from Tsukuba, Japan to the world

NIMS NOW International

National Institute for Materials Science

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RESEARCH FRONTIER

Elucidation of Cryogenic Temperature Ground State at Si (100) Surface

—Providing Indispensable Intellectual Infrastructure for Silicon IT —

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Nanodevice Group
Nanomaterials Laboratory (NML)

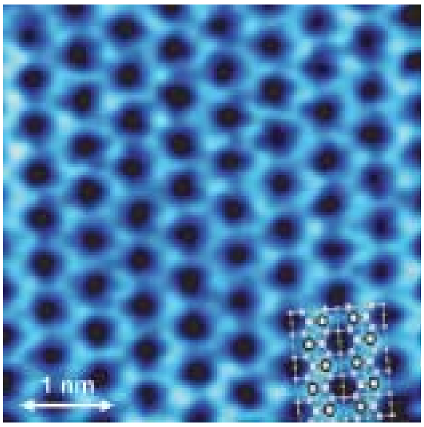


Fig.1: Cryogenic temperature (0.7 K) STM image of Si (100) surface.

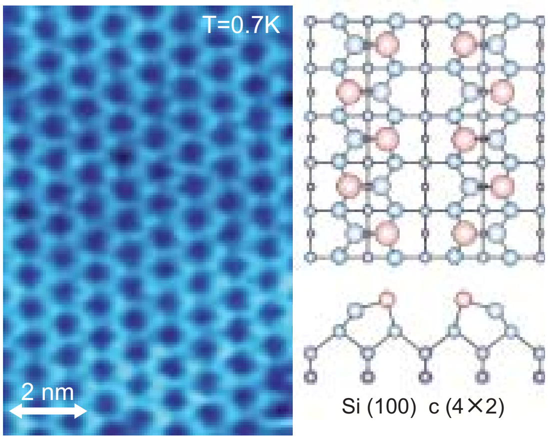


Fig.2: Scanning tunneling microscope (STM) image of Si (100) surface at 0.7 K.

As one basic technology for nanotechnology, the Nanodevice Group is developing scanning tunneling microscope (STM) technology in extreme physical field environments. Using our high resolution/cryogenic temperature STM technology, we succeeded in elucidating the ground state of the Si (100) surface at the atomic level in the sub-1 K temperature region (**Fig. 1**). This allowed us to determine that, among the 3 periodic structures which exist on the Si (100) surface, namely, (2x1), c(4x2), and p(2x2), the most stable structure is c(4x2) (**Fig. 2**). We also demonstrated for the first time that the other structures which had been proposed as the ground state in the past can be freely manipulated by controlling the energy applied from the STM probe (**Fig. 3**).

Silicon wafers with a (100) surface are the most important material supporting IT, and have been investigated by many researchers. However, until now, the ground state (most stable state at cryogenic temperature) of the Si (100) surface had not been determined decisively, and was one key unsolved problem remaining in physics. < Continued on p.4

In this issue

NIMS NOW Name Change

Since July 2003, NIMS has published an English translation of *NIMS NOW*, which had been published in a Japanese-language version until that time, to give a larger number of people around the world an understanding of our activities. This English version has readers in more than 40 countries worldwide.

During this period, the many young international scientists working at NIMS have increasingly expressed a desire to "present research in *NIMS NOW* as a worldwide publication." At the same time, in publishing a newsletter with a worldwide readership, some ingenuity not found in the Japanese- language version had become necessary in the layout and presentation.

To meet these needs, beginning this month, we are changing the name of this publication to *NIMS NOW International*, and will publish the new version as a NIMS newsletter which presents information not for Japan, but for the world as a whole.

Thank you for your continuing readership and support.

First Observation of the Birth of Quasiparticles in Silicon Crystal

—New Knowledge of Quantum Interference Dynamics of Electron Waves/Lattice Waves—

Muneaki Hase, Masahio Kitajima
Reaction and Excitation Dynamics Group
Materials Engineering Laboratory (MEL)

Hrvoje Petek
Dept. of Physics and Astronomy
University of Pittsburgh, U.S.A.

