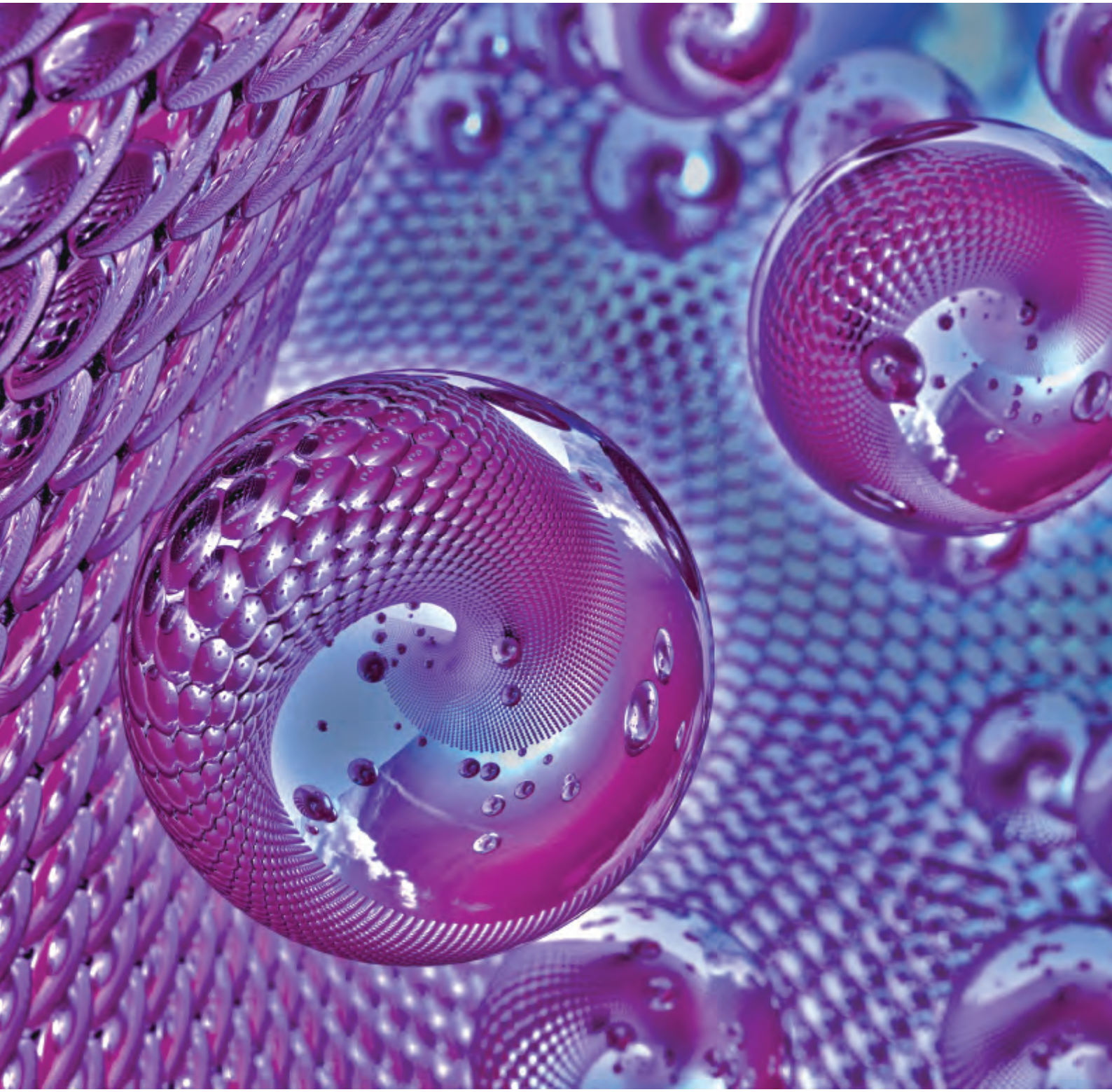
# AiM Research

## RESEARCH HIGHLIGHTS 2011

A publication of the WPI Advanced Institute for Materials Research



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### WPI Advanced Institute for Materials Research

The Advanced Institute for Materials Research (AIMR) at Tohoku University in Sendai, Japan, is one of six World Premier International (WPI) Research Centers established with the support of the Japanese Ministry of Education, Culture, Sport, Science and Technology (MEXT). Since its inauguration in 2007, the WPI-AIMR has been bringing together world-class researchers from Japan and abroad to carry out cutting-edge research in materials science through interdisciplinary collaboration among its four groups: Bulk Metallic Glasses, Materials Physics, Soft Materials, and Device/Systems, along with a newly added Mathematics Unit.

Led by chief scientist and institute director Yoshinori Yamamoto, the center promotes fusion research across the different groups while fostering young researchers through a fusion-research proposal system and the Global Intellectual Incubation and Integration Laboratory ($GI^3$ Lab), where international joint research is carried out in close cooperation with high-profile researchers invited from countries throughout the world.

The WPI-AIMR is host to over 120 leading researchers, with around half from around the world, including 31 principal investigators. In addition to the research hub at Tohoku University, the WPI-AIMR collaborates with research centers in the UK, France, Germany, the USA and China. Close ties with other leading foreign universities are maintained through its Adjunct Professor and Associate Professor programs.

### AIM*Research*

AIM*Research* is an online and print publication that highlights the scientific achievements and activities of the WPI-AIMR. First published in June 2009, AIM*Research* selects the most important papers from the wealth of research produced by WPI-AIMR scientists throughout the year, distilling the essence of the achievements into timely, concise and accessible research highlights that are easy to digest, but retain all of the impact and importance of the original research article. Published monthly on the AIM*Research* website in both English and Japanese, AIM*Research* highlights bring the very best of WPI-AIMR research to a global audience of specialists and nonspecialists alike. AIM*Research* also publishes a range of features articles introducing other activities of the WPI-AIMR's research groups. Visitors to the website can register for monthly email alerts in either Japanese or English to keep abreast of the latest developments and discoveries made at the WPI-AIMR.

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AIM*Research* is a publication of the World Premier International Advanced Institute for Materials Research (WPI-AIMR), a Tohoku University institute funded by the Ministry of Education, Culture, Sports, Science and Technology of Japan.





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**ISSN 1884-491X**

MESSAGE FROM THE DIRECTOR

# A new challenge: Mathematics and materials

As the institute director of the World Premier International Advanced Institute for Materials Research (WPI-AIMR), I have great pleasure in welcoming you to this, the third print edition of AIM*Research*. Last April, the AIM*Research* website entered its third year, and this print publication is a comprehensive collection of the research highlights published on the website in 2011 along with lively journalistic features that turn a spotlight on the people and activities behind the research carried out at the WPI-AIMR.

Since its inauguration in 2007, the WPI-AIMR has consisted of four key research groups — Bulk Metallic Glasses, Material Physics, Soft Materials, and Device/Systems Construction — which have carried out high-caliber research in each discipline, as well as dynamic fusion research between disciplines. Examples of fusion research at WPI-AIMR include the creation of metallic nanoporous catalysts, which combines the fields of modern metallurgy and chemical science; and the development of microelectromechanical devices based on bulk metallic glasses, in which modern metallurgy is combined with device construction. The institute's fusion research outcomes, coupled with the accomplishments in each research group, have established WPI-AIMR as a unique world-class research institute in materials science, where various disciplines work together under one roof. Our recently renovated WPI-AIMR Main Building, completed in July 2011 and in which all four research groups are now based, helps to further enrich the institute's environment of fusion research.

