasz
Institute of Physics, Polish Academy of Sciences, Poland
"Cobalt Spin Arrangement in Co/Nd Multilayers with $^{57}$Fe Probe Layer"
Thursday 10 May 2001

Assoc Prof YAMANE, Hisanori
Institute for Advanced Materials Processing, Tohoku University
"Single crystal growth of GaN"
15 May 2001

Dr KOTERA, Mitsuharu
Chimie Bioorganique, CNRS, Universite Joseph Fourier, France
"Studies on Damage to DNA: Synthesis of Oligodeoxyribonucleotides Containing the 2'-Deoxyribonolactone Lesion"
Thursday 17 May 2001

Prof WEST, Robert
Department of Chemistry, University of Wisconsin, Madison, U.S.A.
"Some New Chemistry of Siloles and Silafluorenes"
Monday 21 May 2001

Prof WINTERFELDT, Ekkehard
University of Hannover, Germany
"Marine Natural Compounds -Biological Activity and Synthetic Exercises"
Monday 28 May 2001

Prof OKUNO, Tsumuko
Department of Human Environmental Sciences, Mukogawa Women's University, Hyogo, Japan
"Surface Modification of Clothing Materials"
Tuesday 12 June 2001

Prof PRAKASH, G. K. Surya
Department of Chemistry, University of Southern California, USA
"New Carbodications"
Monday 18 June 2001

Prof KIBAYASHI, Chihiro
Tokyo University of Pharmacy and Life Sciences, Japan
"Acyl Nitroso Diels-Alder Reactions: Application to Synthesis of Antitumor Marine Alkaloids"
Tuesday 10 July 2001

Prof SAKABE, Shuji
Graduate School of Engineering, Osaka University
"High Intensity Laser-Plasma Interaction and High Energy Ion Production"
Thursday 12, July 2001

Prof DIEDERICH, François
Institute for Organic Chemistry, ETH Zürich, Switzerland
"Covalent Fullerene Chemistry: Regioselective Multiple Functionalization, Chirality, and Advanced Materials"
Monday 23 July 2001

Prof VERKADE, John G.
Department of Chemistry, Iowa State University, USA
"Expanding Applications of $P(RNCH_2CH_2)_3N$ Compounds as Useful Catalysts and Non Ionic Bases in Organic Chemistry"
Friday 27 July 2001

Prof WANG, Guan-Wu
Department of Chemistry, University of Science and Technology of China, Hefei, China
"$^3$He NMR Studies on Fullerenes Derivatives"
Tuesday 31 July 2001

Dr ADAMS, Wade
Air Force Research Laboratory, USA
"Future Challenges in High Performance Fibers"
Tuesday 4 September 2001

Prof FUCHS, Harald
Physics Institute, University of Münster, Germany
"Advances in SXM and the Application for Self-assembling System"
Tuesday 4 September 2001

Prof DE MEIJERE, Armin
Department of Chemistry, Georg-August-Universität Göttingen, Göttingen, Germany
"Small Rings Galore - New Structurally Interesting Cyclopropane Derivatives"
Saturday 8 September 2001

Dr BISOFFI, Giovanni
Legnaro National laboratory, INFN, Italy
"uperconducting Radiofrequency Quadrupoles"
Wednesday 12 September 2001

Prof BORDEN, Weston T.
Department of Chemistry, University of Washington, Seattle, U.S.A.
"Synthesis and Study of Pyramidalized Alkenes"
Thursday 13 September 2001

Assoc Prof IWABUCHI, Yoshiharu
Faculty of Pharmaceutical Sciences, Nagasaki University, Japan
"Development of Catalytic Asymmetric Baylis Hillman Reaction and its Application to Natural Product Synthesis"
Tuesday 18 September 2001

Dr SHIMAZAKI, Makoto
Bayer Yakuhin, Ltd. Japan
"Recent Progress in Combinatorial Chemistry Toward the Development of Medicine"
Tuesday 18 September 2001

Prof ULANSKI, Jacek Pawel
Head of the Department of Molecular Physics, Technical University of Lodz, Poland
"Reticulate Doped Polymer Conducting Systems"
Wednesday 19 September 2001

Dr KISHIDA, Akio
Research Institute, National Cardiovascular Center, Osaka, Japan
"Polymeric Surfaces as Living-Body Interface"
Thursday 20 September 2001

Prof APELOIG, Yitzhak
Technion-Israel Institute of Technology, Israel
"The Chemistry of Novel Silicon-Mercury and Silicon-Lithium Compounds" Friday 21 September 2001