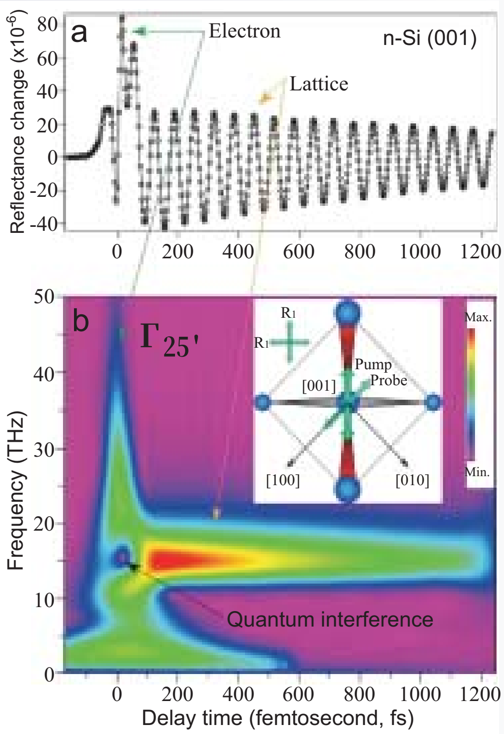


Fig: (a) The change in anisotropic reflectivity from the silicon surface; the abscissa shows the delay time between the pump pulse and probe pulse. (b) The time- frequency map of electro-optic sampling signals obtained by continuous wavelet transform. The frequency unit THz (terahertz) equals 10^{12} Hz.

Crystals such as silicon consist of groups of periodically-arranged atoms (lattice) and the electrons which connect them. Interactions between the lattice and electrons, or so-called phonon-electron interactions, are extremely fast phenomena, normally occurring at the 10 femtosecond level (1 femtosecond, fs = 10^{-15} sec), and therefore have been impossible to observe until now. In the present research, we broke this time barrier and succeeded for the first time in observing the phonon-electron interaction in silicon crystals in the fs time region by performing pump-probe spectroscopy, which is a time-domain measurement method, with a 10 fs pulse laser.

Observations were performed using the time-resolved electro-optic detection method. The light source was a pulse laser with a pulse duration of approximately 10 fs and a central wavelength of approximately 400 nm. The specimens used were n-Si (with doping up to $1x10^{15}$ cm^{-3}). The detection method featured selective extraction of only response components in which the phases of the lattice wave and electron wave were aligned, thereby achieving high experimental accuracy more than two orders better in the past.

The response of the observed signals comprises two components. One is a periodic vibration component caused by lattice vibration, which can be observed at times longer than 50 fs. The other is a nonperiodic response from the electron system, which can be observed only at times shorter than 50 fs and, following this, information on quantum interference between the lattice system and electron system, which appears at times up to 100 fs, as shown in **Fig. (a)**.

This quantum interference can be seen clearly in the frequency-time map obtained by wavelet transform in **Fig. (b)**. The component which extends in the direction of the ordinate around time 0 is the electron response, and the component extending in the direction of the abscissa is the lattice (phonon) response. In particular, what should be emphasized here is that the dip at the intersection between the two components. At this instant, the excited electrons generate a force on the lattice, causing coherent phonon excitation. This is considered to be interference between the electron wave and lattice wave, and would provide experimental evidence of the Fano interference, which was already predicted theoretically more than 40 years ago.

This corresponds to the "entanglement" phenomenon of electrons and the lattice described by the quantum mechanics of many-body systems. In other words, we believe that we have observed a phenomenon corresponding to the birth of "quasiparticles" caused by a quantum- mechanical "entanglement" in silicon. This achievement not only breaks new academic ground in quantum interference dynamics, but is also expected to provide a basis for evaluation of the characteristics of nano-scale electronic devices and development of such devices.

(These research results were published in the English science journal, *nature*, dated November 6, 2003.)

For further information, please visit: http://www.nims.go.jp/nanomat_lab/device.html and http://www.phyast.pitt.edu/

Memorandum of Understanding with Korea Institute of Geoscience and Mineral Resources

The Nanomaterials Laboratory (NML, Director-General: Dr. Masakazu Aono) reached agreement on research cooperation in the field of nano-particles with the Korea Institute of Geoscience and Mineral Resources (KIGAM, Director: Dr. Tai-Sup Lee), a national institute in Korea, and concluded a memorandum of understanding (MOU) with KIGAM on March 24.

