from Tsukuba, Japan to the world

NIMS NOW International

National Institute for Materials Science

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Special Features

Introduction of 20 New Projects and Recent Achievements - Computational Materials Science Center -

For Design of Nanofunctions

Takahisa Ohno
Managing Director
Computational Materials Science Center

The importance of nanomaterials in 21st century science and technology is widely recognized, both in Japan and in other nations, and active research and development are being conducted. In quantum theory, the structural form of nanomaterials is intimately interrelated with the electronic state, giving rise to novel physical properties/functions which are not manifest in the bulk substance. The highest expectations placed on nanomaterials and biomaterials are based on the possibility that those substances can be made to manifest innovative functions and those functions can be freely designed and controlled. This is the foundation of nanotechnology.

The possibility of analyzing/predicting the physical properties/functions of substances with high accuracy using computational science techniques based on quantum theory, as represented by first-principles calculations, has been demonstrated through application to a wide range of materials science. On the other hand, computer power is also increasing dramatically at present, as can be seen in Japan's Earth Simulator and next-generation 10 petaflop-class supercomputer (Keisoku Supercomputer*), which is now in the planning stage. Against the background of this progress in computational techniques and increasing computer power, it has now become possible to realize the challenge of elucidating, in terms of quantum theory, the structures and functions of nanomaterials comprising several 10,000s of atomic groups.

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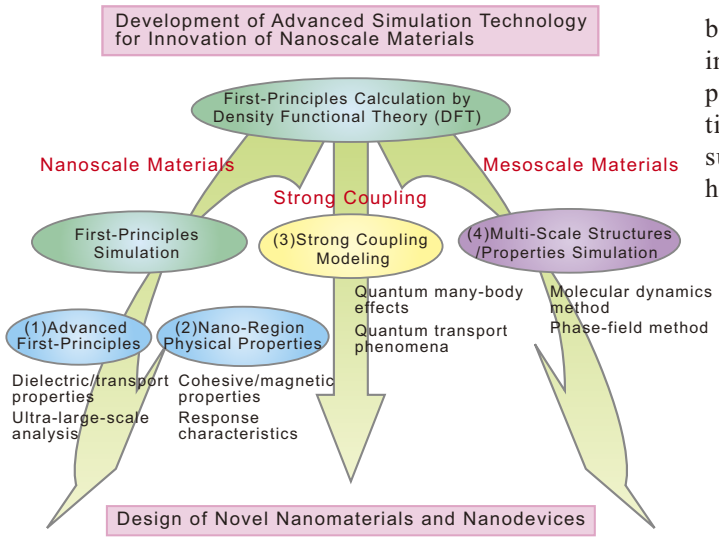

Fig. Outline of advanced simulation techniques for nanomaterials.

in this issue

NIMS News

NIMS Participates in International Science, Innovation and Technology Exhibition INSITE 2006 (South Africa)

Dr. Kitashima, NIMS researcher, explains NIMS' research to Mr. Mangena (center) and H.E. Furuya (right).

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Development of Advanced First-Principles Simulation Techniques

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First-Principles Simulation Group (1)
Computational Materials Science Center

Nanomaterials show novel physical properties/functions which are different from those of bulk substances. As one remarkable example, in bulk form, gold does not have a catalytic function, but in a nanocluster structure (**Fig. 1**), it displays a catalytic function in the oxidation reaction of carbon monoxide (CO). Analysis of the correlation between the structure and functions of nanomaterials which show novel physical properties in this manner is an extremely important challenge from the viewpoint of both pure science and applications.

The objective of the First-Principles Simulation Group (1) is to develop advanced first-principles simulation techniques for analysis of the correlation between structural form, electronic state, and physical properties/functions in nanomaterials. First-principles calculation techniques have been applied to a wide range of fields in materials science, demonstrating that it is possible to analyze/predict the physical properties/functions of substances with high accuracy. Based on this first-principles calculation methodology, we are developing ultra-large-scale analysis techniques for nanomaterials consisting of large numbers of atoms (10^4 order), and are also developing analytical techniques for various physical properties/functions of nanomaterials such as dielectric response, electron transfer, spin conduction, etc.

