from Tsukuba, Japan to the world

NIMS NOW International

National Institute for Materials Science

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NIMS' Policies

NIMS' Policies for the 2nd Mid-Term Program (FY2006-)

- Toward Implementation of NIMS' 2nd Mid-Term Program -

Teruo Kishi
President, NIMS

NIMS embarks on its 2nd Mid-Term Program in April 2006. Although NIMS' policies for this 2nd Mid-Term Program have been described previously on various occasions, here, I would like to present an overview of our objectives for the next 5 years.

First, the direction of our research will be "Nanotechnology Driven Materials Science for Sustainability." While placing strong emphasis on materials research utilizing nanotechnology, which has the potential for exciting new breakthroughs, we will be engaged in materials research which responds to the need to create a safer, more secure social infrastructure and solve environmental and energy problems. To this end, the priority research and development areas which we have established for the 2nd Mid-Term Program are "Nanotechnology Driven New Materials Creation" and "Advanced Materials Responding to Social Needs." **Fig . 1** shows the positioning of the 6 research fields in which NIMS is involved in the flow from substances to products. We plan to carry out work on 20 project research topics corresponding to these research fields.

These research activities include many topics which we began during the 1st Mid-Term Program. However, in addition to developing the results achieved in the 1st Period, in the 2nd Period, we will conduct research with more clearly defined targets. Organizationally, we will create 20 Research Centers corresponding to these respective projects. (Fig . 2)

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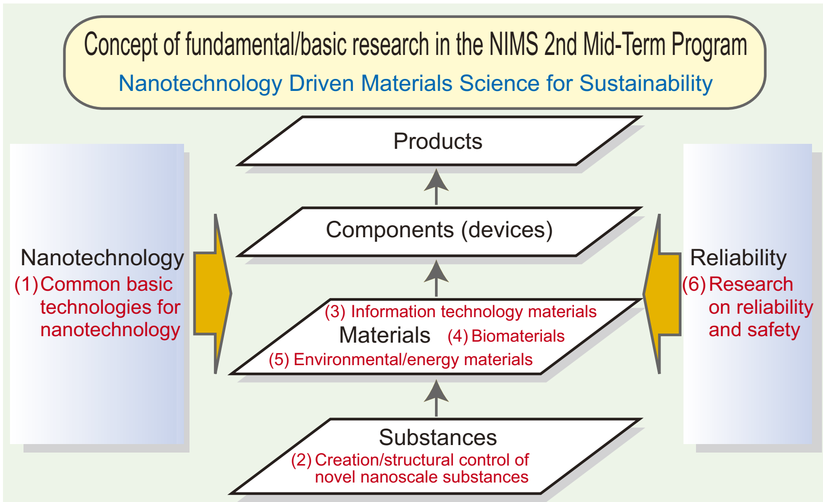

Fig. 1 Position of project research in the NIMS 2nd Mid-Term Program.

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NIMS News

MOU with Springer-Verlag

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Dr. Poerschke, Executive Manager of Springer, right, shakes hands with Dr. Yagi, MITS Director-General, after signing.

NIMS' Policies

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NIMS' activities are not limited to project research. We are also deeply committed to germinal research. Germinal research is an essential type of research, in that it provides the starting point for projects in the next period. From this viewpoint, it is no exaggeration to say that NIMS would have no future without germinal research. Although germinal research is also carried out by researchers engaged in projects in addition to their project research, we plan to create two Laboratories consisting of researchers who will work primarily on germinal research.

NIMS will also actively promote the creation of intellectual infrastructure in the form of datasheets, databases, and similar, as well as sharing of facilities and equipment with outside researchers under our "user facilities" program. As user facilities, we plan to add a new nano-foundry equipped with semiconductor process equipments during the 2nd Period. These efforts are carried out under the responsibility of 8 Stations in the common infrastructure division, and aim at implementing advanced polices and equipment development/maintenance.