Under the MOU, the two institutes agreed to a cooperative relationship in basic and applied research on nano-magnetic particles extending into the future. The arrangement will combine KIGAM's research potential in nano-magnetic particles in the fields of inorganic chemistry and chemical engineering and the research potential of the NIMS Nanomaterials Laboratory, which has been a leader to date in the fields of magnetic fluids, patterned media for high density magnetic recording, and magnetic viscous fluids. Based on the MOU, joint research projects in connection with 2-dimensional arrays of nano-magnetic particles and ultra-high density magnetic recording media were recently proposed to the Korean government.

Athermal Recovery of Silicon Surface from Plasma Damage

—Discovery of Novel Recrystalization Phenomena with Low-Energy Electron (<70 eV)—

Kazushi Miki
Nanoarchitecture Group
Nanomaterials Laboratory (NML)

Masahiro Kitajima
Reaction and Excitation Dynamics Group
Materials Engineering Laboratory (MEL)

In silicon ULSI circuits and magnetic recording media, recent years have seen the appearance of nanoscale functional structures with sizes on the order of 10 nm - 100 nm in plane and several nm in depth. However, at this scale, the artificial structures fabricated by advanced modern techniques collapse under high temperature annealing process to remove defects. A new defect restoration process without high temperature treatment has therefore been desired. Our two groups discovered a phenomenon by using low-energy electron irradiation, even at room temperature, which could restore the damaged surface-layer caused by plasma. This recovery phenomenon is expected to be a principle process open to the technical development of low temperature processing. Such process includes the patterning of some crystal structures where high temperature treatment is not desired, structural modification techniques, and similar applications.

When electron beam irradiation is performed at low energy < 70 eV, we discovered an interesting phenomenon. Here the compressive stress which accumulates as a result of plasma damage was relieved by the introduction of electron beam irradiation. In fact, the strain value returned completely to its initial value (**Fig. (a)**). There are two predominant features of this phenomenon, (1) in contrast to the fact that high-energy electron beams cause defects, the effect of the electron beam becomes completely restorative rather than destructive at around 70 eV, and (2) this is a non-thermal process.

We conjecture that this phenomenon can be explained by an ionization enhanced diffusion model of the Bourgoin-Corbett mechanism type. In this model, attention is drawn to the fact that the charge state of defects changes as a result of electron beam irradiation. Assuming the charge state transition occurs continuously under the electron beam irradiation, diffusion could become possible without the assistance of heat and, as a result, the damaged material undergoes recrystallization.

(These research results were published recently in the English physics journal, *J. Phys.: Condens. Matter*, and were selected by IoPSelect (http://Select.iop.org) as a noteworthy paper.)