The newly established Mathematics Unit, introduced in late 2011, will complement the four existing research groups by further enhancing and catalyzing fusion research, and will contribute to the creation of a new materials science. Professor Motoko Kotani, Deputy Director and Leader of the Mathematics Unit, initiated the collaboration of mathematics and materials science at WPI-AIMR. The power of mathematics has a long tradition of providing common languages to all fields of science and technology, and more recently it has become a global trend for science and technology to amalgamate with mathematics. Mathematics can simplify complicated and diverse phenomena, extracting from them the principles that can make it possible to predict and create new functional material. Over the next five years, the new Mathematics Unit will set us on a unique research direction that will help to further advance WPI-AIMR as a key global research hub for innovation and education in new materials science.

In this fiscal year, site-visit teams and the program committee of the Japan Society for the Promotion of Science (JSPS) undertook an annual evaluation of WPI-AIMR, and an interim evaluation was conducted by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). Released on December 14, 2011, MEXT's evaluation results encourage us to pursue our new research direction of mathematics–materials science collaboration. I am also pleased to announce that Professor Kotani will lead WPI-AIMR from April 2012 as my successor.

Finally, nearly a year has passed since the terrible triple disasters of March 11, 2011 in which more than 15, 000 people died — the 9.0-magnitude Tohoku earthquake, the devastating tsunami with heights of 10 to 20 meters (in some places up to 40 meters), and the subsequent crisis at the Fukushima nuclear power plant.

Although Sendai, along with WPI-AIMR and Tohoku University, has now recovered to a level similar to that before the disasters, many people living in the coastal region are still experiencing serious problems. The situation at Fukushima is gradually improving, but it will take a long time until the problem is completely resolved. Since March last year, people from all over the world have supported us both materially and spiritually, and I wish to extend our deepest gratitude for their generous assistance. It is a pleasure for me to say that WPI-AIMR is quickly recovering from the disasters, and as part of the region's rebuilding process, we are continuing our research activities and education at a faster pace than ever before.

*Yoshinori Yamamoto*
*Director*
*WPI-AIMR*

# AiM Research

**AIM*Research* highlights some of the best materials research at the World Premier International Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Japan.**


AIM*Research* introduces cutting-edge research from the WPI-AIMR through its concise, accessible research highlights, and casts a spotlight on the scientists and laboratories of WPI-AIMR

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# RESEARCH HIGHLIGHTS

The WPI-AIMR advances research in bulk metallic glasses, materials physics, soft materials and device/systems construction, and actively promotes collaboration among these divisions toward the development of ground-breaking technologies that cross the boundaries of conventional fields of study—bridging the disciplines of materials science, physics, chemistry and precision, mechanical, electronics and information engineering. The new Mathematics Unit, established in late 2011, will further complement WPI-AIMR's research activities.

## Thin films

# A tight squeeze

Insight gained into the electronic properties of lead films by combining two characterization techniques suggests new strategies for electronic applications

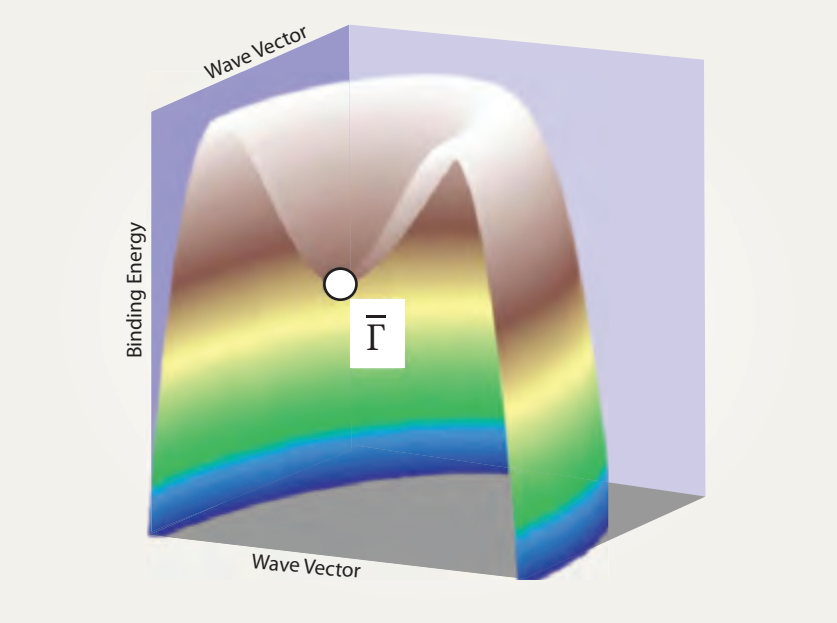
Processing materials into thin films is important for fabricating electronic circuits, solar cells and lasers devices. Often only a few atomic layers thick, thin films are dominated by quantum effects whose properties can offer distinct performance advantages over thicker layers.

Researchers from the WPI-AIMR in collaboration with researchers from Tsinghua University and the Institute of Physics in Beijing, China, have now uncovered how such quantum effects influence the properties of thin films based on the superconducting material lead[1]. Their findings could enable new electronic applications of thin metal films.

Thin films of lead are more unusual than those of most metals. Many of their properties are extremely sensitive to variations in film thickness, even by as little as a single atomic layer. This behaviour is thought to be caused by particularly pronounced quantum effects resulting from the long distances over which the electronic states of the metal extend, says Seigo Souma from the research team. "For most metals, quantum-size effects occur at very small thickness of less than 5 nanometers, whereas lead films, owing to their large electron wave length of 1 nanometers, exhibit significant size effects even at film thicknesses of over 20 nanometers."

To discover the origins of these unusual quantum properties, the researchers studied thin films of lead grown on silicon.

They combined two characterization techniques — surface scanning tunnelling spectroscopy and angle-resolved photoemission spectroscopy — to correlate the relationship between film thickness and any exhibited electronic features.




The electronic structure of lead films. The energetic states of electrons in thin films of lead are plotted as a function of momentum and energy. Quantum effects are responsible for the shape of these electron states, with the top ring in particular being responsible for many of the observed properties.

Charting the kinetic energy of the electrons as a function of their momentum, the researchers discovered that confinement effects caused the electronic states to form an 'm' shape (see image) that changes significantly between films comprising 23 and 24 atomic layers. Of particular interest is the circular structure that forms in the topmost part of the structure, where a very large number of electronic states are concentrated. The energetic position of the ring depends on the film thickness, which in turn causes thickness-dependent oscillations in the electronic properties of the films.

Building on this advancement in fundamental understanding, the next challenge will be to investigate the superconducting properties of these thin films together with systems of different geometries, such as quantum dots, wires and stripes.

"Understanding the electronic structures of these low-dimensional systems lies at the heart of advanced electronic devices," says Souma.

1. Sun, Y. J., Souma, S., Li, W. J., Sato, T., Zhu, X. G., Wang, G., Chen, X., Ma, X. C., Xue, Q. K., Jia, J. F., Takahashi, T. & Sakurai, T. Van Hove singularities as a result of quantum confinement: The origin of intriguing physical properties in Pb thin films. *Nano Research* **3**, 800–806 (2010).