Next, NIMS is also engaged in activities as Japan's core institute in the field of materials research and will continue its efforts in this area, centering on international cooperation, information dissemination, and collaboration with industry and universities in its position as an Independent Administrative Institute (IAI). We plan to further develop and expand several policies which we began during the 1st Mid-Term Program, including holding "World Materials Research Institute Forums" which provide an opportunity for the world's leading materials research institutes to meet in a single venue, publication of "Materials Science Outlook" as a review of trends in the field, creation of a "Materials Research Platform" which allows researchers, mainly in industry and IAI, to gather and exchange information and conduct joint research, and international standardization activities.

From the operational viewpoint, we believe that two large challenges confront us. The first is continuing to secure outstanding human resources. Our aim is to become the world's top materials research institute. In creating a strong group, it is necessary to bring together the strengths of the group's individual members, but this naturally presumes that the group includes strong individuals. Although we have devoted considerable energy to securing human resources to date, we plan to redouble our efforts. Our second major challenge will be introduction of external funding. At present, NIMS' operating subsidy from the Japanese government is its largest source of income, but this will decrease steadily in the years to come. For this reason, an awareness of the need for researchers themselves to secure funding, for example, from private industry or external competitive funds, will become increasingly important. The fact that this is a public research institute does not guarantee a secure future. Just as people must seek food to meet their nutritional needs, funding will be a necessary and indispensable issue with which NIMS must wrestle if the institute is to continue to grow.

Fortunately, NIMS earned an excellent evaluation for its achievements in the 1st Mid-Term Program. In the future, we will devote our utmost efforts to the development of NIMS, bearing firmly in mind the importance of project research, the germinal research from which projects are born, creation and sharing of facilities, and finally, technological innovation. We hope that we will enjoy your continuing support in these efforts.

For more details: http://www.nims.go.jp/

Fig. 2 New organization of NIMS.

NIMS News

MOU with Ruhr University

Prof. Wagner, Rector of Ruhr University (center), Prof. Eggeler, Director of CSMT (right), and Dr. Ishida, Senior Researcher, MEL (left).

(January 20, Bochum) -- The Materials Engineering Laboratory (MEL) signed an MOU on research cooperation with the Institute of Engineering Materials of Germany's Ruhr University Bochum. Exchanges of researchers and research information and joint research in the field of shape memory alloys are planned. Ruhr University manages the Center for Shape Memory Technology (CSMT), which is made up of several domestic institutes, and is actively engaged in the full range of research activities from basic research to applications. The university is also a center for exchanges of researchers, receiving visits from researchers at institutes throughout the world, and plays a role as an information exchange base in Europe.

High Pressure Synthesis of Deep UV-Emitting Boron Nitride Single Crystals

Takashi Taniguchi
High Pressure Team
Advanced Nano Materials Laboratory
Kenji Watanabe
Opto-Electronics Group
Optronic Materials Center

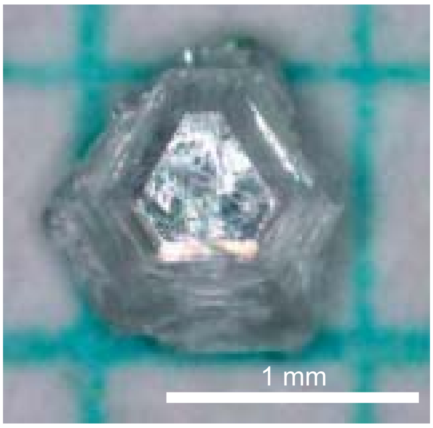

Fig. 1 High purity recrystallized hBN.

In our daily lives, we enjoy the benefits of diverse products which use light emissions from semiconductor materials, beginning with various kinds of pilot lamps and signaling devices. From the development of blue light-emitting devices in the past, the focus of research in Japan and other countries has recently shifted to light-emitting materials extending to the deep ultraviolet (DUV) region, which has shorter emission wavelengths. The development of short wavelength emitting devices is an important research issue, not only for information recording fields such as DVD technology, but also for new demand in the field of environmental protection, for example, as a sterilization technique. Research which is currently in progress is based on the so-called III-V Group compound semiconductors, which include aluminum nitride (AlN) and gallium nitride (GaN).