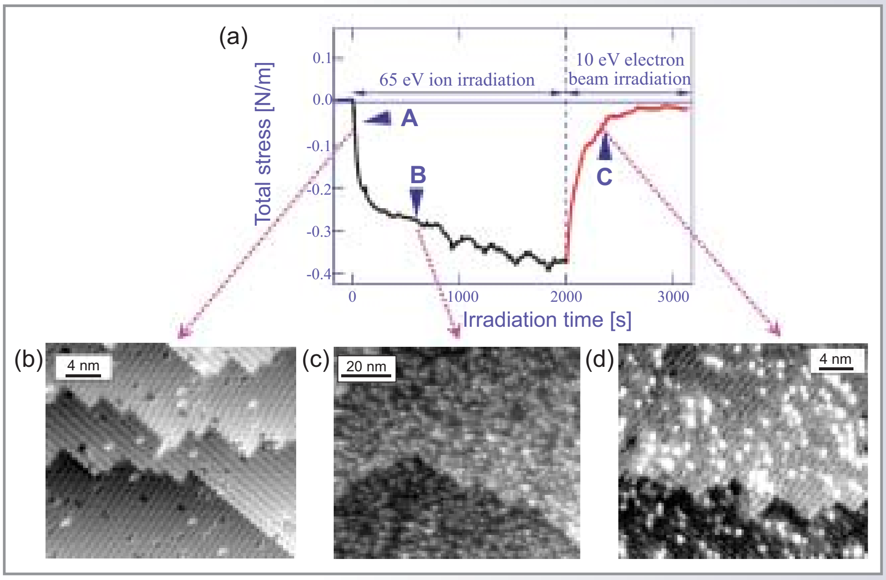


Fig: Change in surface stress during both plasma bombardment and following electron beam irradiation, and scanning tunneling microscope (STM) images: (a) Measured results of the change in surface strain with the optical cantilever method when silicon was irradiated successively both with argon ions at 65eV and then with an electron beam at 10eV. STM images of (b) Si (100) surface before the ion irradiation, (c) surface where defect was introduced, and (d) surface after the defect was removed by electron beam irradiation.

For further information, please visit: http://www.nims.go.jp/nanomat_lab/arc.html and http://www.nims.go.jp/ldynamics/

Symposium Marks Start of ICYS

- Seeking and Training Excellent Young Research Leaders -

Prof. Leo Esaki

A symposium marking the inauguration of the NIMS International Center for Young Scientists (ICYS) was held at Shin-Maru Conference Square in Tokyo on June 1. Prof. Leo Esaki, President of Shibaura Institute of Technology, delivered a speech with numerous suggestions on the development of young researchers, which was followed by presentations of examples and advice on internationalization and human resource development by Prof. Sukekatsu Ushioda, President of the Japan Advanced Institute of Science and Technology, and Prof. Yoshio Nishi of Stanford University in the United States.

During the second half of the symposium, Prof. Yoshio Bando, Director-General of the ICYS, reported on the ICYS's activities up to the present, and Mr. Masaharu Asaba, Chief Editor of the Daily Yomiuri newspaper, and Prof. Toshiaki Ikoma, Director-General of Hitachi Metals, Ltd., expressed their hopes and desires for the ICYS. The enthusiastic gathering included 190 participants and showed the high expectations placed on the ICYS.

Development of Inexpensive, Non-Allergic Dental Devices

Daisuke Kuroda, Takao Hanawa
Reconstitution Materials Group
Biomaterials Center (BMC)

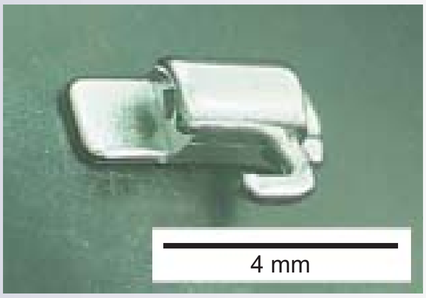


Fig. 1: Small-scale part formed prior to N_2 absorption.

Fig. 2: Ni-free stainless steel wire.

Although Ti-Ni shape memory alloys and 316L austenitic stainless steel are used as materials for dental instruments and other products such as orthodontic wires, these alloys contain nickel, which is considered a problematic as a substance that causes metallic allergy. Non-allergic nickel-free stainless steel, in which mechanical strength and corrosion resistance are improved using nitrogen as a substitute for nickel, has drawn attention as a new metal biomaterial. However, because the material itself becomes extremely hard, depending on the forming and machining conditions, Ni-free stainless steel dental devices and technologies for manufacturing small-scale, complex-shaped dental devices from Ni-free stainless steel have not reached practical application. Moreover, because special melting equipment is required to melt Ni-free stainless steel, the material cost is also high in comparison with the conventional austenitic stainless steel. In view of these problems, the development of a new manufacturing technology which makes it possible to produce dental devices easily and inexpensively using Ni-free stainless steel material has been strongly desired.

To meet this need, we are carrying out joint development of an economical technology for manufacturing small dental devices with complex shapes from Ni-free stainless steel based on a fusion of manufacturing technology for Ni-free stainless steel employing a N_2 absorption treatment proposed by the NIMS Reconstitution Materials Group and the outstanding dental product manufacturing technologies of Dentsply-Sankin K.K.

