



# IMS NOW

## International

National Institute for Materials Science

Vol.4 No.1 January, 2006

New Year 2006

# New Year's Greetings

Teruo Kishi  
President

**A**s we begin 2006, all of us at NIMS would like to express our very wishes to you for a happy New Year.

Approximately 5 years have now passed since NIMS was established on April 1, 2001, and we will conclude our 1st Mid-Term Program at the end of March of this year. During its 1st Mid-Term Program, NIMS has launched many new and innovative initiatives, and we believe that the institute has also grown substantially during this period.

In comparison with the results before NIMS became an Independent Administrative Institution (IAI), our number of published papers has increased 1.9 times, and according to the ISI's Essential Science Indicators database, the number of citations of NIMS papers in the field of materials science has increased 3.4 times. Moreover, our world ranking in this field has risen from 30th before becoming an IAI to 4th after becoming

an IAI. Where patents are concerned, both the number of applications and the number of registered patents have roughly doubled. Although we devote considerable effort to technology transfer to private-sector companies and others, NIMS itself has also created six NIMS-originated venture companies to date to encourage wider use of its research achievements.

The Council for Science and Technology Policy of Japan reviews the science and technology-related activities of IAI, and as a result, has given NIMS its highest ranking in several items. Although we recognize that there are still many areas where improvement is needed, we believe that we have made a very good start in our first 5-year period of operation.

On the other hand, the environment surrounding science and technology changes with each passing year, and NIMS must also respond to these changes. A firm grasp of what should be changed and what should be main-

tained is necessary. In this kind of environment, we believe that the direction which NIMS should follow for the foreseeable future is "Nanotechnology Driven Materials Science for Sustainability." Under our 2nd Mid-Term Program, which begins in April of this year, we plan to carry out 20 project research items in the priority areas of "Nanotechnology Driven New Materials Creation" and "Advanced Materials Responding to Social Needs." Organizationally as well, we will strive to create a simple, flat organization which is capable of sure, steadily implementation of project research.

Exploratory research to cultivate the potential for subsequent projects is also essential. We are committed to promoting both project research and exploratory research in a well-balanced manner, giving due consideration to the allocation of human, financial, and other research resources.

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### NIMS News

## MOU with Shanghai Institute of Ceramics



From the right, Prof. Luo, SICCAS Director, Prof. Chang, BTERC Director, Prof. Tanaka, BMC Director-General, and Prof. Kishi, NIMS President.

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# Strategic Promotion of Nanotechnology Research and Development by Industry, Academia, and Government

Minoru Yonekura  
Deputy Director-General  
Nanotechnology  
Researchers Network Center  
of Japan

Nanotechnology has attracted attention as a technology which holds the key to solving the global-scale problems of the 21st century. In order to promote nanotechnology research and development in a strategic manner, Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT) launched the Nanotechnology Support Project in 2002 under 5-year plan, providing powerful support to all researchers in-

involved in nanotechnology in Japan in private companies, universities, and government organizations (see Fig. 1).

The Nanotechnology Support Project consists of two broad support functions. In the first area, recognizing that advanced measurement technologies, nanoscale fabrication and processing technologies, and synthesis/evaluation technologies, while necessary, are not readily available to many re-

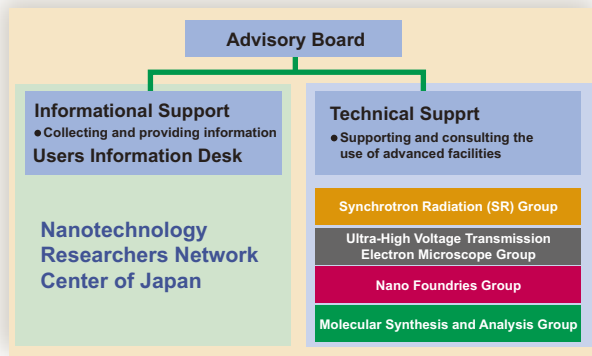


Fig. 1 System for implementation of the Nanotechnology Support Project.