In this connection, it may be noted that the periodic table of the elements shows that boron nitride (BN) is the combination occupying the highest position in the III-V Group compounds, which include the above-mentioned AlN and GaN. Hexagonal BN (hBN; **Fig. 1**) and cubic BN (cBN) are known as the representative crystal structures of BN. The former is chemically and thermally stable, and has been widely used as an electrical insulator and heat-resistant material for many years. The latter, which is a high density phase, is an ultrahard material and is second only to diamonds in hardness. In practical applications, it is an indispensable material for the tools used in machining ferrous metal materials.

Where hBN is concerned, thus far, it has not been possible to obtain single crystals of good quality suitable for various evaluations. In particular, research focusing on light-emitting properties has been inadequate. In the present work, we synthesized high purity single crystals of BN under high pressure, and succeeded in educing interesting properties in hBN single crystals as a result of the reduced concentration of impurities such as oxygen and carbon. As shown in **Fig. 2**, the high purity hBN single crystals obtained in this research display a clear hexagonal idiomorphology, and are colorless and have high transparency. When the optical properties of these crystals were evaluated, high intensity cathode-luminescence (CL) was observed, as shown in **Fig. 2**. Although hBN has a lamellar structure, when parallel plate-shaped crystals of hBN were cut out by cleavage and the crystals were excited by irradiation with an electron beam, it was found that emissions at a wavelength of 215 nm caused several phenomena which are characteristic of laser operation, confirming room temperature lasing (**Fig. 3**).

This new discovery revealed that hBN possesses properties as a direct wide bandgap semiconductor (Eg: 5.97 eV). Control of electrical conductivity in order to realize high efficiency UV emissions will be an important challenge for the future. However, even at present, this material can be used in various kinds of high performance electron-emitting devices. For example, easy construction of compact DUV-emitting devices for wavelengths around 215 nm can be expected by combining this hBN material with diamond, carbon nanotube, or other cold cathode device materials.

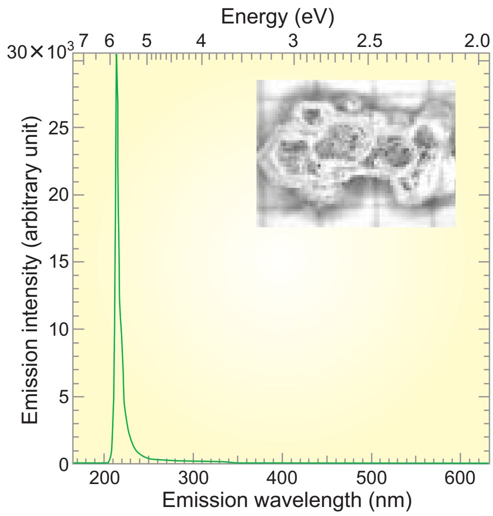

Fig. 2 hBN single crystal and CL spectra.

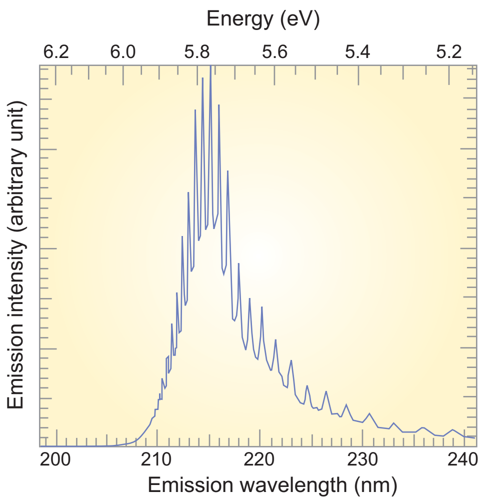

Fig. 3 Example of room temperature laser oscillation spectra from hBN single crystal.