Using stainless steel in the ferritic state, which is soft prior to nitrogen absorption, we found that wire material with a diameter of 1 mm or less and length of more than 4000 mm can be formed easily at room temperature, and dental devices with complex shapes can also be manufactured easily by adjusting the alloy composition (see **Fig. 1** and **Fig. 2**). When these formed parts are held under N_2 gas for 2 hours in a heat treatment furnace heated to 1200 **℃**, 1 wt% N_2 is absorbed by the part, and the entire structure of the part undergoes transformation to austenite, making it possible to obtain the objective Ni-free stainless product. Because the tensile strength, elongation to fracture, torsional strength, and corrosion resistance of the dental products manufactured by this process show high values in comparison with conventional austenitic stainless steel, smaller-scale products can be expected . (see **Fig. 3**)

Future tasks include optimization of N_2 absorption treatment conditions corresponding to the product shape and verification of mechanical durability.

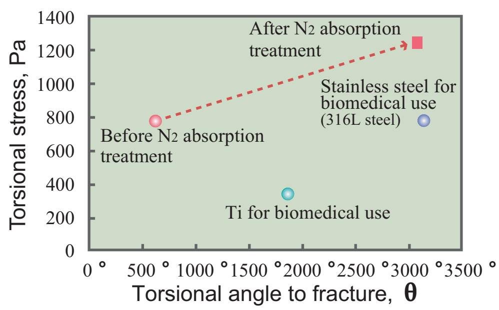


Fig. 3: Comparison of torsional stress and torsional angle to fracture of wire (diameter: 1 mm) before/after N_2 absorption and conventional metallic biomaterials.

< Continued from p.1

Elucidation of Cryogenic Temperature Ground State at Si (100) Surface

From the practical viewpoint, numerous computational simulation methods have been developed for various processes on the Si (100) surface in view of their great industrial importance, and the ability to accurately reproduce the most stable structure of the Si (100) surface with these computational scientific techniques is essential for verifying their reliability. While the achievement reported here provides important basic knowledge for elucidating the ground state of the Si (100) surface, it is also an extremely important discovery in the sense of providing necessary and indispensable intellectual infrastructure for silicon process simulation technologies.

For further information, please visit: http://www.nims.go.jp/nanomat_lab/device.html

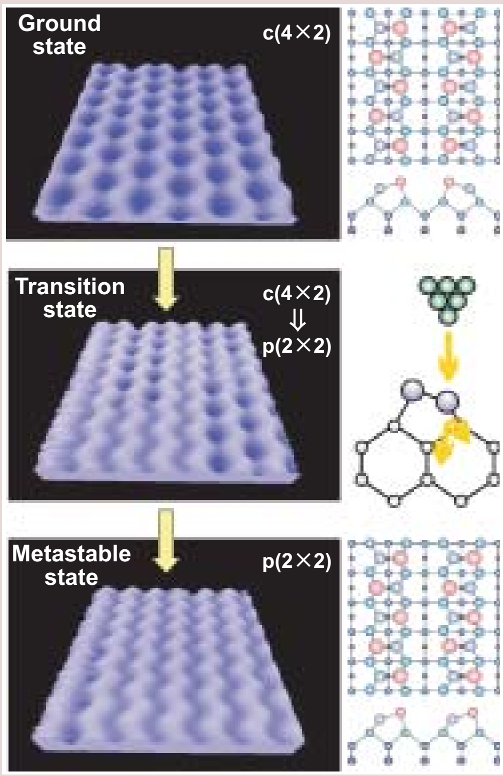


Fig. 3: Structural control of Si (100) surface by STM from ground state to metastable state (up to temperature of 5 K).

Modular Materials
-Introduction of Functional Modules Group-

Dirk G. Kurth
Director, Functional Modules Group
Advanced Materials Laboratory(AML), NIMS
Group Leader, Modular Materials Group Department of Interfaces
Max Planck Institute of Colloids and Interfaces (MPI-KG), Germany

Nature repeatedly demonstrates exquisite control over the weak and competing intra-molecular forces that underlie the very existence of life, ranging from the molecular level, as in the formation of DNA, to the macroscopic length scale, as in bone or wood. As a result, natural materials are intrinsically hierarchical, which is often responsible for some of the unusual properties such as mechanical strength and toughness. Moreover, natural materials often comprise several functions. The cytoskeleton, for instance, determines cell and tissue shape but also affects migration, movement of organelles and cell division. Due to the weak and competitive interactions, biological systems can adapt their structure and function to external stimuli. Inspired by nature, the introduction of specific molecular interactions to guide the association of functional modules is an overarching theme in materials science.