## Energy storage

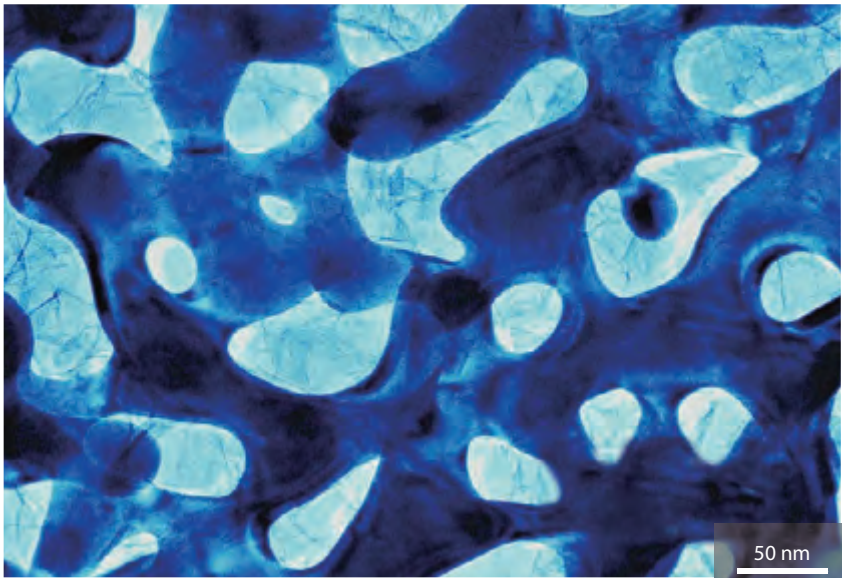
# Supercapacitors with a heart of gold

Growing inorganic crystals inside nanoporous gold films boosts the speed and energy density of charge-storing devices

Wind turbines, solar cells and other 'green' energy technologies often encounter supply-and-demand problems because their energy sources are intermittent. One way to overcome this is by using supercapacitors — devices that can quickly store electricity by organizing positively and negatively charged ions into two distinct electrolyte layers, each in contact with a metal electrode. However, while such double-layer supercapacitors are extremely robust, the energy storage density they offer is not sufficiently high for widespread use.

Xingyou Lang, Akihiko Hirata, Takeshi Fujita and Mingwei Chen from the WPI-AIMR have been working on building supercapacitors using transition metal compounds such as manganese dioxide ($MnO_2$), which can store charge at metal sites by an electron transfer process called 'pseudocapacitance'. Unfortunately, $MnO_2$ has low conductivity, which limits its charging and discharging speeds. The researchers have now shown[1] that a supercapacitor constructed using an $MnO_2$-plated gold film dotted with nanoscale pores has quick-charging properties and unprecedented electrical storage capabilities.

Previous attempts to resolve the conductivity problems of $MnO_2$ have involved incorporating the oxide into conductive polymers or carbon nanotubes. Chen and his team took a different approach by fabricating a nanostructured $MnO_2$–gold composite. First, they selectively etched a silver–gold alloy into a thin gold sheet permeated with numerous nanopores. They then grew $MnO_2$ nanocrystals directly into the pore channels using a gas-phase reaction. This growth step proved crucial to the performance of the supercapacitor — too much crystal deposition would fill the nanopores and impair the double-layer effect, while too little crystal growth would not provide good pseudocapacitance. Finally, the team sealed the resulting nanostructured electrodes and an aqueous electrolyte in plastic, creating a thin and flexible supercapacitor.






Transmission electron microscopy image showing the close contact between gold (dark blue) and crystalline $MnO_2$ (light blue)

The device displayed excellent charge storage capacity with an energy density up to 20 times higher than that of other $MnO_2$ electrodes. The supercapacitor also displayed near-ideal high-speed charging behavior, which high-resolution microscopy revealed to be due to intimate contact between the $MnO_2$ crystals and the conductive gold surface (see image). "We did not expect the formation of such a good interface because of the obvious differences in lattices and chemical properties between gold and $MnO_2$," says Chen.

These properties, in combination with fast ion diffusion through the three-dimensional nanoporous structure, result in an enhanced supercapacitor with promising applications.

Chen and his team are currently investigating how to utilize the $MnO_2$–gold composite for electrodes in lithium-ion batteries, and are attempting to develop other mixed nanoporous materials with even higher energy densities.

1. Lang, X., Hirata, A., Fujita, T. & Chen, M. Nanoporous metal/oxide hybrid electrodes for electrochemical supercapacitors. *Nature Nanotechnology* **6**, 232–236 (2011).

## Metallic glasses

# Local differences

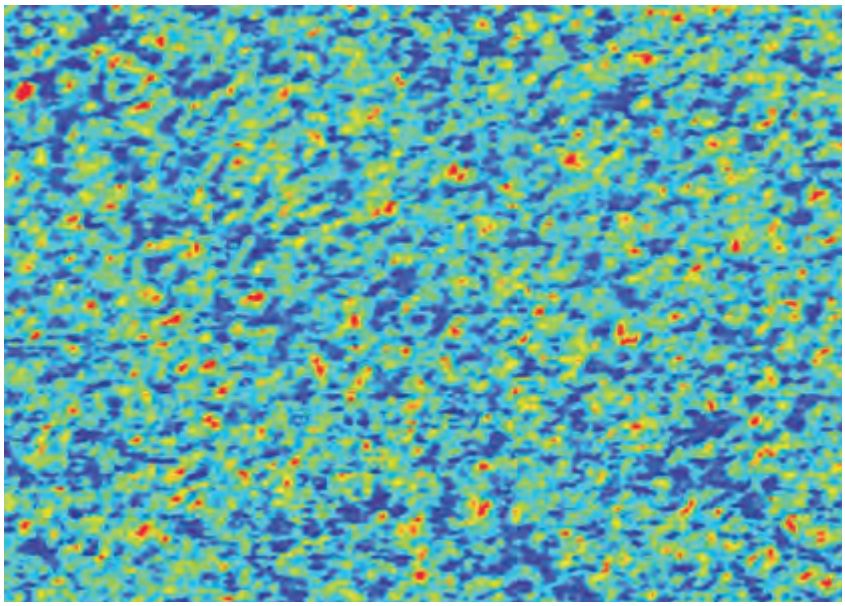
Nanoscale variations in the viscoelasticity of metallic glasses can help explain how they form and break

Most metals are crystalline in structure, with their constituent atoms arranged in a regular pattern. Amorphous or glass-like metals, on the other hand, have little or no atomic ordering, and thus have several advantages over crystalline metals. For example, they can be easily softened and shaped, and are often stronger and more deformable than a crystalline metal with the same composition.

Metallic glasses are formed by cooling a hot metallic melt fast enough to prevent its atoms from rearranging to form a crystal. They are highly conductive, like regular metals, but also exhibit enhanced strength and viscoelasticity. Although metallic glasses have been studied for decades, the initial idea that their properties are homogeneous has recently shifted towards heterogeneity at the nanoscale. Now, Mingwei Chen, Yanhui Liu and colleagues at the WPI-AIMR and the Institute for Materials Research at Tohoku University have characterized the nanoscale elastic properties of metallic glasses[1].

The researchers used radiofrequency magnetron sputtering to form an atomically flat, 2 μm-thick film composed of the metals zirconium, copper, nickel and aluminum, and also showed the film to have a glassy structure.

The researchers then studied its surface using a technique previously developed by Ken Nakajima and Toshio Nishi — members of the research team — for polymeric materials, but they found that it was also suitable for metallic glasses. The technique involves moving a vibrating cantilever with a sharp tip, whose apex is just 1 nanometer in radius, across the surface of the metallic glass film. The tip interacts with the surface of the glass, thus allowing the viscoelasticity-induced energy dissipation of the material underneath the tip to be calculated from the phase change of the tip vibration. In addition, the topography of the glass surface is measured at the same time.





Plot of the phase changes seen as a nanoscale tip is moved over the surface of a metallic glass, giving an indication of variations in the surface's viscoelasticity. The width of the image is around 200 nanometers.

Chen and co-workers found that the viscoelasticity of their metallic glass film was not uniform, but instead varied by around 10% over distances of 3 nanometers (see image).

In comparison, the same variation in film height occurred over distances of around 9 nanometers. The difference between these two numbers supports the interpretation that the phase data reflects inherent viscoelasticity, and is not related to surface roughness.

Heterogeneous viscoelasticity suggests that there are regions of the metallic glass that are more loosely packed than others, which may help scientists to understand how metallic glasses break and form. Regions of higher viscoelasticity, for example, are expected to deform more strongly under applied mechanical stress.

"Our data bridges the gap between atomic modeling and macroscopic models of metallic glasses," says Chen. "In particular, it may help us understand how metallic glasses undergo the transition to liquid-like phases."