For more details: http://www.nims.go.jp/mits/fatigue/index_e.html

NIMS News

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MOU with Springer-Verlag

(January 18, Tokyo) -- The Materials Information Technology Station (MITS) signed a memorandum of understanding (MOU) on cooperation with Springer-Verlag GmbH of Germany. This agreement will establish mutual linkage between the on-line version of the NIMS creep datasheets and the SpringerLink creep databook. As of January 2006, the SpringerLink provided internet access to 2,500 books and 1,250 academic journals. A dramatic increase in the materials information available to researchers can be expected as a result of this cooperation.

NIMS Hybrid Welding Wire and Development of Its Applications

- System for High Quality/High Performance Welds in Pure Argon MIG Welding -

Terumi Nakamura, Kazuo Hiraoka
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Structural Metals Center

TIG (Tungsten Inert Gas) welding is used with high alloy structural materials in structures for cryogenic service, nuclear power structures, and similar applications with high weld quality requirements. In TIG welding, an arc is generated under pure argon gas using a tungsten electrode, and the arc melts the welding wire. In contrast to this indirect melting process, MIG (Metal Inert Gas) welding is a direct melting process in which the arc is generated from the welding wire, thereby melting the wire. In MIG welding, stable, normal welding is not possible unless several % of an active gas (oxygen or carbon dioxide) is mixed in the argon gas. However, the mixed active gas has an negative effect on joint quality, making it difficult to form high quality welded joints equal to those in TIG welding. The NIMS hybrid welding wire was developed based on a new concept which solves all of the problems of MIG welding at once.

A detailed analysis of the phenomena which occur in pure Ar MIG welding revealed that an elongated liquid column of molten metal exists at the tip of the wire, and this moves unstably in all directions (**Fig. 1a**). The arc follows this motion, resulting in unstable arc movement and an unstable, meandering bead (**Fig. 1b**). We conjectured that this molten metal column is the cause of this unstable behavior.

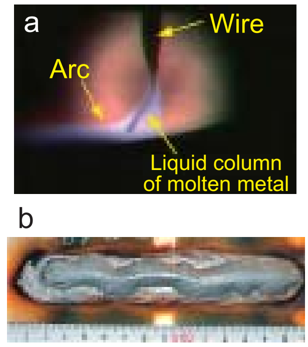

Fig. 1 Results of MIG welding under pure Ar. (a) Behavior of arc and molten metal on the wire tip under pure Ar. (b) Appearance of weld bead.

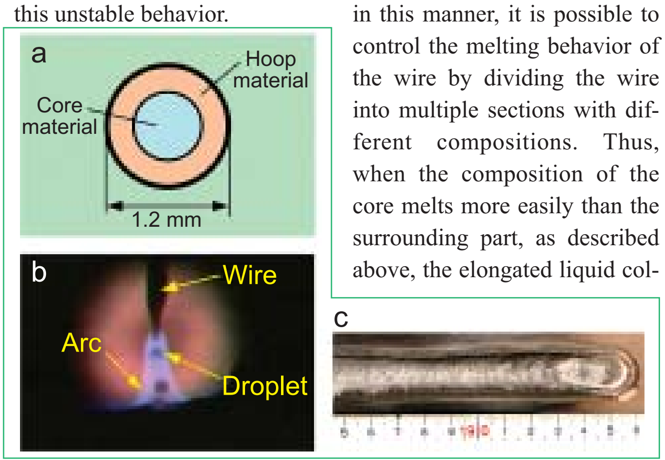

Fig. 2 NIMS hybrid welding wire. (a) Structure of wire. (b) Behavior of arc and droplet on the wire tip under pure Ar. (c) Appearance of weld bead.

