from Tsukuba, Japan to the world

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Special Features

Nanotechnology/Materials Research Supporting the Creation of a Sustainable Society II

Toward Realization of Next-Generation DNA Semiconductors

—Controlling Electric Conductivity in DNA—

Hiori Kino
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Computational Materials Science Center (CMSC)

Existing semiconductor technology will reach the limits of high-density integration in the very near future. In order to develop innovative devices which overcome these limits, the discovery of new circuit elements and microfabrication techniques for realizing those elements will be indispensable. DNA has a thickness of only nanometer scale, and a variety of structures can be created without actual fabrication by appropriately designing the DNA base sequence (that is, by self-organization). Although DNA is essentially an insulator, if a method of obtaining high conductivity by introducing conductive particles in DNA can be established, it would have the potential for the development of innovative nanoscale molecular devices.

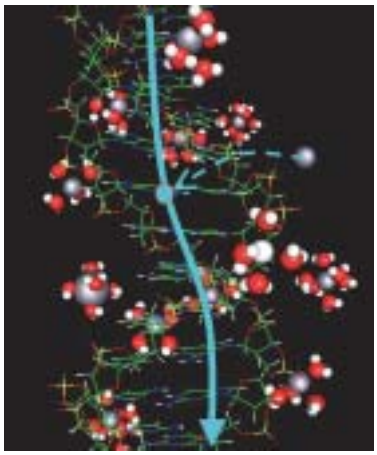

Fig. 1 Mechanism of electric conductivity in DNA. Magnesium (silver circles) with no surrounding water supplies holes (light-blue circles) to the DNA, which is an insulator. The supplied holes move along the DNA (light-blue line).

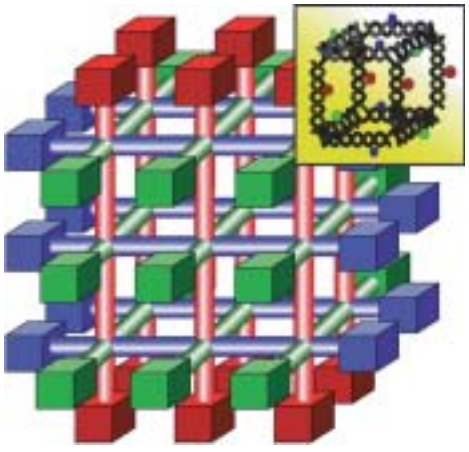

Fig. 2 Example of a three-dimensional crossbar circuit formed from DNA. Each of the cubic structures is formed form the DNA cubes shown in the insert. It is possible to form p- and n-type semiconductors and insulators in the sides of the red, blue, and green DNA columns, respectively, by doping (or not doping) the columns with individual impurities (shown by the circles in the insert). Ends show electrodes.

The present research revealed that holes which had existed in metallic ions when surrounded by water are introduced into the DNA base when the water is removed (**Fig. 1**). The mechanism of electric conductivity in this case resembles the mechanism by which a semiconductor is formed when impurities are introduced in silicon. The conductivity of silicon containing impurities increases as the impurity content increases. In a similar manner, the conductivity of semiconductor DNA increases with the number of holes. < Continued on p.2

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NIMS News

Comprehensive Research Agreement with KAIST, Korea

Prof. Hong (right), Chair of the Department of Materials Science and Engineering, KAIST, and President Kishi of NIMS.

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Analysis of Size Dependence of FePt Particle Ordering by Phase-Field Method