The Functional Modules Group aims at developing strategies to use weak and competing intra-molecular interactions to deliberately combine, position, and orient structural and functional modules in predictable ways. In order to support, handle, manipulate, and operate devices at the nanoscopic length scale, it will be advantageous to collect and arrange the components in surface-confined structures.

Our research objectives also include solution phase functional devices as well as liquid crystals. The modularity of this approach provides extensive control of structure and function from molecular to macroscopic length scale. In addition, the use of modules provides an unsurpassed degree of synthetic simplicity, diversity, and flexibility. Each module can be synthesized and optimized independently before they are assembled as a whole to the final functional device or material. Frequently, we use environmentally safe water-based self-assembly strategies. The ability to control the spatial arrangement of functional constituents is of critical importance with respect to the encoding of new (collective) properties and the exploitation of a material's potential. Studying structure-property relationships of such assemblies forms the basis for identifying potential applications of these materials. Research topics include sensors, electro- and photochromic displays, bio-mimetic catalysts, adaptive as well as magnetic materials.

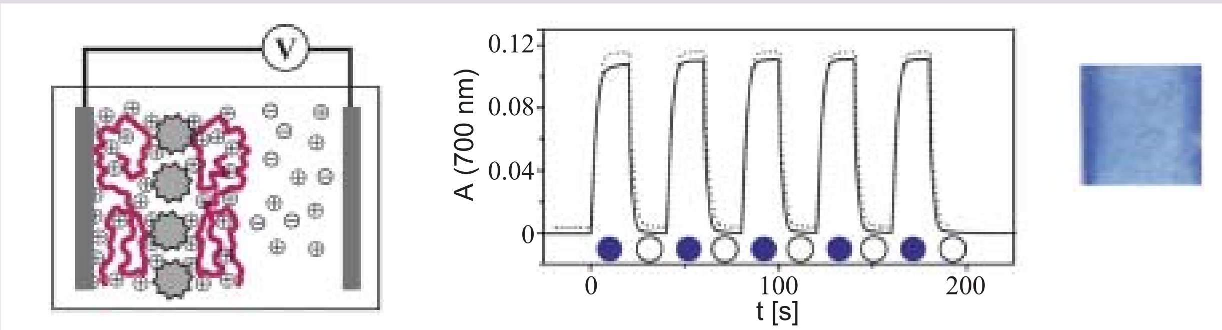


Fig: An electrochromic device made by self-assembly of functional modules. The electrochromic module, a polyoxometalate cluster, is embedded in a polyelectrolyte matrix on a transparent conducting substrate. Left: Schematic of the electrochromic cell. Center: Absorption measured at 700 nm of a 80 nm thick coating. Note the excellent transparency in the visible range of the spectrum. Coloration and bleaching occur within seconds upon applying the appropriate voltage. Right: Photograph showing the nice blue color of the device.

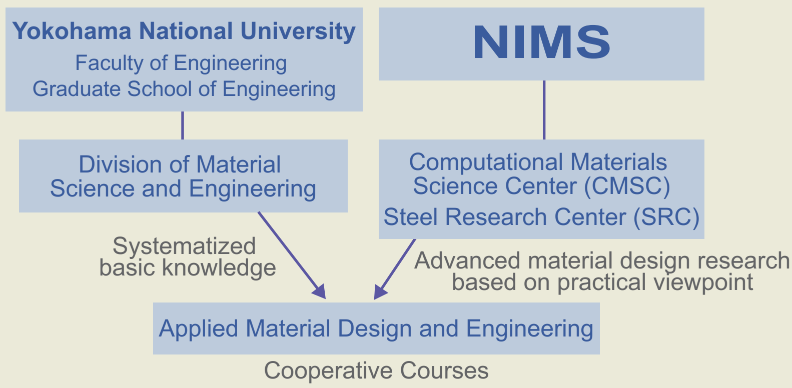
For further information, please visit: http://www.nims.go.jp/amlaml/english/ and http://www.mpikg-golm.mpg.de/gf/

Start of Cooperation with Yokohama National University under Cooperating Graduate School System

Material development is no longer limited simply to achieving high performance, but must now be based on an understanding of the total requirements of the product, including harmony with the environment, safety, and other factors related to the actual use environment.