In order to shorten the liquid column of molten metal, and thereby stabilize the arc, we developed the NIMS hybrid welding wire, which has a different structure from that of the conventional wire. While the average composition of this new wire is the same, the wire is designed so that the central part (core material) melts more easily by adopting a different composition in the core and surrounding part (hoop material) (**Fig. 2a**). Because the components are stirred and alloying occurs as the wire melts in the arc, the welding arc can be thought of as an "all-purpose melting furnace." When the welding process is considered in this manner, it is possible to control the melting behavior of the wire by dividing the wire into multiple sections with different compositions. Thus, when the composition of the core melts more easily than the surrounding part, as described above, the elongated liquid column becomes a spherical droplet (**Fig. 2b**). This enables stable welding under pure Ar gas (**Fig. 2c**) and makes it possible to obtain performance equal to that of TIG welding.

The NIMS hybrid welding wire will enable a changeover from TIG welding, which has the disadvantage of low production efficiency, to high productivity MIG welding. Further development to new MIG welding systems using welding methods and welding designs which differ greatly from the conventional techniques can be expected. Moreover, expensive materials which have poor yield in production can be manufactured at low cost by using multiple combinations of commercial core and hoop materials, and application to small-lot, multi-kind welding wires is expected.

Coating of Titanium by Warm Spray Process

Jin Kawakita
Coating Materials Group
Composites and Coatings Center

Titanium possesses a variety of desirable properties, including high corrosion resistance and biocompatibility, which make it suitable for applications such as offshore structures, energy plants, and medical implants. Considering the importance of this material, the development of a simple titanium coating process which can be used in atmospheric air would be a revolutionary breakthrough from both the scientific and industrial viewpoints.

The obstacle to coating of titanium under an air atmosphere is oxidation, which is caused by the strong affinity between titanium and oxygen and reduces packing density and strength in the final coated product in comparison with wrought products of Ti. NIMS solved the problem of oxidation by developing a warm spray process.

Warm spraying is a technique which is used in depositing various types of materials in air, including metals, ceramics, and plastics (**Fig. 1**). The key technical point is to realize optimum temperature control of the supersonic jet immediately before injection of the feedstock powder by incorporating a mixing chamber where inert gas is introduced between the combustion chamber (section which forms a supersonic jet)

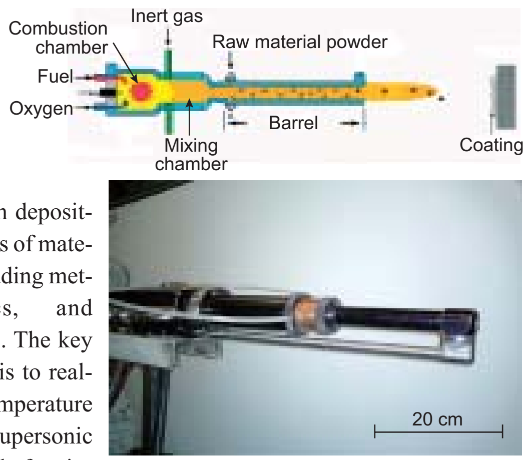

Fig. 1 Conceptual diagram of the warm spray device (upper) and appearance of the actual machine (below).

Development of Simulation Method for the Evolution of the Nanostructure in Real Materials

- Aiming at the Establishment of Practical Design Method for Microstructure Control -

Toshiyuki Koyama
Particle Simulation & Thermodynamics Group
Computational Materials Science Center

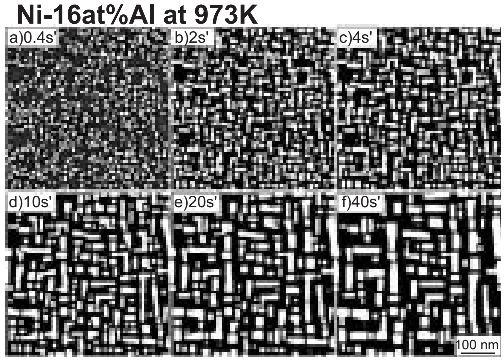

Fig. 1 Coarsening behavior of γ' precipitates (white particles) in a Ni-base superalloy. The shape of the precipitates becomes square due to an elastic constraint, and the particles align in the <100> direction.