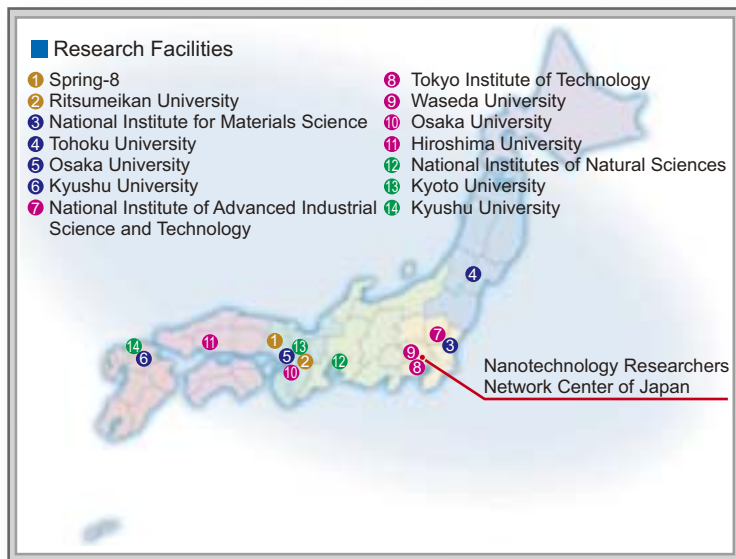


Fig. 2 Institutes providing user facilities.

searchers engaged in nanotechnology-related R&D, the Project offers technical support which gives researchers access to these technologies through use of leading-edge, large-scale facilities as "user facilities." A total of 14 research institutes nationwide have been designated as user facilities. As of the end of FY2004 (March 2005), more than 2,000 research projects had received this type of support. The support system, participating institutes, and results to date are shown in Figs. 1, 2 and 3, respectively. In this Project, NIMS provides support in the use of ultra-high-voltage transmission electron microscopes

(TEM) and synchrotron radiation facilities.

The second large support function of the Project includes the supply of information on research in the vast field of nanotechnology to researchers in industry, universities, and government organizations. Moreover, because nanotechnology requires technology and knowledge in multidisciplinary fields for further development, the Project also provides opportunities for exchanges among researchers and support for the training of new human resources as part of this second function. These functions are administered by the Nanotechnology Researchers Network Center of Japan.

Who Used the facilities? (FY2002-2004)

Support facilities	University	Public Institute	Corporation	Total (number)
Ultra-HV TEM	270	58	97	425
Nano Foundries	272	126	234	632
Synchrotron Radiation	255	42	70	367
Mol. Synthesis and Analysis	433	70	154	657
Total (number)	1230	296	555	2081
(Distribution of the users affiliation (%))	(59%)	(14%)	(27%)	(100%)

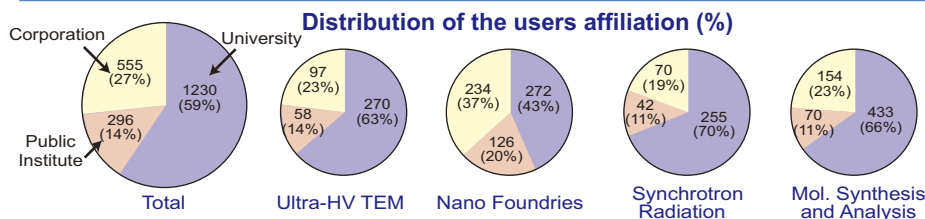


Fig. 3 Results of use of user facilities from FY2002 to FY2004.

Prof. Gillian, LCN, and Prof. Ohno, CMSC Director-General.





Fig. 6 "Nano Adventure" display at Kitanomaru Science Museum, Tokyo.

Continuing progress in nanotechnology requires knowledge and technology in different fields, including chemistry, physics, biotechnology, and the life sciences. The Nanotechnology Researchers Network Center therefore collects advanced information on nanotechnology in diverse fields and makes these resources available through the Center's website and email magazine. The Center also provides important supplementary support for the de-

velopment of nanotechnology by organizing symposiums and other forums for exchanges of advanced information. The main content of this work is outlined below.

The Center collects information on research trends, recent research results, trends in patents, etc. through domestic and international survey activities, and makes the results available through its website, email magazine, and conventional publications (Fig. 4).

As forums for interdisciplinary research exchanges which extend beyond single fields, the Center sponsors or provides support in holding domestic and international workshops and symposiums (Fig. 5).

It is essential to train human resources who are capable of demonstrating international leadership and building enduring international cooperative relationships. Therefore, the Center has implemented a program

of "International Exchanges of Young Scientists," in which young researchers either visit or stay for longer periods at advanced research institutes in several nations based on science and technology cooperation agreements between Japan and the United States, Japan and the United Kingdom, and Japan and Sweden. The Center conducts an "Interdisciplinary School" so that young scientists can deepen their knowledge of different fields. For one of the training program, the Center launched a "Nanotechnology Summer School" for graduate students in FY2005.