1. Liu, Y. H., Wang, D., Nakajima, K., Zhang, W., Hirata, A., Nishi, T., Inoue, A. & Chen, M. W. Characterization of nanoscale mechanical heterogeneity in a metallic glass by dynamic force microscopy. *Physical Review Letters* **106,** 125504 (2011).

## Magnetic memory

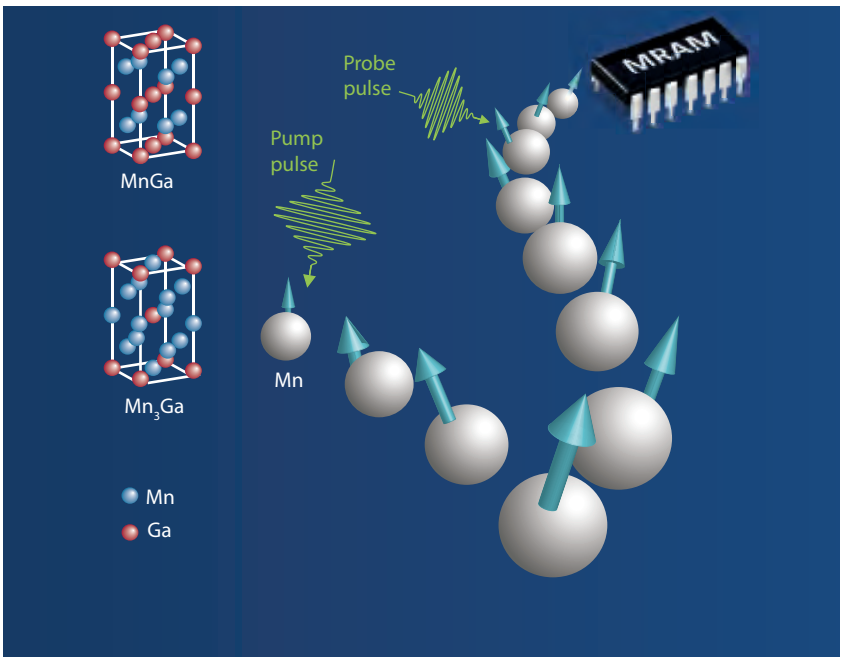
# Less friction, lower power

A manganese–gallium alloy offers the perfect combination of properties for future magnetic memory

Magnetic materials continue to be the dominant storage system for computers. The continuing demand for increased storage densities has resulted in ever-smaller magnetic bits, but as the bits become smaller, the long-term stability of the stored data begins to suffer. In the search for novel materials with enhanced long-term magnetic stability, a team led by researchers from the WPI-AIMR[1] has now discovered that an alloy of manganese and gallium is not only a strong magnet but also has switchable magnetization with low loss — a key requirement for fast, low-power non-volatile magnetic memory.

There are two important requirements for magnetic memory. One is the stability of the magnetic orientation of a domain, a property known as magnetic anisotropy. High magnetic anisotropy is needed to ensure that information, in the form of magnetic orientation, can be retained. The other property is magnetic friction, which describes the losses associated when changes are made to the magnetization direction. "The larger the magnetic friction, the higher the electric power required to record digital information," explains Shigemi Mizukami from the research team.

Similar to any other friction process, magnetic friction can be measured through the slowing of motion. Here, it is the slowing of the precession of magnetization around an axis, similar to the movement of a spinning top when knocked off center (see image). And like spinning tops, this magnetic precession can be set in motion through an external force — in this case by an ultrashort laser pulse. The slowdown of the precession after a given amount of time can be probed by a second laser pulse, which allows the magnetic friction coefficient to be calculated.




The slowdown of spin precession (blue arrows) of manganese atoms in a manganese–gallium (Mn–Ga) alloy can be pumped and probed with two ultrashort laser pulses. The low magnetic friction and high magnetic anisotropy of this alloy may lead to the next generation of computer memory.

So far, all materials with high magnetic anisotropy had also shown a large magnetic friction coefficient. For these manganese–gallium alloys, however, the researchers found the magnetic friction to be surprisingly low.

Theoretical calculations indicate that this reduced friction is caused by a very low density of available electronic states at the topmost electron energies in the material. This means simply that there are relatively few empty states available for electrons to move into as a consequence of magnetic scattering, creating a bottleneck through which magnetic friction is suppressed. This discovery offers unique promise for future magnetic random-access memory devices.

"Other than this alloy, there are no magnetic materials that show both low magnetic friction and high magnetic anisotropy," comments Mizukami. "This combination of properties will be key in developing a replacement for existing computer memories."

1. Mizukami, S., Wu, F., Sakuma, A., Walowski, J., Watanabe, D., Kubota, T., Zhang, X., Naganuma, H., Oogane, M., Ando, Y. & Miyazaki, T. Long-lived ultrafast spin precession in manganese alloys films with a large perpendicular magnetic anisotropy. *Physical Review Letters* **106**, 117201 (2011).

## Nanomaterials

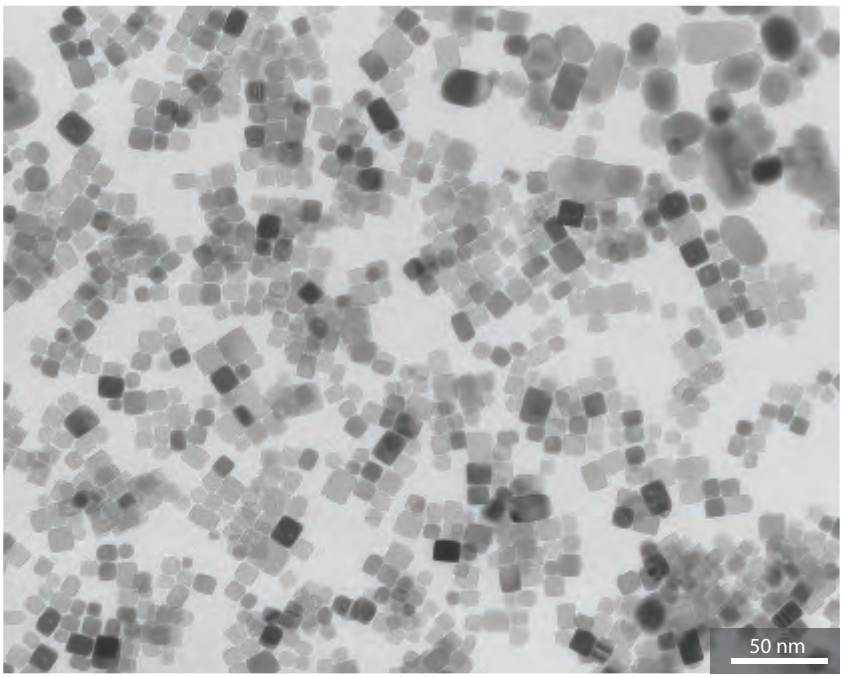
# Cool cubes for catalytic converters

Cerium oxide 'nanocubes' that store more oxygen at lower working temperatures promise to make automobile emissions cleaner

Out of the array of rare earths and precious metals that fill automobile catalytic converters, a compound known as cerium oxide ($CeO_2$) plays a special role. The amount of oxygen inside an engine's combustion chamber determines the amount and composition of emissions that result from burning gasoline. Because $CeO_2$ can both take in and release oxygen atoms without decomposing, this material is critical in balancing oxygen within the catalytic converter to bring emissions to their lowest levels possible. The emission-cleaning capacity of the bulky $CeO_2$ crystals currently used in catalytic converters, however, is held back by the limited amount of oxygen that can be stored on their surfaces.

Now, using organic molecules to precisely control $CeO_2$ crystal growth, Tadafumi Adschiri from the WPI-AIMR and co-workers have prepared $CeO_2$ 'nanocubes' that display almost triple the oxygen storage capacity of typical $CeO_2$ crystals[1].