Dr PEKKER, Sandor
Research Institute for Solid State Physics and Optics, Hungarian Academy of Science, Hungary
"Solid State Reactions of Molecular Carbon"
Saturday 22 September 2001

Dr KIHARA, Daisuke
Donald Danforth Plant Science Center
"An ab initio protein structure prediction method that uses threading-based tertiary restraints."
Monday 15 October 2001

Prof Roger M Leblanc
Department of Chemistry, University of Miami, Miami, U.S.A.
"Recent Advances in the Surface Chemistry of Ultrathin Films"
Tuesday 16 October 2001

Assoc Prof FUJIWARA, Takumi
Department of Chemistry, Nagaoka University of Technology, Nagaoka, Japan
"Formation of optical nonlinear Periodic structure in the glass materials"
Friday 18 October 2001

Prof WATANABE, Junji
Tokyo Institute of Technology, Tokyo, Japan
"Frontier of Research on Polymeric Liquid Crystals"
Friday 19 October 2001

Prof TIAN, Fuli
Department of Chemistry, Inner Mongolia University
"Determination of Free Sugars and Non-Starch Polysacharides in Inner Mongolia Typical Cereals"
Wednesday 24 October 2001

Prof SNIECKUS, Victor
Queen's University, Canada
"From Flatland to Prochiral Metalation: Aiming for New Regio- and Enantioselective Carbanionic Processes for Aromatic Synthesis"
Monday 29 October 2001

Prof MIKOLAJCZYK, Marian
Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Poland
"Asymmetric Cyclopropanation and Synthesis of Aminophosphonic Acids Using Chiral Sulfinyl Auxiliary"
Monday 19 November 2001

Prof SCHMIDT-ROHR, Klaus
Department of Chemistry, Iowa State University, USA
"NMR Studies of Structure and Dynamics of Solid Polymers"
Monday 19 November 2001

Prof KAGAN, Henri
Université Paris-Sud, France
"Some Facets of the Screening of New Catalysts for Asymmetric Catalysis"
Tuesday 20 November 2001

Prof WEVER, Ron
University of Amsterdam, the Netherlands
"Vanadium-dependent halo-peroxidase"
Monday 26 November 2001

Prof COOK, James M.
University of Wisconsin, Milwaukee, U.S.A.
"Enantioselective Synthesis of Sarpagine, Ajmaline and Corynanthe Alkaloids via the Asymmetric Pictet-Spengler Reaction"
Tuesday 27 November 2001

Prof YAMAMOTO, Katsuji
Graduate School of Engineering, Kyoto University, Kyoto, Japan
"Quantum analysis of the Rydberg-atom-cavity detector for dark matter axion search "
Thursday 29 November, 2001

Prof TATSUMI, Kazuyuki
Research Center for Materials Science, Nagoya University
"Challenges for the Synthesis of Highly Ordered Transition Metal-Chalcogenide Complexes towards the Control of the Inorganic Reactions"
Monday 3 December 2001

Prof DEDERICHS P H
Institut für Festkörperforschung, Forschungszentrum Jülich,Germany
"Ab-Initio Calculation of Spin Dependent Transport and Spin Injection"
Wednesday 12 December 2001

Prof KIBAYASHI, Chihiro
Tokyo University of Pharmacy and Life Sciences, Japan
"Total Synthesis of Pumiliotoxin"
Thursday 13 December 2001

Prof CLENNAN, Edward Lawrence
Department of Chemistry, University of Wyoming
"The Persulfoxide; A Key Intermediate in Sulfide Photooxidations"
Monday 17 December 2001

# MEETINGS AND SYMPOSIUMS

## The First Kyoto COE Symposium on "Elements Science"

January 26-27, 2001 (Kyoto)

**Invited speaker**
Prof ASHWELL, G. J.
Cranfield University
"Molecular Architecture of Non-Centrosymmetric Langmuir-Blodgett Films: form Molecular Lego to Molecular Rectification and Second-Harmonic Generation"

Prof CHOY, J. -H.
Seoul National University
"Organic/Inorganic and Bio/inorganic Heterostructured Nanohybrids"

Prof TAYLOR, R.
Sussex University
"Reactions of $C_{60}F_{18}$ and $C_{60}F_{20}$"

Prof MATSUSHIGE, K.
Kyoto University
"Molecular Nano-Electronics and Molecular Computer"

Prof NAKATSUJI, H.
Kyoto University
"Quantum Chemistry of Photosynthetic Bacteria"