It is thought that large numbers of atoms contribute to physical properties/functions in nanomaterials. When considered in the example of the gold nanocluster mentioned above, in addition to the cluster structure itself, the interaction with oxide surface, which includes defects, is also important. In order to analyze this kind of large-scale system by first-principles methodology, we developed an analytical technique called the order-N method. In the first-principles order-N method, large-scale computations are realized by dividing the total analytical system into regions in real space and applying parallel processing to the computations for each region (**Fig. 1**). Ge clusters on the Si (001) surface have attracted attention as a system which realizes quantum dots. Recently, we carried out a first-principles simulation of approximately 23,000 atoms for a Ge cluster on the Si (001) surface. **Fig. 2** shows the contour plot of the calculated electronic charge density, where two Ge layers (green) are sitting on the Si substrate (blue) and the Ge cluster (the top is red) is placed on these Ge layers. To our knowledge, this is the largest first-principles simulations performed so far. As seen in the Earth Simulator and the planned 10 Pflop Keisoku Supercomputer, computer power is increasing at a dramatic rate. High expectations are placed on the first-principles order-N method as a powerful technique for analyzing nanomaterials and biomaterials.

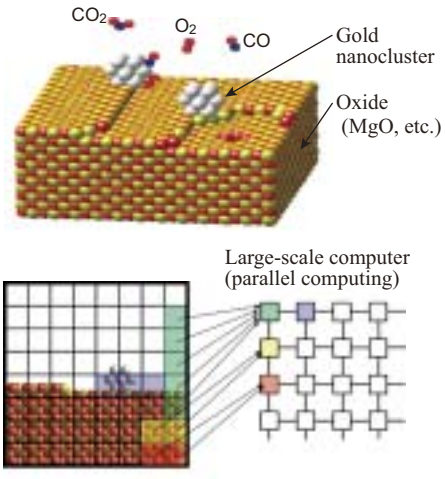

Fig. 1 Gold nanocluster on oxide and schematic diagram of first-principles order-N method.

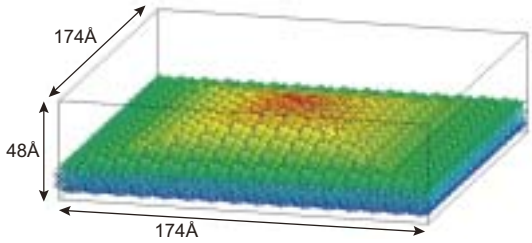

Fig. 2 First-principles simulation of approximately 23,000 atoms for Ge cluster on Si (001) surface: Charge density contours of electron density are shown here by color (blue: low, red: high). (From phys.stat.sol.(b)243,989(2006)) .

For more details: http://www.nims.go.jp/cmsc/fps1/

Special Features

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For Design of Nanofunctions

The Computational Materials Science Center consists of four groups, the First Principles Simulation Group (1), First Principles Simulation Group (2), Strong Coupling Modeling Group, and Particle Simulation & Thermodynamics Group. The Center's objective is the development of simulation techniques which will make it possible to search for novel functions, in order to analyze comprehensively the correlation between structural form, electronic state, and physical properties/functions in nanomaterials and nano-hybrids (see **figure**). (1) In first-principles simulations, the Center is involved in the analysis of various physical properties/functions of nanomaterials such as dielectric response, electron transport, spin conduction, etc. based on first-principles computational techniques, and the development of analytical techniques, etc. for ultra-large-scale system. (2) In the field of strong coupling modeling, we are developing modeling techniques for analysis of the quantum many-body effects and transport phenomena which appear in strongly coupled systems. (3) In multi-scale structures/property simulations, we are developing analytical techniques for meso-scale substances, including particle computation techniques such as the molecular dynamics simulation method, etc. and statistical thermodynamics simulation methods including the Phase-field method and others. New function search nanosimulation techniques are expected to form the foundation for the construction of a new manufacturing paradigm for creating nanomaterials with innovative functions by designing the structural form of the material, thereby making it possible to propose novel physical properties/functions.

*The Keisoku Supercomputer, which will have theoretical performance (computing speed of 10 Pflops/sec) exceeding that of the Earth Simulator (40 Tflops/sec) which is currently in operation, is now in the planning stage with start of operation scheduled for 2012.

For more details: http://www.nims.go.jp/cmsc/top_e.html

Elucidation of Physical Properties by the Nanoscale Analysis

- Control of Electronic and Magnetic Properties using the tools of First-Principles Electronic Structure Calculations -

Taizo Sasaki, Igor Solovyev
Kazuaki Kobayashi, Masao Arai
Shigeru Suehara, Ryo Maezono
First-Principles Simulation Group (2)
Computational Materials Science Center

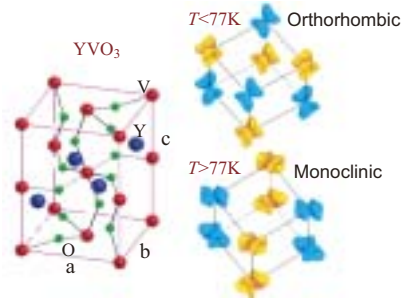

Fig. 1 Distorted perovskite structure and the shape of electron densities around V sites in orthorhombic (upper right) and monoclinic (lower right) phases of YVO_3. The surfaces in the figure at the right shows the electronic distribution on V. Different magnetic sublattices are shown by different colors.