It is also important to gain the understanding of the Japanese people by providing easily-understood explanations of nanotechnology. For this purpose, the Center has created a series of programs called "The Nano Adventure" using animation and computer graphic technology. The currently-available versions of this program cover biotechnology, IT, and energy and the environment. The Center has a stand-

ing exhibition at the "Kitanomaru Science Museum, Tokyo" and other institutions, as well as traveling exhibitions at science museums throughout the country (Fig. 6). As popularization activities, the Center introduces the work of the Nanotechnology Support Project through various exhibits and domestic/international seminars so that a larger number of researchers can make use of the Project's services.

As the second function of the Project, the Nanotechnology Support Project responds to various types of inquiries regarding introductions to and use of large-scale and special facilities such as ultra-high-voltage transmission electron microscopes, nano foundries, synchrotron radiation facilities, and molecular synthesis and analysis facilities.

We hope to contribute to the development of nanotechnology in Japan through these activities.



Fig. 4 Project website (<http://www.nanonet.go.jp/english/>). Number of pages viewed; 279,118 (As of October, 2005).



Fig. 5 JAPAN NANO 2005.

For more details: <http://www.nanonet.go.jp/english/>

## NIMS News



# MOU with London Centre for Nanotechnology

(November 9, Tsukuba) -- The Computational Materials Science Center (CMSC) signed an MOU on research cooperation for development and applications of large-scale DFT simulations with the London Centre for Nanotechnology (LCN). The two institutes plan to exchange researchers, conduct exchanges of research information, and carry out joint research in connection with theoretical research using linear-scaling DFT calculations. LCN is a research center under the joint administration of two of the world's leading nanotechnology research institutes, Imperial College London and University College London, and is home to a large number of outstanding researchers.

# Achievements in Supported Nanotechnology Research

Kazuo Furuya  
Director-General  
High Voltage Electron  
Microscopy Station (HVEMS)

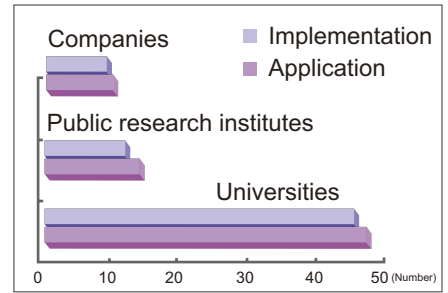


Fig. 2 Number of applications/implemented nanotechnology support topics and project structure (FY2004).

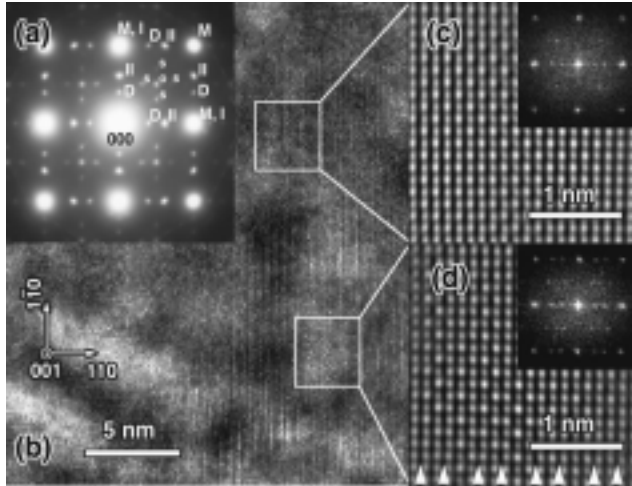


Fig. 1 Example of observation results obtained with NIMS support: Structure of recrystallized region formed by annealing after implantation of ions in a semiconductor specimen. (a) Diffraction image, (b) high-resolution image, (c) matrix, and (d) enlarged view of antiphase boundary (APB) and Fourier transform image.

In nanotechnology, simultaneously with techniques for manipulating atoms and molecules, techniques for observing and analyzing atoms and molecules with high accuracy and high speed are also indispensable, and it is fair to say that the success or failure of these techniques determines the progress of nanotechnology. Because the transmission electron microscope (TEM) achieves resolution in the 0.1 nm region, and thus can easily observe atoms and molecules, this technique is increasingly important in the field of nanotechnology. Among TEMs, ultra-high-voltage electron microscopes are particularly large in scale, making it difficult for general research institutes to introduce these instruments. Therefore, beginning in FY2002, the Japanese Ministry of Education, Culture, Sport, Science and Technology (MEXT) began a "Nanotechnology Support Project/Support for Analysis by Ultra-high-voltage Electron Microscope" to enable joint use of this type of electron microscope. As part of this program, NIMS is the organization responsible for supervising "Analytical support with in-situ, high resolution, and analytical electron microscopy" and is making three ultra-high-voltage electron microscopes with distinctive features appli-