And 8 oral and 57 poster presentations

## Workshop: "Study of Plant Transcription Factor in the Post-genome Era"

Organized by AOYAMA, Takashi and YANAGISAWA, Shuichi
Saturday 26 March 2001 (Fukuoka)

## The 1st International Symposium on the Kyoto University COE Project "Elements Science: Characteristics and Functions in Organic and Inorganic Frameworks"

(Post-Conference of ISCOM2001: The 4th International Symposium on Crystalline Organic Metals, Superconductors and Ferromagnets)

September 17-18, 2001 (Kyoto)

Prof KUNITAKE, Toyoki
The University of Kitakyushu
"Preparation of nano-precision films of organic and inorganic components"

Prof HADDON, Robert C.
University of California at Riverside
"Chemistry of carbon nanotubes"

Prof MICHL, Josef
University of Colorado at Boulder
"Advances in the chemistry of carborane anions and radicals"

Prof AIDA, Takuzo
The University of Tokyo
"Design and applications of supramolecular porphyrin/fullerene nanohybrids"

Prof KOMATSU, Koichi
Kyoto University
"Synthesis of π-conjugated systems having raised HOMO levels by σ-π interaction"

Prof ULANSKI, J. et al.
Technical University of Lodz
"Comparison of optoelectronic properties of silicon- and carbon-backbone polymers substituted with carbazole groups"

Prof ASHWELL, Geoffrey J.
Cranfield University
"Molecular rectification: dipole reversal without molecular reorientation"

Prof KARL, Norbert et al.
University of Stuttgart
"Organic field effect transistors, influences of structural order/disorder"

Prof YOKOYAMA, Masaaki
Osaka University
"Optical logic devices based on a new phenomenon in organic thin films, photocurrent multiplication"

Prof SATO, Naoki et al.
Kyoto University; Kumamoto University
"Unoccupied electronic states in lithium phthalocyanine thin films of different morphologies examined by inverse photoemission spectroscopy"

Prof DAY, Peter
The Royal Institution of Great Britain
"Joining organic and inorganic layers in hybrid materials"

Prof POEPPELMEIER, Kenneth R.
Northwestern University
"Noncentrosymmetric inorganic-organic materials"

Prof ITO, Tasuku et al.
Tohoku University; University of California , San Diego
"Intramolecular electron transfer on the vibrational time scale in the mixed valence state of bridged dimers of triruthenium cluster"

Prof CASSOUX, P. et al.
Laboratory of Coordination Chemistry, CNRS
"From molecule-based conductors and magnets to thin films and nanowires deposited on conversion coating substrates"

Prof OUAHAB, Lahcene
University of Rennes
"Conducting and magnetic organic-inorganic hybrid materials"

Prof AWAGA, Kunio et al.
Nagoya University
"Unusual phase transitions in heterocyclic thiazyl radicals"

Assoc Prof ONO, T. et al.
Osaka University; Kyoto University
"Electrical transport in nano-magnet"

Prof TAKANO Mikio
Kyoto University
"Iron in unusual valence states"

Prof TAKAGI, Hidenori.
The University of Tokyo
"Guided tour to spinel oxides; from geometrically frustrated antiferromagnet or charge ordered insulator to heavy fermion metal"

Prof YAMANAKA, Shoji
Hiroshima University
"High-pressure synthesis and properties of silicon clathrate and related compounds"

Prof YAGUBSKII, Eduard B.
Russian Academy of Science
"Effect of metal type (M) and counterion on crystal structure and properties of $M(dddt)_2$ cationic complexes

Prof LYUBOVSKAYA, Rimma N.
Russian Academy of Science
"Design of novel solids based on fullerenes"

Assoc Prof YAMOCHI, Hideki et al.
Kyoto University
"A new type phase transition observed in the charge-transfer complexes based on a sulfur based donor molecule, EDO-TTF"

And 41 poster presentations

## Post OMCOS-XI Symposium, Thirty Years of the Cross-Coupling Reaction

Organized by TAMAO, Kohei (Kyoto University), HIYAMA, Tamejiro (Kyoto University), and MIYAURA, Norio (Hokkaido University).
27-29 July 2001 (Kyoto)

## Workshop:" Ion Beam Cooling -- toward the Crystalline Beam -"

November 12-14, 2001 (Kyoto)

1. Laser Equipped Cooler Storage Ring, LSR at ICR, Kyoto University
   Prof NODA, Akira
   Insititute for Chemical Research, Kyoto University, Japan