—Guidelines for Nanostructure Control of Magnetic Recording Media—

Toshiyuki Koyama
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Hard disk capacity has increased dramatically in recent years. To realize this, it is necessary to refine the minimum region where information is stored on the magnetic recording surface to the nanoscale level. However, it is known that recorded data are lost in some cases due to thermal vibration when the size of these regions is reduced beyond some point. Therefore, a material which will guarantee data storage with small recording regions has been needed. As one important candidate for this, the FePt phase, which has an $L1_0$ ordered structure (structure having alternating layers of Fe and Pt in every other atomic layer), has been the subject of considerable interest, and research is proceeding worldwide. In experimental work, the Metallic Nanostructure Group of Materials Engineering Laboratory (MEL) at NIMS recently discovered that, although the FePt phase has a high magnetic recording storage capability when it has the $L1_0$ ordered structure, when the FePt phase consists of nanoscale particles, the ordered structure breaks down, changing to a disordered phase (condition in which Fe and Pt are arranged randomly within crystals), and its magnetic recording storage capability drops sharply. Because this is a serious problem for realizing high density in magnetic recording, elucidation of the minimum size limit at which the $L1_0$ ordered structure can be maintained has emerged as an important issue.

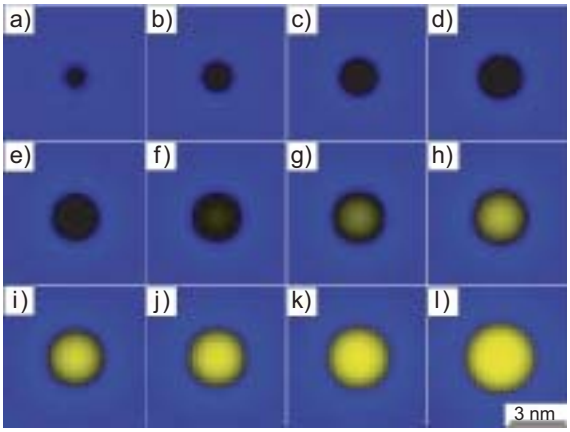

Fig. 1 Phase-field calculation for ordering of FePt particles.

The present research was the result of an attempt to obtain an answer to this question using the phase-field method, which has attracted attention in recent years as a powerful computational method for modeling the evolution of the microstructure in materials. In the phase-field method, the morphology of microstructure in materials is expressed based on a model for a continuous medium, and analysis is performed using evolution equations for temporal/spatial changes in a complex microstructure.

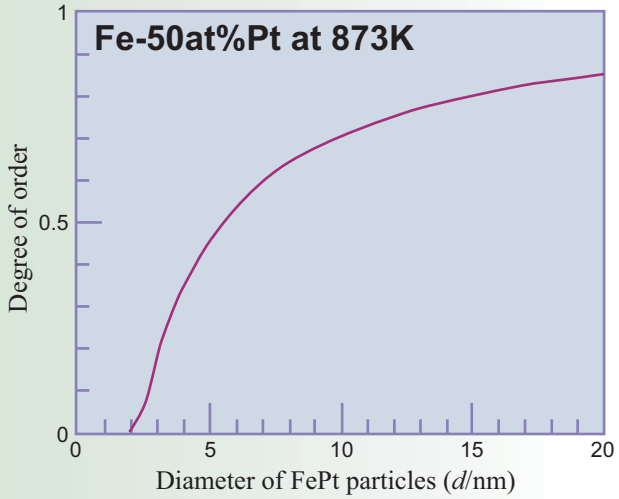

Fig. 2 Size dependence of ordering in the FePt phase.

Figure 1 shows the results of a calculation of the size dependence of the stable state of the FePt phase using conditions of temperature, 873 K and particle composition, Fe-50at%Pt. The circular areas are FePt particles, and the yellow color within the particles represents the degree of $L1_0$ ordering. It can be understood that a disordered condition (shown by black) exists when the particles are small, and the ordered condition (yellow) becomes stable as the particle size increases, with approximately diameter d = 2-4 nm corresponding to the borderline for stable ordering. **Figure 2** is a graph in which changes in the degree of ordering were calculated for the diameter d. Because the value of d when the material is completely disordered is roughly 2 nm, it can be understood that the limit for use as a magnetic recording medium is approximately 2 nm. We believe that obtaining a quantitative understanding of the guidelines for nanostructure control based on theoretical considerations will be indispensable for future material and device design at the nanoscale level.