able to nanotechnology available for use by outside researchers. **Figure 1** is an example of support provided to a university. This is an example of observation of the structure of the recrystallized region formed when an ion-implanted semiconductor specimen was annealed. Because various kinds of defects can occur in the recrystallized region, a detailed understanding of the structures of these defects is indispensable in micro-processing of devices. At the same time, because the recrystallized region forms in a region approximately several 100 nm in thickness from the surface, the electron microscope is the most effective method of observation. This support mainly involved observation of high-resolution images. The 3-dimensional structure of defects which were repeated periodically in each of several atomic layers was clarified by using electron beam diffraction images and high-resolution images photographed from various irradiation orientations. This analytical support program is now in its 3rd year and

cable to nanotechnology available for use by outside researchers.

is functioning smoothly in both administration and use. As a larger number of researchers participate, the program is also beginning to produce research results (**Fig. 2**). At the same time, however, because this analysis support program is widely recognized among nanotechnology researchers, we now also receive proposals for research topics in a diverse range of fields, as shown in **Fig. 3**. Consequently, there is a feeling that it is necessary to develop suitable new techniques and methods, and not simply advanced devices. In view of the actual results and future outlook of research with this analytical support, we intend to carry out a further study of the directions in which technology should be promoted and systems for producing important results in the field of nanotechnology by ensuring that a greater number of researchers can use electron microscope technology.

For more details: <http://www.nims.go.jp/hvems/>

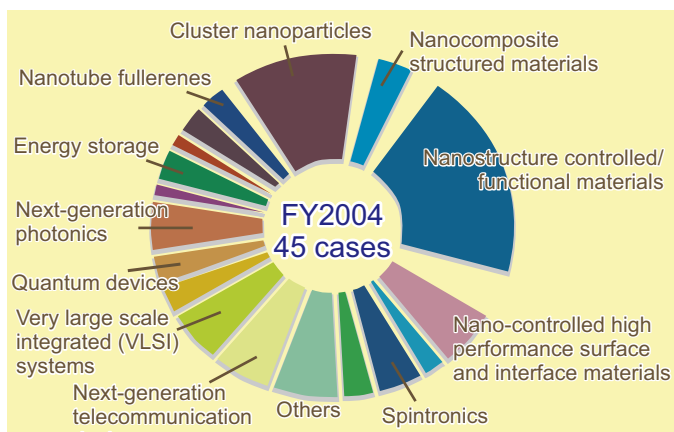


Fig. 3 Composition of nanotechnology support and supported fields.

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**NIMS News**



## MOU with Shanghai Institute of Ceramics

(November 22, 2005, Tsukuba) -- The Biomaterials Center (BMC) signed an MOU with the Biomaterials and Tissue Engineering Research Center (BTERC) of the Shanghai Institute of Ceramics, Chinese Academy of Sciences (SICCAS). BTERC oversees biomaterials research in the Chinese Academy of Sciences as a whole and is actively engaged in the development of ceramics, macromolecular materials, nanomaterials, and composite materials and their application to regenerative medicine. In the future, the two sides will actively promote exchanges of human resources and information and cooperatively develop high functional/porous base materials for regenerative medicine.

# NIMS Dedicated Synchrotron Radiation Beamline Available to Outside Researchers and Nanotechnology Research Support by Beamline Staff

At the NIMS dedicated beamline, which is part of the synchrotron radiation facility SPring-8 (SP-8), NIMS makes 20 % of annual machine time available to outside users for Japanese nanotechnology research and provides comprehensive support, ranging from guidance in measurements, assistance in the use of the device, and analysis to the publication of related papers.

SPring-8 is a 3rd-generation synchrotron radiation facility which boasts the world's highest-class luminescence beam. As part of this facility, the NIMS beamline is designed to produce a beam with high parallelism, while also enabling free use of X-rays over a wide

energy range (1-60 keV), and is equipped with the necessary measuring devices, making it possible to cope with the diverse measurement methods required in materials research, which include X-ray diffraction (XRD) and various kinds of X-ray spectrometry (XPS / XAS / XFS). As a result, since the start of the Nanotechnology Support Project, the NIMS beamline has been used in a total of 41 supported research topics for a cumulative time of approximately 2,500 hours (2002-first half of 2005).