2. Electron Cooling for hot ion beam
   Mr FADIL, Hicham
   Faculty of Science, Kyoto University, Japan

3. Single and multiple Coulomb strings of ions in heavy ion storage ring
   Dr HASSE, Rainer W.
   Gesellschaft für Schwerionenforschung, GSI, Germany

4. Observations of Ordered Ion Beams in CRYRING
   Dr DANARED, Hakan
   Manne Siegbahn Laboratory, Sweden

5. Systematic investigation on electron cooling at the Heidelberg heavy ion storage ring
   Dr GRIESER, Manfred
   Max-Planck-Institut für Kernphysik, Heidelberg, Germany

6. Electron Cooling at HIMAC
   Dr NODA, Koji
   National Institute of Radiological Sciences, Japan

7. The heating rate during crystallization
   Dr SHOBUDA, Yoshihiro
   High Energy Accelerator Research Organization, KEK, Japan

8. Beam Crystallization at Low Line Densities
   Prof OKAMOTO, Hiromi
   Hiroshima University, Japan

9. Electron Cooling of Positrons and Possibilities of Positron Beam Crystallization
   Dr SIDORIN, Anatoly
   Joint Institute for Nuclear Research, JINR, Dubna, Russia

10. Design of Cooler Storage Ring at ICR, Kyoto University
    Mr SHIRAI, Toshiyuki
    Insititute for Chemical Research, Kyoto University, Japan

11. Diagnostics of Laser-Cooled Ion Beams
    Prof HANGST, Jeffrey S.
    University of Aarhus, Denmark

12. Crystalline Beam at PALLAS
    Mr SCHAETZ, Tobias
    Ludwig-Maximilians-Universitat , Munchen, Germany

13. Sympathetic cooling of molecular ions and mass spectrometry
    Mr BABA, Takashi
    Advanced Research Laboratory, Hitachi, Ltd., Japan

14. Strong Effects of Low-level Background Clouds on Crystallization of Clumps in Coulomb-Interacting Particle System

Prof KIWAMOTO, Yasuhito
Faculty of Integrated Human Studies
Kyoto University, Japan

15 Beam cooling at MUSES project
Prof KATAYAMA, Takeshi
University of Tokyo/ Institute of Physical and Chemical Research, RIKEN, Japan

16 An electron target/cooler for extremely low-energy ion beams at the electrostatic storage ring
Prof TANABE, Tetsumi
High Energy Accelerator Research Organization, KEK, Japan

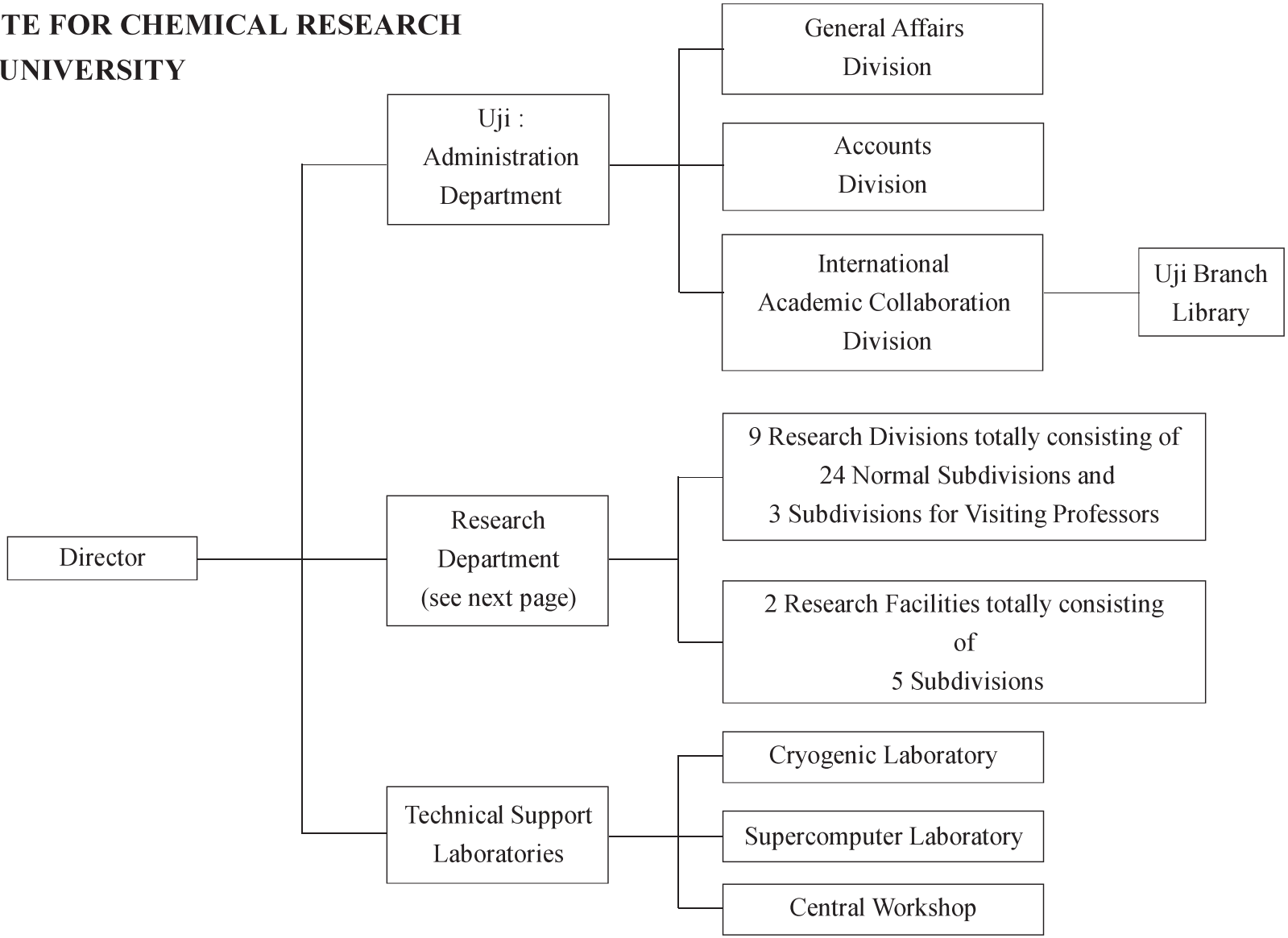
17 Intense high energy particle generation by ultraintense laser-matter interactions"
Prof NAKAJIMA, Kazuhisa
High Energy Accelerator Research Organization, KEK, Japan