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Toward Realization of Next-Generation DNA Semiconductors

It is possible to construct nanometer-size micro-transistors utilizing the self-organizing capability of DNA and the semiconductor-forming mechanism described above. First, DNA with a base sequence designed for self-organization in a designated shape is allowed to self-organize to the designed shape in water. Semiconductor-forming metal ions are then mixed in the solution, the water is removed, and the DNA is dried. Three-dimensional nanostructures can be created using only this simple process. For example, a three-dimensional nano-crossbar circuit was formed from DNA by combining the DNA nanostructure called Seeman's cube (**Fig. 2**).

As this work illustrates, creation of nano-molecular devices which exceed the current limits of high-density integration can be expected by a fusion of biotechnology and nanotechnology. This work was carried out as joint research with Tohoku University and the National Institute of Advanced Industrial Science and Technology (AIST).

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

Analysis of Hydrogen Embrittlement Phenomena by First-Principles Simulation

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Takahisa Ohno
Director-General
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In spite of its small size, the hydrogen atom causes many macroscopic phenomena of interest in materials. Hydrogen embrittlement, the phenomenon in which materials get quite brittle due to the existence of solute hydrogen, is one of them. In particular, hydrogen embrittlement of structural materials based on iron is a serious problem from the viewpoint of safety. However, the hydrogen solubility in iron is extremely low and the direct observation of hydrogen is quite difficult using present techniques. What the state of hydrogen is in such iron-based materials and how such small amounts of hydrogen cause macroscopic failure of the materials are still open questions.

First-principles simulations show their predictive power in investigation of such microscopic phenomena that are difficult for experiments to observe. We have first examined the hydrogen-trapping energy of monovacancy, Vac, in iron (**Fig. a** center), and demonstrated that the $VacH_2$, the monovacancy trapping two hydrogen atoms, is energetically dominant at ambient conditions. This result indicates that the conventional theory on the number of trapped hydrogen atoms may need revision.

The energetics of the Vac and $VacH_2$ bindings was also investigated. In the case of the monovacancy without hydrogen, Vac, it is found that binding is energetically favourable irrespective of the alignment of the monovacancies and a more compact structure is likely to be formed. These results suggest that a vacancy cluster with a spherical structure, as shown in **Fig. (b)**, is energetically more preferable to the separate monovacancies.

Regarding the binding of $VacH_2$, on the other hand, the alignment in the <111> direction and keeping the hydrogen-iron bonds is found to be energetically more favourable. This suggests that the formation of anisotropic plate-shaped clusters on the (100) or (110) plane, as shown in **Fig. (c)**, occurs in the existence of hydrogen.

Since the (100) planes are the cleavage planes in iron, the planar vacancy clusters parallel to these planes could enhance the cleavage. The enhancement of the vacancy clusters on the (110) planes, on the other hand, can increase the dislocation (linear defects) intersections, because the cutting of the dislocations is usually accompanied by leaving vacancies on the slip planes. This enhancement of the intersections can be closely linked with 'Hydrogen-enhanced local plasticity', which recently has been regarded as one of the most promising mechanisms of hydrogen embrittlement.

Analysis from the atomic level as in this study is expected to play a crucial role in future research on the hydrogen embrittlement mechanism.