To produce these unique box-shaped crystals, the team turned to a technique known as supercritical hydrothermal synthesis. First, a $CeO_2$ precursor, a short hydrocarbon chain and a water solvent were locked together in a pressure-resistant chamber and then heated to 400 °C. At supercritical temperature and pressure conditions, the organic molecules mix homogenously with the metal centers in aqueous solution, and attach to the most reactive faces of small $CeO_2$ crystals, hindering growth in that direction. Transmission electron microscopy showed that this method generated distinct $CeO_2$ cubes less than ten nanometers across (see image). Testing the oxygen storage capacity of the ultrasmall cubes revealed surprising temperature-dependent properties.






Transmission electron microscopy image of 10 nanometer-wide $CeO_2$ nanocubes

Whereas conventional irregular-shaped $CeO_2$ crystals only take in oxygen when heated to 400 °C, Adschiri's nanocubes adsorbed significant amounts of oxygen at a much lower 150 °C, indicating a much higher catalytic activity.

"Oxygen storage capacity is directly related to the mobility of oxygen in a material," says Adschiri.

Normally, metal oxides need high temperatures to make oxygen atoms travel through their crystal framework. But because the $CeO_2$ nanocubes exhibit high mobility at lower temperatures, these compounds could potentially clean up emissions over a wider range of operating conditions. This could be a boon for vehicles and reduce the amount of precious metals used for catalytic emission cleaning.

Adschiri notes that controlling the growth of crystals by manipulating their exposed surfaces is the key to tuning the catalytic activity of $CeO_2$. The researchers are now exploring how other capping molecules and different supercritical reactions conditions can lead to completely new methodologies for catalyst fabrication.

1. Zhang, J., Kumagai, H., Yamamura, K., Ohara, S., Takami, S., Morikawa, A., Shinjoh, H., Kaneko, K., Adschiri, T. & Suda, A. Extra-low-temperature oxygen storage capacity of $CeO_2$ nanocrystals with cubic facets. *Nano Letters* **11**, 361–364 (2011).

## Sustainable chemistry

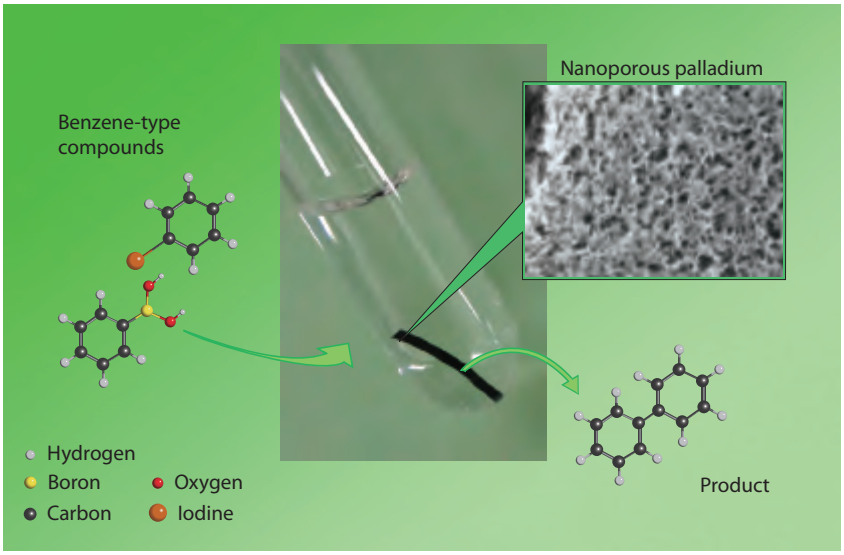
# Made of greener stuff

Fabricating catalysts into robust, nanoporous metallic glasses eliminates leaching problems during carbon coupling reactions

Convincing two organic molecules to connect through the formation of a carbon–carbon bond is never straightforward. The discovery that precious metals such as palladium can catalyze precisely such coupling reactions under mild conditions led to revolutionary advances in a range of fields, including the synthesis of pharmaceuticals and organic semiconductors. Unfortunately, palladium catalysts are toxic, expensive and difficult to separate completely from the final product. Handling issues can be circumvented through the use of a solid support, but gradual leaching of the metal into the surrounding solution can contaminate reactions.

Naoki Asao, Yoshinori Yamamoto and colleagues from the WPI-AIMR at Tohoku University[1] have now developed a solid palladium-based 'metallic glass' that can repeatedly catalyze carbon coupling reactions with negligible leaching of the catalyst into the solvent. And thanks to an electrochemical fabrication technique that permeates the metallic glass with a uniform, nanoporous framework, the team's recyclable catalyst shows excellent activity. Together, these two developments represent critical improvements for industries facing demands for safer, more sustainable chemical procedures.

Metallic glasses are stiff, strong alloys made by quickly cooling a mixture of atoms — in this case palladium, nickel and phosphorus — into an amorphous solid. The very dense packing of atoms in these materials affords them high resiliency, but the bulk metallic glasses are not catalytically active because only a small proportion of palladium atoms are sufficiently exposed to interact with organic reagents. The team solved this problem by exploiting one of the 'noble' properties of palladium metals — a strong resistance to electrical corrosion. Asao explains that dipping a palladium–nickel–phosphorus metallic glass into an electrochemical etching solution dissolves the nickel and phosphorus atoms, while the palladium atoms agglomerate into a clustered, three-dimensional network. Due to the homogenous composition of the initial alloy, the resulting catalyst has a uniform distribution of pores of about 30 nanometers in diameter.




A nanoporous palladium material (center) that catalyzes coupling reactions between benzene-type compounds can be used many times without breaking down or losing activity

When the team performed a typical coupling reaction between two benzene rings bearing iodine and boron functional groups, they saw that the nanoporous catalyst gave the desired product in close to maximum yield (see image). Even after reusing the catalyst four times, the coupling proceeded extremely efficiently.

Further analyses also revealed that the amount of palladium lost into solution during the reaction was less than 0.0005% of the precious metal in each cycle.

"Contamination with palladium must be avoided, especially when the products are medicines," says Yamamoto. "Our results demonstrate one way to solve the leaching problem, and give us hope that more innovations are possible, allowing nanoporous palladium to be developed as a robust 'green' catalyst."

1. Tanaka, S., Kaneko, T., Asao, N., Yamamoto, Y., Chen, M., Zhang, W. & Inoue, A. A nanostructured skeleton catalyst: Suzuki-coupling with a reusable and sustainable nanoporous metallic glass Pd-catalyst. *Chemical Communications* **47**, 5985–5987 (2011).

## Spin electronics

# Magnetism under control

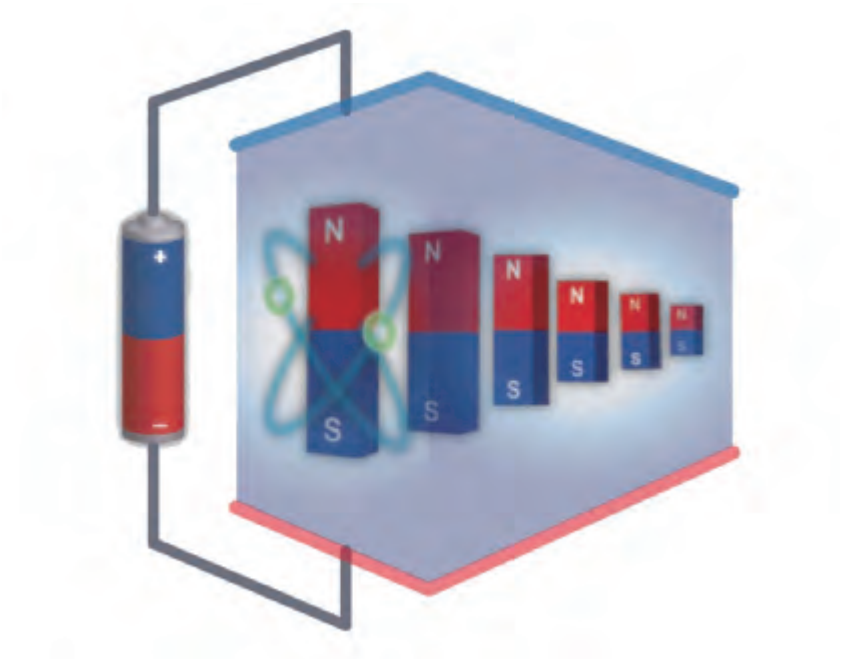
A switchable magnetic semiconductor that operates at room temperature could lead to enhanced electronic devices

The ability to switch the magnetic properties or electron 'spin' of a semiconductor in a similar way to charge in conventional devices opens up new possibilities for fast, low-power data storage and 'spintronics' applications. The magnetic semiconductor materials needed for such applications at room temperature, however, have proved elusive as most magnets are either metals or insulators. Now, researchers from the WPI-AIMR in collaboration with colleagues from the University of Tokyo have developed a magnetic semiconductor system with controllable ferromagnetism at room temperature[1].