As one example, here, we will introduce the results of an investigation of the catalytic conditions necessary in order to perform nanoscale wiring with

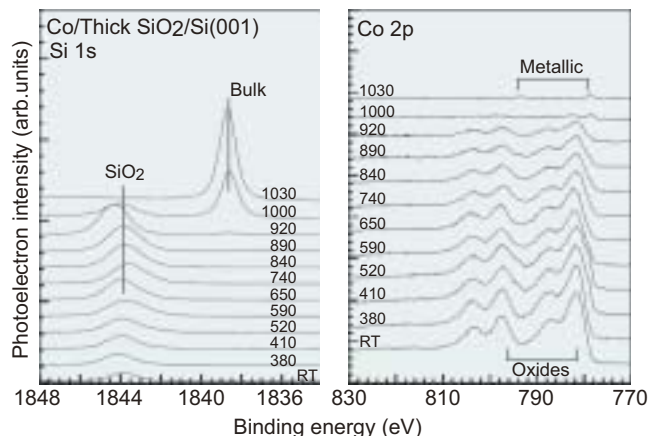


Fig. 1 Change in photoelectron spectra due to temperature of Si 1s and Co 2p.

Masahiko Tanaka, Hideki Yoshikawa  
Advanced Beam Analysis Group  
Advanced Materials Laboratory (AML)  
Hiroki Nakazawa  
NIMS Fellow

carbon nanotubes (CNTs) (Fig. 1). This study, in which X-ray photoelectron spectroscopy (XPS) was used, was a joint research project involving NIMS, the major Japanese telephone

both Co and Fe, which are oxides in the initial-stage condition, undergo metallization and display catalytic activity as the temperature of the substrate increases. So long an SiO<sub>2</sub> layer

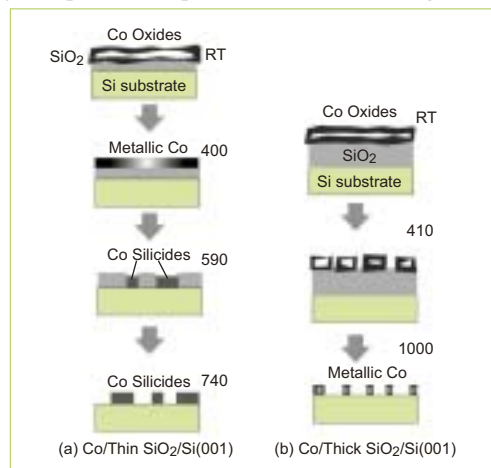


Fig. 2 Chemical state on Si substrate estimated from temperature changes of photoelectron spectra (thin = 1 nm, thick = 100 nm).

company NTT Corporation, and NTT Advanced Technology Corporation. CNTs are formed by a gas-phase growth process from hydrocarbon gases in the presence of metallic particles of Fe or Co as a catalyst. When these metallic particles are arranged on an Si substrate, it should be possible to create nanowiring in which the CNTs form bridges between the metallic particles. Therefore, the relationship between the catalyst metal and Si substrate under high temperature was observed systematically using high energy XPS. As a result,

exists, Fe shows catalytic activity in a metallic condition, but when the SiO<sub>2</sub> layer is exhausted, the Fe forms silicide and becomes catalytically inert. With Co, formation of silicide proceeded locally, even in the presence of an SiO<sub>2</sub> layer, and the Co became catalytically inert. These observation results revealed that the existence of an SiO<sub>2</sub> layer and its film thickness largely control the catalytic activity of catalytic metals, and thus provided an important clue for a nanowiring technique using carbon nanotubes (Fig. 2).

For more details: <http://www.nims.go.jp/abg/eng/>

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New Year 2006

## New Year's Greetings

Moreover, we will forcefully promote activities as a core institute for materials research. The key items for this are strengthening of internationalization and dissemination of information, strengthening of intellectual infrastructure, and strengthening of cooperation with industry and academia. These various efforts were already begun during the 1st Mid-Term Program. Among its concrete policies, NIMS holds "World Materials Research Institute Forums" where representative research institutes

which are world leaders in materials research can meet in a single venue, publish "Materials Science Outlook" as a summary of trends in materials research, and have constructed a "Materials Research Platform" which enables researchers to gather, exchange information, and carry out joint research. In addition to these, we will implement other new policies during the 2nd Mid-Term Program in order to play our full role as a core institute.

We expect dizzying changes in the surrounding environment in the future, includ-

ing a changeover to a system where we are no longer public employees and a reduction in our operating subsidy, but NIMS must respond flexible to these changes and continue to grow. Our goal is to build a new NIMS with sustainability, where staff can enjoy research and will constantly maintain an active and aggressive stance toward new challenges.