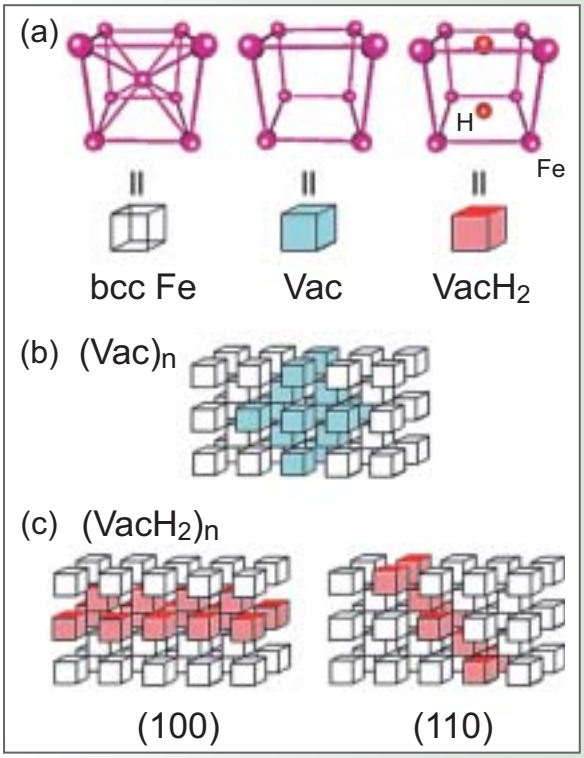

Fig. (a) Structures of iron crystal (bcc Fe), monovacancy (Vac), and major monovacancy-hydrogen complex ($VacH_2$) and their schematic diagrams. (b) Stable structure of vacancy cluster in iron in case where hydrogen is not present. (c) Plate-shaped $VacH_2$ clusters on the (100) plane and (110) plane, which are suggested to be stable structures in the presence of hydrogen.

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

Visit by Czech Science and Technology Delegation

(May 25, NIMS) -- NIMS was honored with a visit by a science and technology delegation from the Czech Republic, which was headed by Dr. Kolar, Vice Minister of Education, Youth and Sports, and Prof. Paces, President of the Academy of Sciences. After a general explanation of NIMS by President Kishi, the delegation enthusiastically observed laboratories conducting research on non-oxide ceramics, nanomaterials, and nanoelectronics. NIMS launched an International Joint Graduate School Program with Charles University in Prague three years ago and now receives five doctoral students from its Czech counterpart each year. Although research exchanges between NIMS and the Czech Republic are progressing steadily through this program, the Czech delegation expressed a desire to further deepen cooperation with NIMS in the future.

Czech delegation with students in the International Joint Graduate School Program.

Transport Properties of Single Organic Molecules

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Takahisa Ohno
Director-General
Computational Materials Science Center (CMSC)

In recent years, with progress in experimental technologies, the physical properties of nanosize materials have attracted attention. Among these, electron transport phenomena are one type of property which has been energetically investigated. In particular, extremely interesting work on nanosize electron transport phenomena is now being done. This is linked to molecular devices, nanowire conduction, and similar technologies which have recently become important areas of research. However, because there are few systems which can actually be manipulated or controlled, investigation is currently limited to trial-and-error methods. It would therefore be extremely useful for future development if systems with the required properties and the properties of systems which the researcher wishes to manipulate could be predicted.

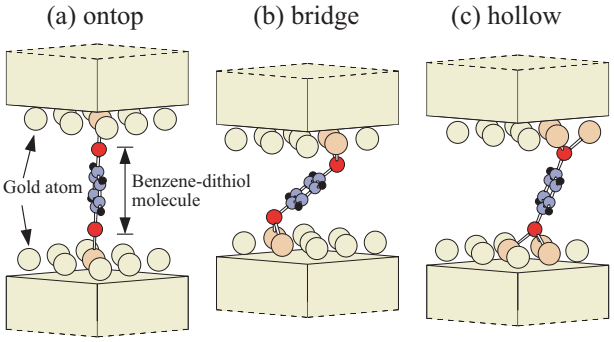

Fig. 1 Structure of benzene-dithiol molecule and gold electrode.

Based on scattering theory, we calculated the transport properties of benzene-(1,4)-dithiol between gold electrodes as a typical example to investigate the transport properties of nanowire. Three contact structures were considered, ontop site contact, bridge site contact, and hollow site contact (**Fig. 1**). Transmission, which is an index of the ease with which electricity flows, was calculated for these contact structures, as shown in **Fig. 2**. With ontop site contact, three peaks with comparatively narrow widths were found in the range of -1 eV ~ -2 eV. In contrast to this, with bridge site bonding, a high, wide peak at -3 eV and a low peak at -1 eV can be seen, while the hollow site had only one extremely wide peak centering on -2.0 eV. As can be understood from this example, transport properties differ greatly depending on the contact structure.