This cooperative arrangement is intended to train human resource who understand and can realize the requirements of more complex, higher-level material development through cooperation between university researchers whose aim is to create systematized basic knowledge and leading NIMS material design researchers whose work is based on the viewpoint of practical use.

Concretely, a cooperative course in Applied Material Design and Engineering will be established in the Yokohama National University Graduate School. Three NIMS researchers will be named as guest faculty members in this specialty, and will give courses in Computational Modeling of Phase Equilibria, Computational Modeling of Phase Transformations and Microstructure Evolutions, and Structural Materials Design Engineering. NIMS also expects to give research guidance to interested graduate students.



Hello from NIMS

Jimmy Stokes (Univ of Minnesota in Minneapolis, U.S.A.)
Visiting Researcher (Jun. 2004-Jul. 2004)
Macromolecular Function Oxides Group
Advanced Materials Laboratory (AML)

[With colleagues, center front]

My name is Jimmy Stokes and I am a third year undergraduate student in chemical engineering from the University of Minnesota in Minneapolis. With funding support from the National Science Foundation and the Georgia Institute of Technology, I was able to work this summer in the Macromolecular Function Oxides Group at NIMS under the supervision of Dr. Izumi Ichinose and Dr. Sharmistha Paul. My primary goal this summer was to investigate the ion exchange between biomolecules on a protein layer assembled on a ZrO_2 surface. Understanding the fundamental chemistry behind this exchange will give a much better description of the protein's behavior when it is immobilized on a surface.

I would like to thank everyone at NIMS for all of their support and for giving me the opportunity to perform first class research. Japan is an excellent place to live because of the superb food and the overwhelming generosity shown by the people. For example, anyone who has ever been to a major department store in Japan will undoubtedly be greeted by a hearty "irashaimase".

Tsukuba is a wonderful "melting pot" city where many different cultures can coexist and international collaboration is common. Although my stay in Tsukuba was extremely short, I would like to reemphasize my appreciation for having this magnificent research opportunity. I will continue to stay in contact with all of my co-workers in the future and I hope to visit Tsukuba again one day.

■ Life, so far, in Japan! ■

[With colleagues, back, third from the left]

Richard Buchanan (Scotland, UK)
JSPS Fellow (Jan. 2004-Sep. 2004)
Eco-Energy Materials Group
Ecomaterials Center (EMC)

Hello, I am Richard Buchanan, a JSPS-funded Post-Doctoral Fellow at NIMS' Namiki site, after finishing a PhD at the University of St Andrews. I am working with Dr.Toshiyuki Mori (Ecomaterials Centre) on investigating the dependence of the conductivity of $Gd_xCe_{1-x}O_{2-x/2}$ ceramics (x=0.10-0.25) on grain size. These materials could be used as SOFC electrolytes operating at ≤800 ℃, as they have higher oxide ion conductivity than yttria-zirconia electrolytes.

I think I'm used to normal everyday things in Japan. Japan's hotter, with typhoons and earthquakes. Work-wise, Japan's working week would be illegal under European law but there's less 'group politics', which is a relief.

I've been to Mt. Tsukuba (difficult to get to) and some areas of Tōkyō. Akihabara has anime/ manga-related items in 'hobby' shops and places that sell English-language goods. For books and magazines, go to Shinjuku or Shiubya. In May, I went to the Edo-Tōkyō museum, watched Sumo at the Ryōgoku Kokugikan and in June, I tried on a kimono. My other exposure to Japanese culture is in manga and anime but why is anime more expensive in Japan than in the UK or USA? Finally, I haven't tried much Japanese food but I like 'butadon' (pork rice bowl).

Tsukuba is surrounded by a rich natural environment, with the second largest lake in the country, Kasumigaura, in the east. The area boasts Japan's largest production for hasu (lotus root) and it is famous as a local food as well as the processed fish products from the lake.

Hasu (Lotus flower)
July 20

Independent Administrative Institution
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