In the New Year, we request the guidance and support of all of our friends and colleagues in Japan and other countries, and we sincerely hope that all of you will have an active and productive year.

# Atomic Images of Quasicrystal Surface and Step Structure

H. R. Sharma, Masahiko Shimoda  
Reaction and Excitation Dynamics (RED) Group  
Materials Engineering Laboratory (MEL)

The solids called quasicrystals (QC) do not possess periodicity like that displayed by ordinary crystals. This does not mean that the atomic arrangement is entirely random, as QC display a special ordered structure called quasiperiodicity. However, their lack of periodicity makes it extremely difficult to determine their structure,

face by scanning tunneling microscopy (STM).

**Figure 1** is an atomic image of the surface of a QC alloy consisting of aluminum, copper, and iron. Atoms arranged in a regular pentagonal shape, which is a distinctive feature of the quasiperiodic structure, and a condition in which these formed larger regular penta-

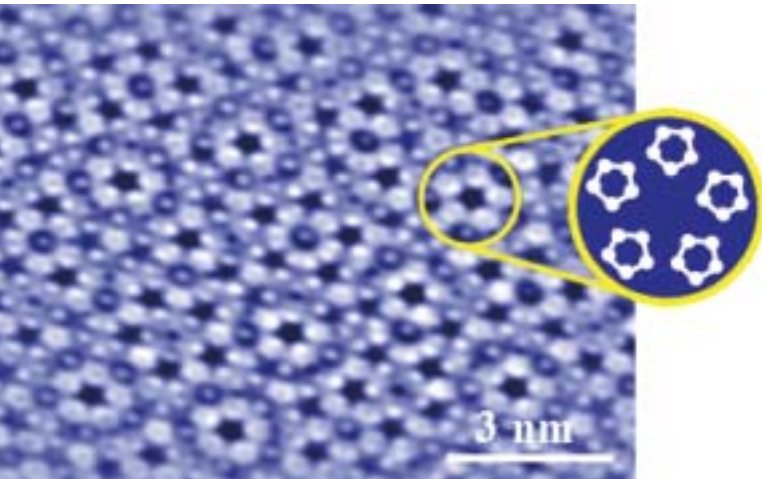


Fig. 1 Atomic image of surface of AlCuFe quasicrystal.

and investigation using various techniques is necessary. We are attempting to elucidate the structure of QC by observing atomic images of the QC sur-

face by scanning tunneling microscopy (STM). Looking at the largest region of the surface, a step-terrace structure can be seen (**Fig. 2**). Although this step-terrace forma-

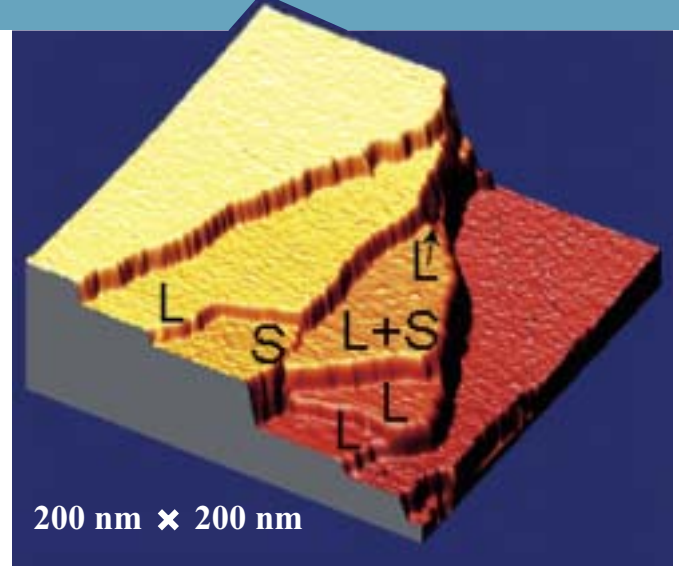


Fig. 2 Steps on surface of AlCuFe quasicrystal.

tion is commonly observed in ordinary crystals, in the case of this quasicrystal, two kinds of steps were found, these being large (L) and small (S) steps with different heights. The ratio of these two steps,  $L/S$ , is approximately the same as the golden ratio (irrational number of 1.618...). Moreover, L and S steps appear in a sequence like LSLLSLSL..., which is called the Fibonacci sequence (sequence starting from L, formed by repeated substitution of L SL, S L). Generally, it is known that the golden ratio and the Fibonacci sequence are intimately related to the structure of quasicrystals.