The contribution of molecular orbitals was also investigated. The numbers in **Fig. 2** indicate the molecular orbital. **Fig. 2** shows which molecular orbitals caused the peaks on the transmission spectra. As shown in **Fig. 2**, even with the same molecular orbital, the contribution of the orbital differs greatly depending on the contact structure. In particular, with the ontop site contact, molecular orbitals 19 and 20 make a large contribution to transport properties, whereas the same orbitals make almost no contribution with the other two contact structures. In other words, not all molecular orbitals contribute to transport properties.

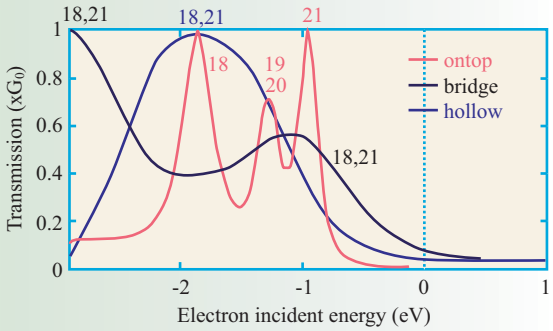

Fig. 2 Transmission spectra.

As described above, calculations of the transport properties of multiple structures revealed that their transmission and the contribution of molecular orbitals are strongly dependent on the contact structure between molecules and electrodes. This shows that consideration of the contact structure is extremely important when researching molecular devices.

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

NIMS News

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Comprehensive Research Agreement with KAIST, Korea

(June 8, NIMS) -- NIMS concluded an agreement on comprehensive research cooperation with the Korea Advanced Institute of Science and Technology (KAIST). KAIST is a research-type university which was established by Korea's Ministry of Science and Technology to train first-class researchers. KAIST is devoting great effort to research on nanotechnology. KAIST Nano Research Institute was established in 2001, and at the end of 2004, the institute completed construction of a joint-use facility equipped with state-of-the-art nanofabrication equipment, which it has opened to Korean universities and research institutes. The comprehensive agreement was concluded based on a judgment by both sides that it is necessary to strengthen cooperation between KAIST and NIMS in a wide range of materials research fields in the future, centering on nanotechnology.

NIMS Signs MOU with a British Centre for Industrial Collaboration

Prof. Fisher, Director of BITE-CIC (right), and Prof. Tanaka, Director-General of the BMC.

(May 25, U.K.) -- The Biomaterials Center (BMC) signed a cooperation agreement with the Centre for Industrial Collaboration in the field of Biomaterials and Tissue Engineering (BITE-CIC), UK. The three UK universities known as the "White Rose Universities" (Universities of Leeds, York, and Sheffield) are world-class research institutes in biomechanics, molecular biology, and biomaterials evaluation, respectively. BITE-CIC serves as an organization for promoting various types of cooperation between the three White Rose Universities and industry. To date, the Centre has produced a number of international top-level medical device companies. The aims of this MOU are to promote exchanges of researchers, information, and technology between the three universities and NIMS and to accelerate practical application of biomaterials developed at NIMS.

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

Discovery of New States of Material

—Theoretical Research on Superconductivity Vortex Systems —

Xiao Hu
Strong-Coupling Modeling Group
Computational Materials Science Center (CMSC)

Solids melt into liquids as their temperature increases. This everyday phenomenon is deeply related to the magnetic-field response of the superconducting state, which is governed by quantum mechanics, and exposes extremely interesting aspect of physics. When a magnetic field is applied to a superconducting state, vortices form as the superconducting current attempts to shield the field. The theory that vortex lines (flux quanta) parallel to the field form a regular vortex-line lattice because of the mutual repulsive force was first advanced by Dr. Alexei A. Abrikosov, who won the 2003 Nobel Prize in Physics for this achievement. The change of the vortex lattice to a vortex liquid as temperature rises accompanied by a thermodynamic first-order phase transition with finite latent heat was observed only in the past 10 years. The fact that superconductivity is lost simultaneously with this melting transition was seen clearly in our large-scale computer simulations.