## International Symposium: "New Era of Transcription Factor Research in Plants"

Organized by TAKATSUJI, Hiroshi and AOYAMA, Takashi
Thursday 29 to Friday 30 November 2001 (Tsukuba)

# ORGANIZATION AND STAFF

**INSTITUTE FOR CHEMICAL RESEARCH**
**KYOTO UNIVERSITY**



# INSTITUTE FOR CHEMICAL RESEARCH, KYOTO UNIVERSITY

As of 31 December 2001

RESEARCH DIVISION (G: Laboratory for Visiting Professors)

| | Research Division | Subdivision (Laboratory) | Related Graduate School<br>*Graduate School/Division of* | Professor | Associate Professor | Instructor |
|---|---|---|---|---|---|---|
| Director<br>TAMAO, Kohei | States and Structures | I. Atomic and Molecular Physics | *Science / Physics I* | | ITO, Yoshiaki | NAKAMATSU, Hirohide |
| | | II. Electron Microscopy and Crystal Chemistry | *Science / Chemistry* | ISODA, Seiji | | OGAWA, Tetsuya<br>NEMOTO, Takashi |
| | | III. Polymer Condensed States | *Engineering / Polymer Chemistry* | KOHJIYA, Shinzo | TSUJI, Masaki | URAYAMA, Kenji<br>TOSAKA, Masatoshi |
| | Interface Science | I. Solutions and Interfaces | *Science / Chemistry* | NAKAHARA, Masaru | UMEMURA, Junzo | MATSUMOTO, Mutsuo<br>MATSUBAYASHI, Nobuyuki<br>OKAMURA, Emiko |
| | | II. Molecular Aggregates | *Science / Chemistry* | SATO, Naoki | ASAMI, Koji | KITA, Yasuo<br>YOSHIDA, Hiroyuki |
| | | III. Hydrospheric Environment Analysis | *Science / Chemistry* | SOHRIN, Yoshiki | UMETANI, Shigeo | SASAKI, Yoshihiro<br>OKAMURA, Kei |
| | Solid State Chemistry | I. Artificial Lattice Alloys | *Science / Chemistry* | SHINJO, Teruya | HOSOITO, Nobuyoshi | FUJITA, Masaki |
| | | II. Quantum Spin Fluids | *Science / Physics I* | YAMADA, Kazuyoshi | MIBU, Ko | IKEDA, Yasunori |
| | | III. Solid State Chemistry | *Science / Chemistry* | TAKANO, Mikio | TERASHIMA, Takahito | AZUMA, Masaki |
| | | IV. Amorphous Materials | *Engineering / Molecular Engineering* | YOKO, Toshinobu | UCHINO, Takashi | TAKAHASHI, Masahide<br>HIMEI, Yusuke |
| | | G. Structure Analysis | | KIKKAWA, Shinichi | YAMANAKA, Akio | |
| | Fundamental Material Properties | I. Molecular Rheology | *Engineering / Molecular Engineering* | OSAKI, Kunihiro | WATANABE, Hiroshi | INOUE, Tadashi |
| | | II. Polymer Materials Science | *Engineering / Polymer Chemistry* | KAJI, Keisuke | KANAYA, Toshiji | NISHIDA, Koji |
| | | III. Molecular Dynamic Characteristics | *Engineering / Molecular Engineering* | HORII, Fumitaka | TSUNASHIMA, Yoshisuke | KAJI, Hironori<br>HIRAI, Asako |