The phase-field method is a simulation technique which is based on a continuum model and can be applied to studies of the phase transformation and microstructure evolution of materials at the nano/meso scale. Recent years have seen increasing use of this method in various fields of materials science and engineering.

The phase-field method is a computational method in which the microstructural morphology of materials is expressed based on a continuum model, and the temporal/spatial changes in complex microstructures are analyzed using the evolution equations. The objects of simulation by this technique now extend to the field of materials science as a whole, and use is continuing to grow as a total microstructural evolution analysis/simulation method. In the present research, we developed a simulation method for the microstructural evolution of practical real materials based on the phase-field method. (The **figures** demonstrate examples of recent simulations.)

Prediction of the microstructure evolutions in various types of practical materials is an extremely important issue from the viewpoint of engineering, but the advent of a "dream" technique which enables prediction of the complex microstructural evolution in practical materials by non-empirical simulations is perhaps still far in the future.

However, even today, quantitative and phenomenological modeling of actual microstructure evolution using a combination of experimental evidence and simulation techniques is possible. In particular, because the phase-field method enables virtually quantitative modeling of the evolution of complex microstructural morphologies, with connecting a thermodynamic basis in materials science, this method is expected to become a powerful tool for material design.

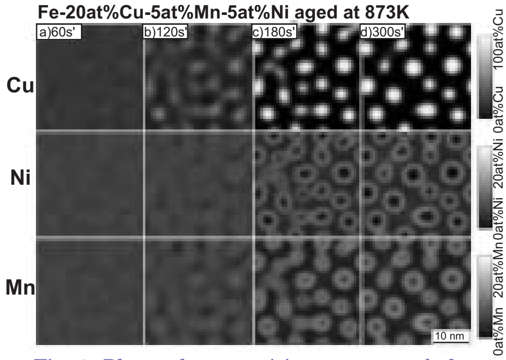

Fig. 2 Phase decomposition process of the α phase (bcc) in Fe-Cu-Mn-Ni quaternary system. The Mn and Ni components initially concentrate in the Cu precipitation phase, but segregate to the interface as the Cu concentration in the particles increases.

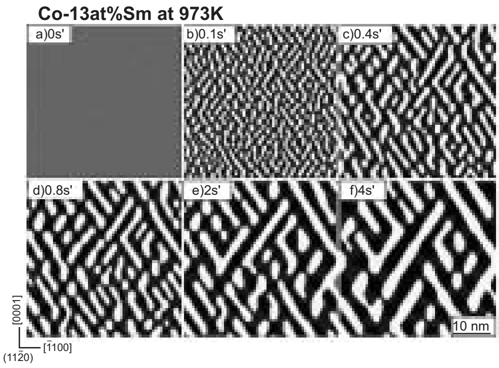

Fig. 3 Phase decomposition process in Sm-Co-Cu alloy (white: $Sm(Co,Cu)_5$, black: $Sm_2(Co,Cu)_{17}$). A modulated microstructure evolves by the mechanism of spinodal decomposition.

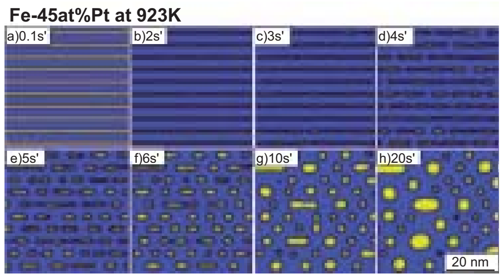

Fig. 4 Spheroidization process in a lamellar microstructure. With the lamellar structure as the initial state, the lamellar structure breaks down and spheroidization proceeds during diffusion controlled microstructure evolution.

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and barrel (acceleration zone) in a commercial high velocity oxy-fuel (HVOF) spray device. The mechanism of particle stacking involves acceleration of the supplied powder to supersonic speed maintaining its temperature below melting point, and continuous deposition using mainly impact energy as the driving force.