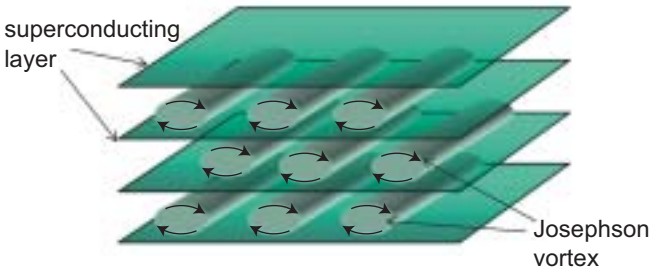

Fig. 1 High-temperature superconductor and Josephson vortex quantum.

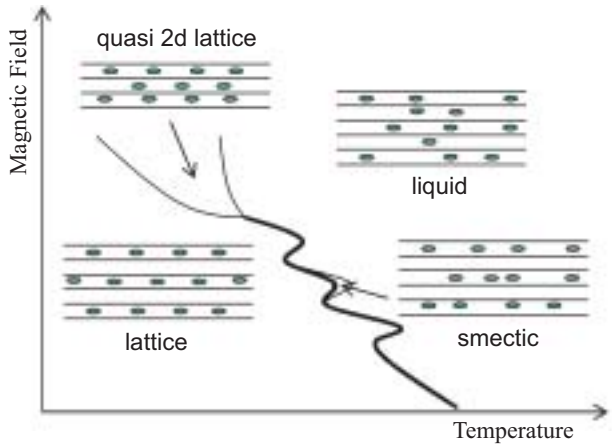

Fig. 2 Field-temperature phase diagram of Josephson vortex quantum. The thick and thin lines show discontinuous and continuous phase transitions, respectively.

On the other hand, in high-temperature superconductors, superconducting planes and semiconductor planes are stacked alternately at the nanometer scale and interlayer coupling occurs between the superconducting planes due to the quantum tunneling effect (in this case, called the Josephson effect), which results in intrinsic, multiple Josephson junctions. When a magnetic field is applied parallel to these planes, the vortex lines will avoid the superconducting planes and enter the semiconductor layers (**Fig. 1**). Because the interaction between vortex lines is extremely anisotropic, and the superconducting planes exert a pinning effect on motions and fluctuations of the vortex lines in the direction perpendicular to the planes, the states which the Josephson vortex system can take and the melting processes are extremely abundant.

According to our recent computer simulations, under a magnetic field strong enough to ensure that vortex lines are introduced into all semiconductor layers, a state in which vortex-line arrays with good in-plane order can slide mutually appears in an intermediate temperature region. When this happens, the vortex lattice melts through a process of two continuous phase transitions. Furthermore, our density-functional-theory study revealed the existence of a so-called smectic phase at appropriate magnetic fields and temperartures, where semiconductor layers with more and less Josephson vortices appear alternately (period m=2) and within each layer vortex lines take a liquid state with short-range correlations. The melting process in this field regime consists of a first-order phase transition and a second-order phase transition (**Fig. 2**).

The knowledge of these new material states will be useful for developing terahertz laser emission based on intrinsic Josephson junctions in high-temperature superconductors. The present study also provides insights for the physical properties of the lipid/DNA superlattice used in DNA manipulation and the charged stripe state seen in the matrix of high-temperature superconductors.

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

NIMS Exhibits in Thailand

Mr. Thapparansi (center) and Dr. Nongluck (right) visiting NIMS' exhibition booth.