The compound studied — titanium dioxide containing a small amount of the magnetic element cobalt — has previously been suggested by some of the same researchers to be ferromagnetic at room temperature. "We have now unambiguously demonstrated not only that titanium cobalt dioxide is a ferromagnetic semiconductor, but also that it can be used for transistors using switchable ferromagnetism," says Masashi Kawasaki from the research team.

The researchers achieved control of the magnetic properties of the material by modulating the density of electrons it contains: an accumulation of electrical charge enhances its magnetic properties, while the depletion of charge turns the magnetization off (see image). In previous studies, injecting sufficient charge into the material to drive this switching functionality had met with limited success because the voltages required were too high, destroying the sample.

To achieve high charge concentrations, the researchers used a recently developed approach that involves delivering electrical charge into the material using a liquid electrolyte rather than by the solid-state capacitor used previously. Such electrolytes are known to carry large quantities of charge, which has led to their use for electrical energy storage in applications such as supercapacitors in electrical cars. The use of a liquid electrolyte resulted in a system for which only a few volts were needed to switch the magnetism of titanium cobalt dioxide on and off.




Electrical charge induces magnetism in the semiconductor titanium cobalt dioxide

The development of a magnetic semiconductor providing switchable magnetic properties at room temperature offers intriguing possibilities for high-performance devices that use not only the charge of an electron but also its 'spin' or magnetic properties. Although the use of a liquid electrolyte has its practical limitations and cannot, for example, be integrated easily on computer chips, Kawasaki is confident such hurdles can be overcome. "There are two possibilities. One is to search for a more practical way of switching, and the other to look for applications where liquids are suitable. The important point is that we know that switching can be achieved in the first place."

1. Yamada, Y., Ueno, K., Fukumura, T., Yuan, H. T., Shimotani, H., Iwasa, Y., Gu, L., Tsukimoto, S., Ikuhara, Y. & Kawasaki, M. Electrically induced ferromagnetism at room temperature in cobalt-doped titanium dioxide. *Science* **332**, 1065–1067 (2011).

## Single-molecule spectroscopy

# A new gold standard?

Thin wrinkled sheets of nanoporous gold make particularly suitable surfaces for single-molecule detection

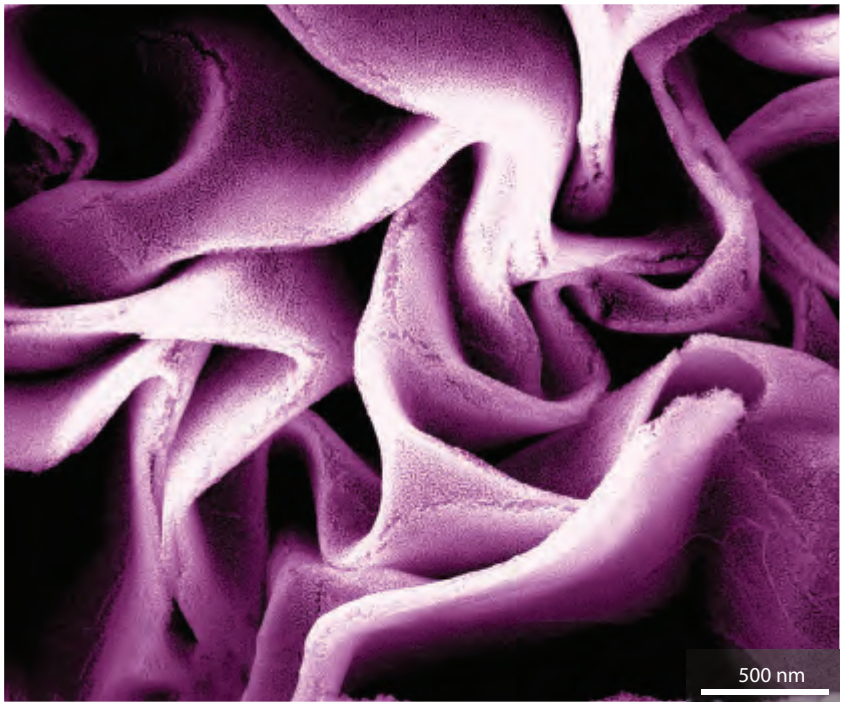
Wrinkly films of nanoporous gold just 100 nanometers thick make an excellent surface for ultra-high sensitivity chemical diagnostics, a team of WPI-AIMR researchers led by Mingwei Chen has shown[1]. The nanoporous surface allows even a single molecule of an analyte to be detected using a technique known as surface-enhanced Raman spectroscopy (SERS).

Raman spectroscopy takes advantage of the fact that many molecules interact with light and scatter it in a characteristic way. Because different molecules scatter light at different wavelengths, the technique can be used to identify an unknown chemical. For many molecules, however, the scattering effect is very weak, which means that the scattered light is extremely difficult to detect.

The nanoporous gold surface prepared by Chen and his colleagues amplifies the Raman effect to an extent that SERS can be used to detect the presence of single molecules. Other SERS substrates with this capability have been prepared in the past, but they tend to have drawbacks such as low stability or poor reproducibility. "In our research, we developed a controllable method to fabricate large-scale, stable and reproducible SERS substrates," says Ling Zhang, a postdoctoral fellow of the research team.

To fabricate their wrinkled gold substrate, the researchers attached flat gold sheets with nano-sized pores onto a pre-strained polymer substrate. Heating caused the polymer to shrink, which in turn caused the overlying nanoporous layer of gold to wrinkle up (see image).

Different wrinkle structures were obtained by varying the size of the nanopores, with the best results obtained using 26-nanometer holes.






A scanning electron microscopy image of the wrinkled Raman-active gold surface

Key to the Raman-enhancing effect of the gold surface is the way that its three-dimensional wrinkled texture interacts with light. The nanogaps formed on the wrinkled surface allow light to induce collective oscillations of electrons at particular points or 'hotspots' on the surface by an effect known as surface plasmon resonance. The plasmonic effect is known to amplify the Raman scattering signals of nearby molecules on the surface, but this is the first time that such a plasmonic-based surface has been produced reliably.

The local SERS enhancement factor at 'hotspots' on the wrinkled gold surface can be larger than 100 million, the researchers showed. "This is comparable to the best Raman-active nanomaterials and enables single-molecule detection," says Chen.

The team is continuing work to improve the performance of their gold surface for practical analytical chemistry applications. "We are now optimizing the chemical composition and structure of the wrinkled films to further increase the density and local enhancement factors of the 'hot spots'," says Chen.

1. Zhang, L., Lang, X., Hirata, A., & Chen, M. Wrinkled nanoporous gold films with ultrahigh surface-enhanced raman scattering enhancement. *ACS Nano* **5**, 4407–4413 (2011).