According to the principles of quantum mechanics, the properties of a material are completely determined by the motion of electrons in it, that is, the electronic structure. If this is derived theoretically, without any experimental data, the result is termed a "first-principles" electronic structure calculation. The First-Principles Simulation Group (2) is involved in elucidating various phenomena at the nano-scale by the electronic structure calculations and investigating properties/functions as materials. We will introduce a part of our activities, mostly by Dr. Solovyev here.

From the viewpoint of materials science, the most attractive point of electronic structure calculations is a possibility of theoretical elaboration and design of materials with a desired set of properties. In this respect, a particular attention is paid to transition-metal oxides, where the application of external magnetic or electric fields, or the stress tension may cause the dramatic changes of the electronic structure, which is frequently accompanied by the metal-insulator transition. Moreover, one can always reveal a small group of electronic states, which is mainly responsible for this intriguing behavior. Therefore, for the transition-metal oxides, we may have a real chance to *design* the electronic and magnetic properties through the *design* of their electronic structure.

In order to achieve this goal, we use a unified approach, which combines first-principles electronic structure calculations with the model analysis. Namely, we perform conventional electronic structure calculations; derive parameters of the model Hamiltonian; and analyze the obtained data in terms of some model categories and trends. By doing so, we can combine the accuracy and predictable power of first-principles calculations with the flexibility and insights of the model analysis.

The basic idea can be illustrated for one of transition-metal oxides with the distorted perovskite structure, YVO_3 (**Fig. 1**). A broad interest to this and related materials is related with a large variety of magnetic structures, which is apparently related with tiny distortions in the perovskite structure. For example, YVO_3 may be found in two distinct antiferromagnetic configurations, the existence of which is closely related with the orthorhombic-monoclinic structural phase transition at T=77 K. We succeeded in not only reproducing this effect, but also presenting a transparent physical picture by the theoretically constructed model. The model explains how the lattice distortion (the changes in *a*, *b*, and *c*, and the angles between them in **Fig. 1**) affects the distribution of electron densities around (the so-called orbital ordering) and controls the form of interatomic magnetic interactions in these compounds. The same method was successfully applied to $YTiO_3$ shown in **Fig. 2**.

We believe that such strategy can be successfully applied to nano-materials with nanostructures one can directly design the electronic structure with the desired properties.

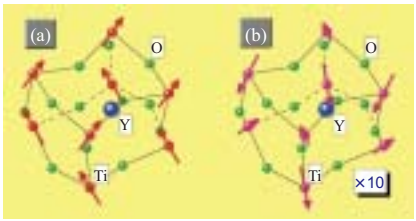

Fig. 2 Magnetic configuration of $YTiO_3$ derived from first-principles electronic structure calculations. (a) Electron spin part, (b) electron orbital orbital. The size of the arrows expresses the magnitude of the magnetic moment. In (b), the magnitude of the magnetic moment has increased tenfold.

For more details: http://www.nims.go.jp/cmsc/fps2/INFO/abste.html

NIMS News

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NIMS Participates in International Science, Innovation and Technology Exhibition INSITE 2006 (South Africa)

(September 24-27, South Africa) -- The International Science, Innovation and Technology Exhibition INSITE 2006 was held in South Africa. A total of 39 organizations from 10 countries participated in this exhibition, representing a wide range of fields such as information/communication, human resources, systems, tourism resources, automobiles, home electrical appliance, and others. From NIMS, the High Temperature Materials Center, which has concluded an MOU with a South African research institute (CSIR-M&Mteck and MINTEK), introduced research at NIMS and exhibited the results of recent research on Ni-base single-crystal superalloys containing platinum group metals. The NIMS booth received many visitors, increasing recognition of research at NIMS and giving a feeling the heightened interest in NIMS' work. On September 25, the NIMS booth received a visit from the South African Minister of Science and Technology, Mr. Mosibudi Mangena, and Japan's Ambassador Extraordinary & Plenipotentiary to South Africa, His Excellency Akihiko Furuya, who were extremely interested in research at NIMS.