(May 23-27, Thailand) -- The Thailand Institute of Scientific and Technological Research (TISTR), with which NIMS has signed an MOU, invited NIMS to its 42nd Anniversary Ceremony and General Exhibition. NIMS introduced its research activities including the nanotechnology support activities by posters and videos, and exhibitions of shape memory alloys and photocatalysts. The Anniversary Ceremony was held on May 25 with numerous dignitaries in attendance, including Thailand's Minister of Science and Technology, Mr. Thapparansi, the Director of TISTR, Dr. Nongluck, and members of the diplomatic missions of Russia, Germany, and Vietnam. NIMS was honored to have the opportunity to explain its research activities directly to Thailand's Minister of Science and Technology, who listened with keen interest.

Hello from NIMS

Vladimir Matolin (Jul. 2005 - Feb. 2006)
(Charles University in Prague, Czech Republic)
NIMS Overseas Fellow/ICYS Visiting Advisor

[Working with Dr. Yoshitake of the Nanoassembly Group (right) at the NIMS Sakura Site]

My name is Vladimir Matolin. I am a Professor and Head of the Department of Electronics and Vacuum Physics of Charles University in Prague (CU). CU is one of the oldest in Europe, having been founded in 1348, and has over 42,000 students, including international students, who have come to the university to obtain their degrees.

The Department of Electronics and Vacuum Physics has more than 70 people (5 professors), including PhD students, working in the fields of surface and interface physics and plasma physics with a strong emphasis on materials science. In addition to our activities in the Czech Republic, we built the Materials Science Beamline facility at the Synchrotron Light Laboratory Elettra in Italy. I visited NIMS for the first time in 1997 when we established the first scientific contacts for the study of metal-oxide interactions. Since then, our mutual contacts have developed rapidly, and in 2002 I was appointed as the Coordinator of the International Joint Graduate School Program established by NIMS and CU.

I am really glad to be able to develop my scientific cooperation with NIMS, which is one of the World Wide Centers of Excellence in Materials Science. My contacts with NIMS give me new possibilities to meet excellent scientists, participate in challenging scientific programs, and bring our students and my colleagues closer to this fascinating scientific institution. I am also proud of my appointment as the 1st NIMS Overseas Fellow, Research Advisor of Nanomaterials Laboratory (NML) and Ecomaterials Center (EMC), and Visiting Advisor of International Center for Young Scientists (ICYS), as well as coordinator of the MOU between NIMS and CU signed in July, 2005.

[Meeting with President Kishi, supervisors of NIMS, and Czech students]

My visits to NIMS are always satisfying and pleasurable experiences for me. Time after time, I am delighted to meet friendly Japanese people and to wonder at Japanese culture. My travels to Tsukuba and my responsibilities at NIMS represent for me gratifying obligations to do my utmost for the further development of our cooperation.

■ Hello NIMS NOW readers! ■

Emily Collins (U.K./RIKEN)
Visiting Researcher (Oct. 2004-Sep. 2005)
Magnet Development Group
High Magnetic Field Center (Tsukuba Magnet Laboratory)

[Under the full bloomed cherry blossom]

My name is Dr Emily Collins and I am from Norwich, England. I came to Japan last year after completing my PhD in England and then working as a Marie-Curie fellow at the Center for Biological Magnetic Resonance in Frankfurt, Germany and am working as a visiting researcher in the Magnet Development group at NIMS Sakura site.

I am a postdoctoral researcher in the Protein Research group of RIKEN GSC, Yokohama and am working on determining the 3D structures of proteins as part of the Protein 3000 project. Knowing the structure of a protein can elucidate information about its function and binding partners and help in such things as drug development. NIMS has ideal facilities for my research as I am fortunate enough to be able to use the 920MHz NMR spectrometer, the highest field solution-state spectrometer in the world, which was developed and built here at NIMS.

My husband is also working at NIMS as fellow in the International Center for Young Scientists (ICYS) in Namiki and we feel very fortunate that we are able to work in the same institute here in Japan. We have very much enjoyed living and working in Tsukuba, a clean modern safe environment. In particular I like the food, the parks, the spa, the shopping and especially all the friendly, helpful people at RIKEN, NIMS and my residence; Ninomiya House.

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PUBLISHER
Dr. Masatoshi Nihei

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