## Superconductors

# Dirac cones come in pairs

The superconductor compounds known as pnictides have a double Dirac cone energy structure that dramatically affects their magneto-transport properties

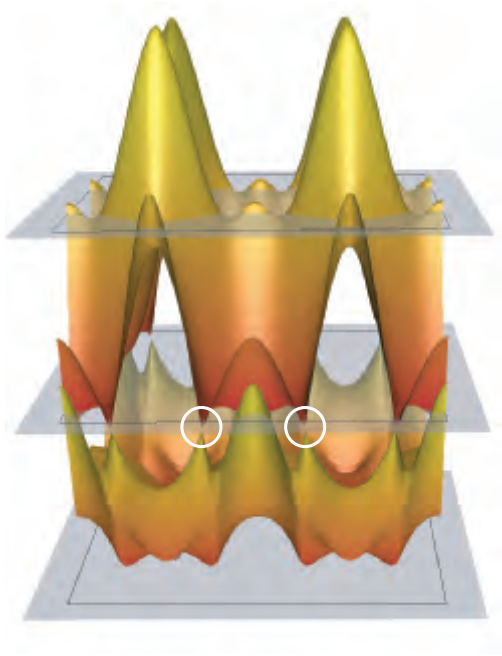
The Dirac cone is a surface that describes in theoretical terms the unusual electron transport properties of materials like graphene and the even newer class of materials known as topological insulators. Scientists can both predict and measure the existence of a Dirac cone from the relationship between electron energy and momentum, and through such studies have confirmed that the class of iron-based superconductor compounds known as pnictides have this characteristic energy structure. Katsumi Tanigaki and colleagues from the WPI-AIMR and Tohoku University have now demonstrated the effect that such Dirac cones can have on the electron transport properties of these materials[1].

The researchers investigated samples of the pnictide $Ba(FeAs)_2$. There is a fundamental difference between the Dirac cones of the pnictides and graphene, however. "The Dirac-cone state of graphene derives from a single 'π-electron' band, while the Dirac-cone states of $Ba(FeAs)_2$ are made from multiple '*d*-electron' bands," explains Tanigaki.

This multi-band origin creates a greater chance for the development of a more versatile Dirac-cone structure (see image), depending on the material.

The main observable effect of a Dirac cone is a linear relationship between resistance and applied magnetic field, or magnetoresistance, above a certain 'crossover field', below which the relationship is parabolic. These curves can be well explained using existing models as due to the effect of Landau level splitting.

Under a magnetic field, the electron energy is split into Landau levels, the lowest of which exhibits linear behavior, similar to the feature described by the Dirac cone. On increasing the magnetic field, the level splitting increases and all of the electrons move to this lowest level, which makes the magnetoresistance effect linear. Importantly, this should occur at magnetic fields easily accessible using existing magnets.



Electronic band structure of $Ba(FeAs)_2$, showing the Dirac cones (circles)

A crucial conclusion that can be drawn from the detailed analysis of the data is that the observed magnetoresistance must be caused by a combination of two Dirac cones, one for electrons and also one for their opposite number, holes — a finding that had not been anticipated.

Tanigaki believes that the results could be important for superconductivity, as engineering the compounds to enhance the contribution of Dirac cones could lead to superconductors that operate at higher temperature.

There could also be practical consequences. "High-mobility field-effective transistors are made using superlattice structures in III-V semiconductors. However, we can hope in the future that high-mobility transistors can also be constructed from compounds with Dirac-cone states," says Tanigaki. The observed linear magnetoresistance could also lead to highly sensitive magnetic field sensors.

1. Huynh, K. K., Tanabe, Y. & Tanigaki, K. Both electron and hole Dirac cone states in $Ba(FeAs)_2$ confirmed by magnetoresistance. *Physical Review Letters* **106,** 217004 (2011).

## Superconductors

# Taking charge of the future

A fundamentally new way to search for superconductivity using ionic liquids could lead to the discovery of entirely new classes of superconductors

Since the discovery of superconductivity more than a hundred years ago, new superconductors have typically been discovered by looking for new compounds that, when cooled to extremely low temperatures, show a vanishing electrical resistance. Masashi Kawasaki and colleagues from the WPI-AIMR in collaboration with researchers from the University of Tokyo have now devised an entirely new way of searching for superconductors — by artificially introducing large amounts of electrical charges into known materials[1]. Using the approach, the researchers have discovered superconductivity in the compound potassium tantalum oxide ($KTaO_3$).

Superconductivity arises from a pairing of electrons in a material, which makes them immune to external disturbances such as scattering off atoms in the crystal. Given this key role of free electrons, many materials could be made to superconduct by introducing a surplus of free electrons by chemical 'doping'. Unfortunately, however, there are constraints on the maximum charge that can be introduced in this way.

The alternative developed by Kawasaki and his co-workers is to introduce the electrons externally. This can be done through the use of an ionic liquid, which is able to transport large amounts of charge. By bringing the ionic liquid into contact with the surface of an electrical circuit containing the material (see image), an electric double layer is formed at the material–liquid interface. Applying an electrical voltage then separates the charges. On lowering the temperature, the researchers found that the compound, in this case $KTaO_3$, transformed from its original insulating state into a semiconductor, a metallic conductor and eventually a superconductor.



Photograph of the electric double layer transistor with a drop of ionic liquid for testing for superconductivity in $KTaO_3$

"Through this ionic liquid-based method, we achieved a charge density in the material about ten times higher than that achievable by conventional methods," says Kawasaki.

Superconductivity had not previously been observed in $KTaO_3$, and although the phenomenon was observed at very low temperature, the appearance of superconductivity is only possible because of the high electrical charge densities. The real potential of this new technique therefore lies in the discovery that superconductivity can be induced in materials under circumstances not investigated previously. "We do not have the same limitations as with chemical doping," comments Kawasaki. "There are many compounds that could become superconducting by providing sufficient charge carriers but which have not been examined yet."

In particular, while the discovery of superconductivity in $KTaO_3$ is exciting in itself, the approach used to make the discovery is more exciting for its potential to uncover superconductivity at higher temperatures than achieved so far.

1. Ueno, K., Nakamura, S., Shimotani, H., Yuan, H. T., Kimura, N., Nojima, T., Aoki, H., Iwasa, Y. & Kawasaki, M. Discovery of superconductivity in $KTaO_3$ by electrostatic carrier doping. *Nature Nanotechnology* **6**, 408–412 (2011).

## Photovoltaics

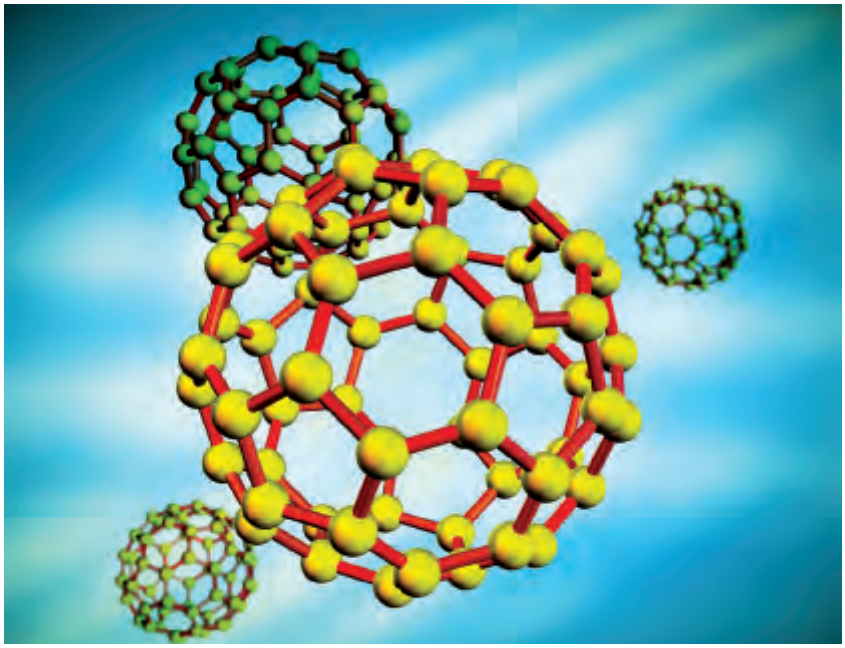
# Making light work of organic solar cells

A novel method for producing functionalized fullerenes could lead to lower-cost organic solar cells

With growing demand for renewable energy sources, devising new methods to improve the efficiency of photovoltaic materials is a key challenge in the production of next-generation solar cells based on organic materials rather than silicon. A team led by Tienan Jin from the WPI-AIMR in collaboration with researchers from China have now developed a novel strategy to produce organic solar cells using functionalized carbon 'fullerenes' with high yield and at low cost[1].