Strong Correlated Electron Systems in Copper Oxides and Design of Novel Functions

Xiao Hu, Yoshihiko Nonomura
Akihiro Tanaka, Masanori Kohno
Strong Coupling Modeling Group
Computational Materials Science Center

Theoretical analysis of novel functional materials resulting from strong coupling among spin, charge, and crystal structure, and proposal of guidelines for developing new materials based thereon is our goal. The following introduces research on the magnetic/electrical properties of copper oxides as one example of the recent research activities of this group.

The synthesis of a new copper oxide, $Sr_8CaRe_3Cu_4O_{24}$, which possesses a perovskite structure, and spontaneous magnetization of this oxide above room temperature (T_c = 440 K) were reported in 2003. Although this material does not have magnetic ions like Fe and Ni, it is extremely interesting because its magnetic phase transition temperature (T_c) is more than 10 times higher than that of other known copper oxide magnetic materials. According to first-principles calculations, two species of copper (Cu) atoms exist in this material. The e_g orbit of Cu1, which has up spin, the $d_{3z^2-r^2}$ orbit of Cu2, which has down spin, and the p orbit of oxygen are ordered, and a strong pd **σ** bond forms, resulting in ferrimagnetism with a high transition temperature (see **figure**). The phase transition temperature and temperature dependency of magnetization can be explained with high accuracy by a quantum Monte Carlo analysis of a spin model based on the results of first-principles calculations.

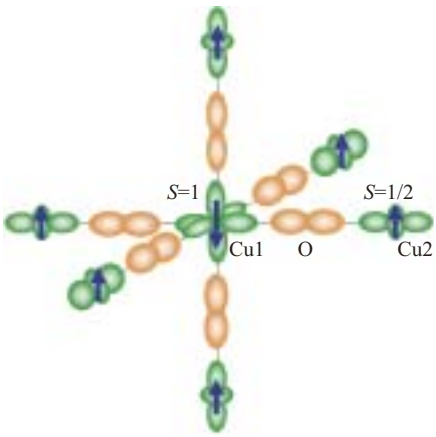


Fig. Orbital order and ferrimagnetism of copper oxide $Sr_8CaRe_3Cu_4O_{24}$ which is expected to provide the stage for novel spintronic functions.

Other unique properties were also discovered. In this material, the rhenium (Re) atoms have virtually no magnetic moment, but the magnitude of the Jahn-Teller distortion in the oxygen octahedron surrounding Cu2, which is caused by the electronegativity of this element, is important in determining the properties of this system. This fact means that it is possible to control the electronic band structure with a down spin if an element having lower electronegativity can be substituted for Re. With this strategy, theoretical design of novel materials would become possible. We therefore performed first-principles calculations in which the Re sites were substituted with tungsten (W) or molybdenum (Mo). The electronic state of Cu2 changed as expected, and the fact that its band crosses the Fermi level was clarified. As a result, it has been predicted theoretically that the new material will become a so-called half-metal, in which the electrons in one spin channel behave like in metal and those in the opposite channel like in insulator.

For more details:
http://www.nims.go.jp/cmsc/scm/index_en.html

NIMS News

Visitors from Finnish Finding Agency for Technology and Innovation

(October 30, NIMS) -- Mr. Reijo Munther, Director, Mr. Tapani Nummelin, Senior Technical Advisor, Dr. Jukka Viitanen, Councellor, and Dr. Mitsuru Niwano, Technology Consultant, of the Finnish Funding Agency for Technology and Innovation (Tekes) visited NIMS.

Tekes is now preparing national technology development program and "Development of advanced composite materials" is one of the important topics of the program. To see research activities in the related field, they had laboratory tour in Composites and Coatings Center and Fuel Cell Materials Center.

From left to right: Prof. Kagawa (NIMS), Mr. Munther, Mr. Nummelin, Dr. Niwano, Dr. Viitanen.

MOU with India's Jawaharlal Nehru Centre for Advanced Scientific Research

(August 22, India) -- NIMS' International Center for Young Scientists (ICYS), Nanoscale Materials Center, and Fuel Cell Materials Center signed an MOU with the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur, India.

This MOU is for collaboration on the Basics and Fabrication of Nanomaterials with the Chemistry and Physics of Materials Unit of JNCASR. For the strengthening of this cooperation, Dr. C.N.R. Rao, Honorary President of JNCASR, assumed the ICYS Executive Adviser on September 1.