| | | G. Composite Material Properties | | TANAKA, Yoshinobu | YOSHINOBU, Jun | |
| | Organic Materials Chemistry | I. Polymeric Materials | *Engineering / Polymer Chemistry* | FUKUDA, Takeshi | TSUJII, Yoshinobu | OHNO, Kohji<br>MURAKAMI, Syozo |
| | | II. High-Pressure Organic Chemistry | *Engineering / Energy & HC Chemistry* | KOMATSU, Koichi | KITAGAWA, Toshikazu | MORI, Sadayuki<br>NISHINAGA, Tohru<br>MURATA, Yasujiro |
| | Synthetic Organic Chemistry | I. Synthetic Design | *Engineering / Energy & HC Chemistry* | TAMAO, Kohei | TOSHIMITSU, Akio | KAWACHI, Atsushi<br>YAMAGUCHI, Shigehiro |
| | | II. Fine Organic Synthesis | *Pharmaceutical Sci / Pharmac. Chem.* | FUJI, Kaoru | KAWABATA, Takeo | TSUBAKI, Kazunori |
| | | G. Synthetic Theory | | KIBAYASHI, Chihiro | IWABUCHI, Yoshiharu | |
| | Bioorganic Chemistry | I. Organoelement Chemistry | *Science / Chemistry* | TOKITOH, Norihiro | NAKAMURA, Kaoru | KAWAI, Yasushi<br>SUGIYAMA, Takashi<br>TAKEDA, Nobuhiro |
| | | II. Bioactive Chemistry | *Pharmaceutical Sci / Drug System* | SUGIURA, Yukio | FUTAKI, Shiroh | NAGAOKA, Makoto |
| | | III. Molecular Clinical Chemistry | *Medicine / Internal Medicine* | UEDA, Kunihiro | TANAKA, Seigo | ADACHI, Yoshifumi |
| | Molecular Biofunction | I. Chemistry of Molecular Biocatalysts | *Agriculture / Agricul. Chem.* | SAKATA, Kanzo | HIRATAKE, Jun | MIZUTANI, Masaharu<br>SHIMIZU, Bun-ichi |
| | | II. Molecular Microbial Science | *Agriculture / Agricul. Chem.* | ESAKI, Nobuyoshi | YOSHIMURA, Tohru | KURIHARA, Tatsuo<br>MIHARA, Hisaaki |
| | Molecular Biology and Information | I. Biopolymer Structure | *Science / Biophysics* | | HATA, Yasuo | HIRAGI, Yuzuru<br>FUJII, Tomomi |
| | | II. Molecular Biology | *Science / Biophysics* | OKA, Atsuhiro | AOYAMA, Takashi | SAKAI, Hiroe<br>KAWASHIMA, Shuichi |
| | Bioinformatics Center | I. Bioknowledge Systems | *Science / Biophysics* | KANEHISA, Minoru | GOTO, Susumu | NAKAYA, Akihiro |
| | | II. Biological Information Network | *Informatics / Intelligence Science and Technology* | AKUTSU, Tatsuya | SUGISAKI, Hiroyuki | |
| | | III. Pathway Engineering | *Informatics / Intelligence Science and Technology* | MIYANO, Satoru<br>(Adjunct Prof) | | |
| | Nuclear Science Research Facility | I. Particle and Photon Beams | *Science / Physics II* | NODA, Akira | IWASHITA, Yoshihisa | SHIRAI, Toshiyuki |
| | | II. Beams and Fundamental Reaction | *Science / Physics II* | | MATSUKI, Seishi | |

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# KEYWORD INDEX