In titanium coatings fabricated by the warm spray process, it is possible to control porosity over a wide range while maintaining the same level of purity as in the feedstock powder. In particular, in comparison with other coating techniques which are used under an air atmosphere, the Ti coatings produced by the warm spray process displays the world's highest levels of purity and density (closely packed structure) (**Fig. 2**).

This warm spray technique was developed through joint research by NIMS, university, and industry. Because it is easily incorporated in commercial thermal spray devices, introduction of the technology is comparatively simple. Wide application is expected in the future, taking advantage of the following features:

1) Because the temperature of the supplying particles is controllable, the structure, composition, phase, and other properties can be kept intact and deposition in accordance with the material design is possible.

2) Because the kinetic energy of the particles is controllable, it is possible to improve the physical properties of the coatings such as the packing density (closely packed structure) and the mechanical properties such as adhesion at the substrate/coating interface.

Fig. 2 Photograph of the cross-section of laminated titanium on a metal substrate fabricated by the warm spray process.

■ Hello from ICYS, NIMS ■

Ajayan Vinu (India)
Senior Researcher
Nano Ionics Materials Group
Fuel Cell Materials Center

[Visiting Nagoya Castle with my wife, Siji, and Japanese friends living in Nagoya]

I am Ajayan Vinu. I come from Kanyakumari, which is one of the most beautiful places in the world, surrounded by hills, colorful seashores, beautiful waterfalls, and paddy fields, and is located at the extreme southern tip of the Indian subcontinent in Tamil Nadu, India, where I did all my schooling and college studies. After three successful years of research life in the University of Kaiserslautern, Kaiserslautern, Germany, I received an opportunity to continue my research as an independent Research Fellow in the International Center for Young Scientists (ICYS), NIMS, in January 2004. ICYS has an excellent research system which offered me a lot of research freedom, an international environment, "coffee break meetings," and a fantastic working atmosphere with cutting edge facilities and an English support system (kind and friendly administrative staffs) to do both exploratory as well as the fundamental research. I really enjoyed my stay and the freedom in the ICYS, collaboration with the NIMS permanent researchers, especially Dr. Katsuhiko Ariga, Dr. Toshiyuki Mori, and Dr. Dmitri Golberg, and utilized all the opportunities given me by the ICYS to convert my original research thoughts and ideas into reality. Moreover, I would like to say that this is also the turning point of my research life from ICYS Fellow to NIMS permanent Senior Researcher, which also came through the ICYS research system. I feel that this is a great opportunity for me to honor NIMS for introducing a nice research system which not only provides career position for many young scientists from different countries, but is also a place to develop friendships with different people from different countries having different cultures, characters, and attitudes, who are doing work in various research fields.

[Celebrating our marriage party which was organized by a Japanese family in Nagoya]

The area of my research in NIMS is mainly the synthesis of novel mesoporous, silica, carbon, and nitride materials and their application toward adsorption, catalysis, and fuel cells, with special focus on the immobilization of large biomolecules such as proteins, enzymes, vitamins, etc., onto mesoporous silica and carbon molecular sieves. Very recently, I have discovered many novel materials like the carbon nanocage, carbon nitride nanocage, mesoporous carbon nitride, boron nitride, and boron carbon nitride materials which possess very high surface areas, pore volumes, and uniform pore size distributions. If anybody is interested in using the above materials, please feel free to contact me at vinu.ajayan@nims.go.jp, as I am very interested in developing internal and international collaboration. Apart from my research, I am really enjoying the stay in Tsukuba, Japan. The Japanese people are kind, helpful, caring, friendly, affectionate, and gracious. My two year stay in Tsukuba really helped me to understand the magnificent country and the character of polite and nice Japanese people, and convinced me to change my mind and accept a permanent position in NIMS. Life in Japan is interesting, challenging, and exciting. I really hope that I can contribute something to NIMS as well as to the wonderful country of rising sun.

Traveling in Spring

Kiyomizudera Temple, Kyoto
April 7

Gate of Heian Jingu Shrine, Kyoto
April 7

Photo by M. Sato

National Institute for Materials Science

PUBLISHER
Dr. Hisao Kanda

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