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

Left to right: Dr.Vinu, Senior Researcher, Fuel Cell Materials Center, Prof. Bando, ICYS Managing Director, Dr. C.N.R. Rao, and Dr. M.R.S. Rao, President, JNCASR.

Microstructure Analysis by the Phase-Field Method
- Application to Pb-Free Solder Alloys -

Hidehiro Onodera, Katsuyuki Kusunoki
Toshiyuki Koyama, Masato Shimono
Masahiko Katagiri, Taichi Abe
Machiko Ode
Particle Simulation & Thermodynamics Group
Computational Materials Science Center

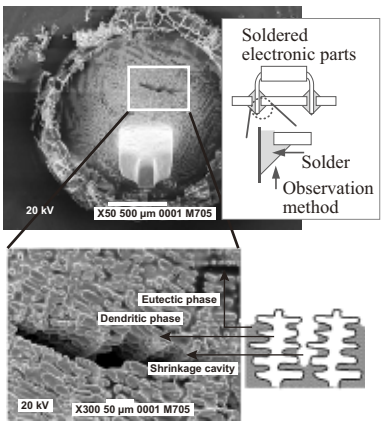


Fig. 1 Electron microscope image of soldered connection (courtesy of Mr. Uejima, Senju Metal Industry Co., Ltd.).

When materials which appear featureless to the naked eye are observed with a microscope, a variety of patterns can be seen. These are called the "internal structure" and have a large influence on material properties.

The Particle Simulation & Thermodynamics Group conducts research on the internal structure at the nano- to micro-scale making full use of various computational techniques. As one example, the research by Dr. Ode using the Phase-field method will be introduced here.

Based on environmental considerations, the EU has banned the use of harmful heavy metals in electrical/electronic equipment. Because these regulations require the use of lead-free (Pb-free) solder, electonics manufacturers had investigated the Sn-Ag-Cu composition system as a substitute alloy. However, various problems arose in connection with practical application. As one such problem, a dendritic microstructure (tree-like type of microstructure) appears on the soldered surface, causing surface to be rough, and this made it difficult to discover defects such as "solder crack."

Figure 1 shows the surface microstructure of a soldered connection. The part with the tree-like appearance is called the "dendritic phase," and the parts buried between the dendritic parts are called the "eutectic phase." The opening is called a "shrinkage cavity," and is a phenomenon which is frequently seen when the amount of eutectic phase is small. Although shrinkage cavities do not impair the function of the soldered connection, they closely resemble the defect called solder crack and are difficult to distinguish from such cracks. Using a trial-and-error process, makers discovered an alloy composition which minimizes the ratio of dendritic phase to eutectic phase, but it was not possible to explain the reason for the reduced dendritic content in terms of equilibrium thermodynamics. Using the Phase-field method, which is based on non-equilibrium thermodynamics, calculations were performed in order to investigate the factors which determine the ratio of eutectic phase and dendritic phase.

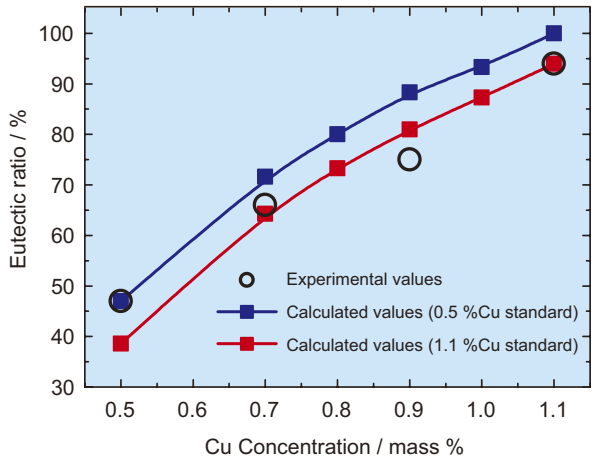


Fig. 2 Relationship between Cu content and eutectic ratio.

Figure 2 shows the relationship between the Cu composition and the eutectic ratio. The white circles (○) are the experimental results, and the closed squares (■) are the values calculated by the Phase-field method. One point in the experiment is used as a standard, the eutectic ratio of the other concentrations is obtained. Phase-field calculations consider the non-equiribrium phenomena, such as diffusion and segregation, the results are more reliable than those based on the equilibrium theory, Because the calculated and experimental values are in good agreement, it was understood that the amount of Cu composition had determined the eutectic ratio.

In addition to the above, we are also performing analyses of various other microstructures with the aim of contributing to materials design/development.