According to a structural model, QC can be considered to consist of blocks of densely concentrated atoms and the large and small gaps which separate them. When the distinctive features of the above-mentioned atomic arrangement and

steps were investigated in detail, it was found that all of the facts can be explained if the areas where the gap width is especially large and the block density is also high are considered to be the surface of the QC. This not only demonstrated the correctness of the structural model, but also clarified the relationship between the surface and the bulk.

Based on these results, we are currently attempting to create thin films of various metals on the surface of QC. This is an attempt to produce novel physical properties by arranging a quasiperiodical structure in a substance which is not by nature a quasicrystal using a substrate with quasiperiodicity. This work was carried out as joint research with Dr. Shoji Yamamoto, NIMS Fellow, of the Advanced Materials Laboratory (AML) and Prof. Tsai An-Pang of Tohoku University.

For more details: [http://www.nims.go.jp/dynamics/QC/QC\\_Surface\\_e.html](http://www.nims.go.jp/dynamics/QC/QC_Surface_e.html)

## NIMS News

### MOU with University of St. Andrews and Korea University

(November 2005) -- The Ecomaterials Center (EMC) signed an MOU on research cooperation in connection with materials for high performance fuel cells with the University of St. Andrews (UStA; Nov. 8) and Korea University (KU; Nov. 24). UStA, which was established in 1413, is the oldest university in Scotland and the third oldest in the entire UK. KU is one of Korea's most prestigious private universities and will celebrate its 100th Anniversary this year. The aims of these MOU are to bring together the research "seeds" possessed by NIMS and the two universities and accelerate the development of materials for next-generation high performance fuel cells through exchanges of information and human resources.



Signing ceremony with KU, Prof. Lee second from left.

# Encapsulation of Bi Nanolines in Silicon

-Verification of Nanoline Structure by "Invisible Light"-

Kazushi Miki  
Nanoarchitecture Group  
Nanomaterials Laboratory (NML)  
Osami Sakata  
Japan Synchrotron Radiation  
Research Institute (JASRI) / Spring-8  
David Bowler  
International Center for  
Young Scientists (ICYS)

Nanometer-scale structures created until now have generally been single, independent structures. However, functional layering consisting of a combination of multiple nanostructures is essential for practical application

rication of an interconnect structure. Because the size of Bi atoms is larger than that of Si atoms, Bi atoms cause large strain if embedded in a silicon crystal. However, during epitaxial growth of Si, this strain causes these

possibility that the microscopic structure will also be destroyed during specimen preparation. The structure should ideally be elucidated by a nondestructive technique. However, even with a combination of high-brilliant

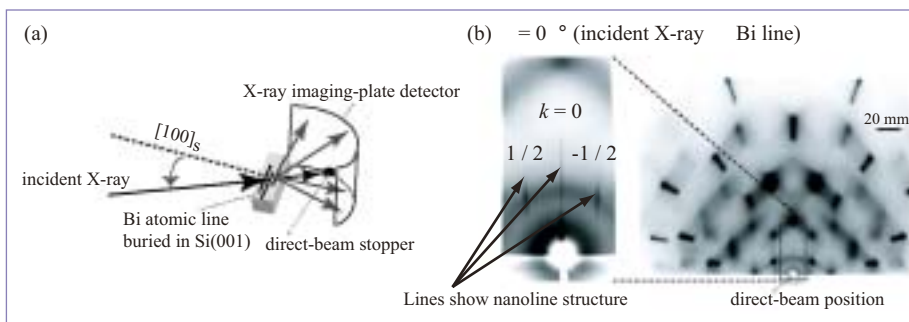


Fig. 1 Structural evaluation method for atomic lines (a) Arrangement of experimental apparatus, (b) X-ray diffraction pattern of case where the irradiated X-ray is perpendicular to the atomic line. The linear diffraction pattern in the figure shows one dimensional structure of the Bi nanoline.

in devices. As one example of this, we are conducting research with the aim of creating interconnects (wiring structures) in crystals.

In this work, we succeeded in developing a technique for encapsulating (layering) nanolines consisting of bismuth atoms in silicon by epitaxial growth of Si, which is the first step toward the fab-

atoms in the Bi atomic lines to be replaced by the Si as it grows. The Bi atomic lines are destroyed by this surface segregation phenomenon, and as a result, are not embedded in the Si. To solve this problem, we temporarily used a third process material called a surfactant. Surface segregation is avoided because the surfactant layer remains on the surface throughout growth, making it possible to embed the Bi atomic line structure in the Si. We are pleased to note that this report is the first describing the possibility of utilizing crystal growth to embed atomic lines.