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

NIMS News

MOU with SUNY at Stony Brook, USA

(October 20, USA) -- The NIMS Sensor Materials Center (Dr. Hajime Haneda, Director General), the International Center for Young Scientists (Dr. Yoshio Bando, Director General), and the Optoronic Materials Center (Dr. Naoki Ohashi, Leader of the Opto-Electronics Group) signed an MOU with the College of Engineering and Applied Sciences (Dr. Yacov Shamash, Dean) and the Center for Nanomaterials and Sensor Developments (Assoc. Prof. Perena Gouma, Director) at State University of New York (SUNY) at Stony Brook. Stony Brook is familiar to material scientists because Prof. Prewitt, who published the table of ionic radius with Dr. Shannon, was there. Recently, Stony Brook is drawing international attention for its development of 10 peta-flops-class supercomputer.

This MOU is for effective cooperation on the study of nano-materials synthesis and their properties. The exchange of graduate students has already been initiated with the NIMS International Internship Program and a graduate student at Stony Brook has come to the Sensor Materials Center at NIMS this fall. Both institutes are now planning further steps, including researcher exchange or cooperative research focusing on sensors and sensor related materials and structures.

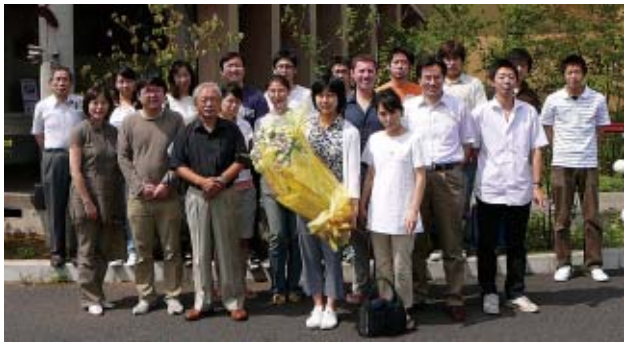
At the office of Dean Shamash, Stony Brook. From the left: Dr. Ohashi, Dean Shamash, Dr. Haneda, and Prof. Gouma.

Hello from NIMS

Science and Mountain Trekking

Hello everybody. My name is Michal Jerzy Wozniak. I came to NIMS from the Faculty of Materials Sciences and Engineering, Warsaw University of Technology, Poland and joined NIMS as a Junior Researcher in the Clinical Technology Group of the Biomaterials Center. My host researcher was Dr. Guoping Chen. My research at NIMS was divided into two parts. One was magnetic encapsulates (ferromagnetic nanocrystals in multiwalled carbon shells) for targeted drug delivery systems, which is also the subject of my Ph.D. thesis. The other was evaluation of the electrical and mechanical properties of biodegradable polymer scaffolds for tissue engineering by scanning probe microscopy (SPM).

Michal Jerzy Wozniak (Warsaw University of Technology, Poland)
Junior Researcher (February 2006-October 2006)
Clinical Technology Group, Biomaterials Center



[Having a good time with Prof. Tetsuya Tateishi (Managing Director of the Biomaterials Center), Dr. Chen, and other friends from my group]

[Somewhere in the Japanese Alps]

I found that NIMS was an excellent place for carrying out my research and I want to return here as a postdoctoral researcher. I enjoyed not only NIMS but the whole of Japan, which I found to be a beautiful country. During weekends, I traveled all over Japan. I had very good experiences trekking in the Japanese mountains. I found that the Japanese and Polish people are very similar, in that we know there is a time for working hard and a time for having fun as well. Even our cuisines are sometimes very similar, with the exception that the Japanese people eat a lot of rice, but the Polish, a lot of potatoes. I am very grateful to my friends from NIMS. They made my life in Japan much easier and comfortable. I hope I can meet them again in the near future.

NIMS News

Launch of the NIMS Alumni Association

The NIMS Alumni Association has been formed this year to promote cohesive network between the alumni and the researchers in NIMS. All researchers who stayed for more than 1 month at NIMS since its establishment in 2001 can obtain the alumni membership. To maintain international links, NIMS begins by providing memberships to non-Japanese alumni. The total number of the non-Japanese researchers since the establishment is about 600, and about 200 of them are currently in NIMS. Along with this November issue and NIMS 21, NIMS Alumni Membership Card will be sent to the members. If you are supposed to be a member but have not received the postal mail, please contact us.

Membership Card.

Contact: NIMS Alumni Association, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047 Japan
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NIMS National Institute for Materials Science

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