Observation of structures embedded in crystals is generally difficult because direct observation (as would be the case on the surface) is impossible. Although methods such as observation by electron microscope after destroying the structure are frequently used, there is a large

synchrotron radiation and X-ray technology, which has already been established and is a representative nondestructive technique, structural evaluation of nanostructures like that in the present work is exceedingly difficult. In the measured specimen, the volume of a Bi atomic line is a minute quantity, being approximately 1/10 that of a monolayer (equivalent to one atomic layer), and it was impossible to evaluate the structure due to the weak signal strength. We were able to improve detection sensitivity by using the reciprocal lattice imaging method and thereby succeeded in obtaining diffraction images (Fig. 1). Based on the structural information from these experiments, we modeled the optimum atomic structure (Fig. 2).

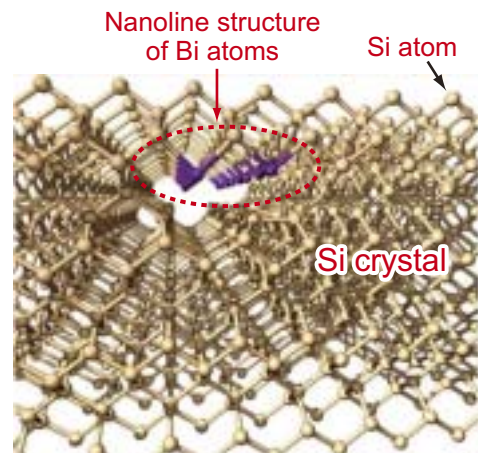


Fig. 2 Structural model of Bi atomic line encapsulated in Si. The Bi atoms form a paired structure and maintain a bonding angle of approximately 90°. Because Si atoms prefer a regular tetrahedral structure, Bi cannot bond with all 4 adjacent atoms.

## Japan-Russia Workshop Held at NIMS



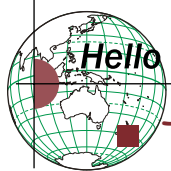
Workshop participants.

(December 12-13, 2005, Tsukuba) -- A Japan Workshop entitled "Advanced Nanomaterials in Russia" was held at NIMS. By receiving support from Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT), the Moscow-based International Science and Technology Center holds a series of Japan Workshops to invite outstanding scientists in Russia and the CIS countries to Japan and contribute to the implementation of new projects through introduction of their research. The workshop, which was jointly sponsored by NIMS, featured presentations on recent research trends in advanced nanomaterials in the three fields of physics, chemistry, and biotechnology by 9 researchers each from Russia and Japan, and was accompanied by lively discussions.



Signing ceremony with UStA, Prof. Irvine at right.

For more details: [http://www.nims.go.jp/nanomat\\_lab/index\\_e.htm](http://www.nims.go.jp/nanomat_lab/index_e.htm)



## Hello from NIMS

### ■ Tsukuba - The Unique City ■

After knowing Tsukuba for 9 years, the excitement of living here and working at NIMS continues... Tsukuba is a huge campus city which cannot really be identified as Japanese. Come vacation time and even the Japanese abandon it to visit their hometowns. In recent times, Tsukuba has been rapidly changing into a commercial city like numerous others. Although it does not have the natural sights and sounds of an old city like the neighboring Tsuchiura, the pleasure of living in a garden city with a truly international society is unique. In fact, a visiting friend who is a reporter from Geneva compared it to her native city! We can interact and make friends

Alok Singh (India)  
Senior Researcher  
Light Materials Group  
Materials Engineering Laboratory (MEL)



[ TWMC Christmas party showing the international character of Tsukuba (the author is Santa) ]

with people from various countries at various forums, including my hiking club (Tsukuba Walking and Mountaineering Club; TWMC), which has meetings every week. There are places to learn traditional and modern arts with your friends, and it's a city especially made for the play and safety of children. In my opinion, the schools are good and sensitive to the needs of foreign children. If you are single, you may also find a life partner here from another country. After living here, my wife also became a scientist (she had no choice about that!). Enjoy living here, contribute to it, and enrich your personal and professional experience!

### Japanese New Year

For Japanese people, it is a tradition to do *hatsumode*, the year's first visit a temple or shrine during New Year. Popular temples and shrines like the ones below attract millions of people. There, we pray for happiness and health, and purchase lucky charms for a fortunate New Year.

Photos by M. Sato

Kaminarimon Gate, Asakusa  
Sensoji Temple, Tokyo



Ohtenmon Gate, Heian  
Jingu Shrine, Kyoto



Fukuroda Falls, Ibaraki



Ornamental kites with New Year design; animal symbols, Chinese character for the year of the Dog, etc.



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