Photovoltaic cells generate electricity from light based on a system of charge transfer between electron donor and acceptor molecules. Fullerenes — soccer ball-like spheres of carbon atoms — are widely used as an acceptor molecule in organic solar cells in the form of phenyl-$C_{61}$-butyric acid methyl ester (PCBM), but this complex molecule is expensive to make and attempts to reduce production costs have so far met with limited success. Jin and his co-workers turned to the naturally occurring fullerene $C_{60}$ as a lower-cost alternative to the $C_{61}$ derivative. Functionalizing $C_{60}$ to achieve the same level of electron acceptor performance, however, required the development of a new synthesis strategy.

The researchers functionalized the $C_{60}$ fullerene (pictured) by grafting on alkyl chains. This type of modification has been performed in the past using magnesium- or lithium-based reagents, but these reactions often result in over-alkylation. Milder, more selective conditions are needed to produce the mono-functionalized fullerenes that are most suitable for use in organic solar cells. "We have previously developed a number of transition metal-catalyzed molecular transformations at carbon–carbon multiple bonds, so we investigated whether we could functionalize $C_{60}$ in the same way," explains Jin.



$C_{60}$ is a spherical form of carbon that can be functionalized for use in photovoltaic applications

After an exhaustive search of possible catalysts and reaction conditions, the researchers found that a cobalt-based compound was the most efficient catalyst for this grafting reaction. Adding the $C_{60}$ and an alkyl halide compound to a solution of the cobalt catalyst and a manganese reducing agent gave the mono-alkylated $C_{60}$ fullerenes in 88% yield in 2 days. Using this efficient procedure, Jin and his colleagues were able to produce fullerenes bearing a zinc porphyrin, a branch-like dendrimer, and even another fullerene to afford a fullerene dimer or 'dumbbell' — all of which are difficult to synthesize by previous methods.

A simple organic solar cell with a bulk heterojunction structure constructed using the new fullerene derivatives achieved higher solar-to-electricity conversion efficiency than a comparable device prepared using the conventional PCBM electron acceptor. "Based on this promising result, we plan to design and synthesize other new fullerene derivatives with possible photovoltaic applications," says Jin.

1. Lu, S., Jin, T., Bao, M. & Yamamoto, Y. Cobalt-catalyzed hydroalkylation of [60] fullerene with active alkyl bromides: selective synthesis of monoalkylated fullerenes. *Journal of the American Chemical Society* **133**, 12842–12848 (2011).

## Catalysis

# A tale of two metals

A nanoporous palladium-nickel catalyst shows promise for improved catalytic performance in fuel cell applications

Platinum-based materials are traditionally the catalysts of choice for incorporation in fuel cells. In recent years, however, palladium-based materials including bimetallic alloys have become more attractive due to their high electrocatalytic activity in key oxidation and reduction reactions.

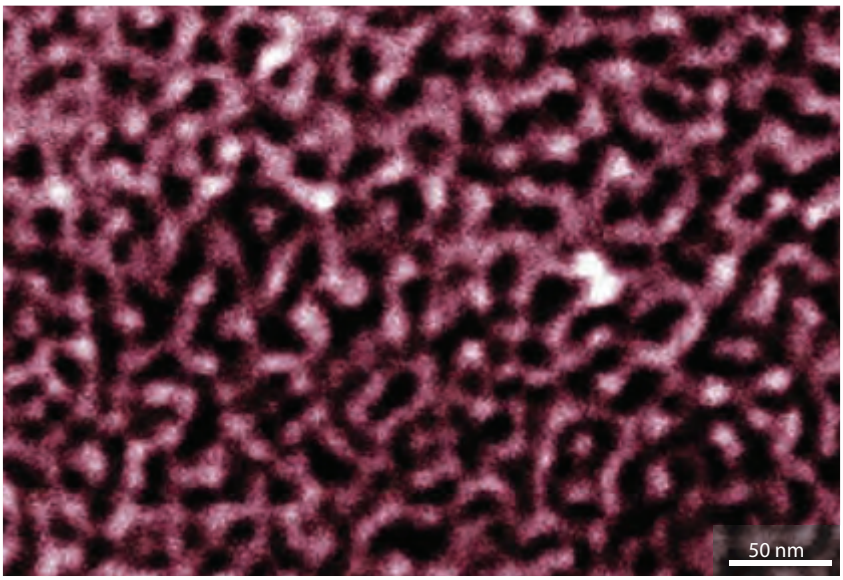
On the nanoscale, catalysts formed from palladium or platinum nanoparticles have shown high performance owing to their large surface areas and outstanding mechanical and electrical properties.

Mingwei Chen at the WPI-AIMR at Tohoku University, Japan, and colleagues have now prepared a bulk palladium-nickel alloy with a nanoporous structure that combines some of these advantages to produce an easily recyclable, low-cost and high-performance catalyst[1].

In a series of electrochemical studies, they have demonstrated that their novel nanoporous Pd–Ni alloy (np-PdNi) is a superior catalyst for small molecule electro-oxidation and oxygen reduction reactions.

The np-PdNi material is made by electrochemically dealloying a $Pd_{20}Ni_{80}$ bimetallic alloy in a sulfuric acid solution. Nickel partially leaches out of the alloy through control of the etching potentials. The structure of np-PdNi comprises crystalline metallic ligaments and nanoporous channels in a bicontinuous arrangement (see image).

A combination of X-ray photoelectron spectroscopy and ion etching techniques reveals that the distribution of nickel within the metallic ligaments varies depending on depth — the core is nickel-rich, whereas the shell is palladium-rich.




A scanning electron microscopy image of the nanoporous PdNi alloys

For the electro-oxidation reactions of methanol or formic acid, np-PdNi shows a higher catalytic activity than nanoporous pure palladium and commercial nanoparticulate Pd–C catalysts.

In addition, the onset potential for catalytic activity is more negative for np-PdNi than for nanoporous Pd, which implies that the kinetics of the electro-oxidation reaction are enhanced.

The np-PdNi material also exhibits excellent electrochemical stability — after 500 cycles of the electro-oxidation of methanol, the loss of electrocatalytic activity is only around 8%, a better result than that of commercial Pd–C catalysts.

"The current catalytic performance of the np-PdNi in the oxygen reduction reaction is just comparable to commercial platinum catalysts," says Chen. "In the future, we need to further optimize the morphology and composition of the np-PdNi to improve catalytic performance so that it surpasses the expensive platinum catalyst."

Potential applications of the material include the development of various green energy devices, including commercial fuel cells, hydrogen sensors and nanostructured electrodes.

Chen and his co-workers are currently investigating how the control of dealloying potentials and alteration of the alloy precursors could be further extended to make an even wider range of nanoporous materials with compositions that can be finely tuned.

1. Chen, L., Guo, H., Fujita, T., Hirata, A, Zhang, W., Inoue, A. & Chen, M. Nanoporous PdNi bimetallic catalyst with enhanced electrocatalytic performances for electro-oxidation and oxygen reduction reactions. *Advanced Functional Materials* Published online: 8 Sep 2011

## Oxide interfaces

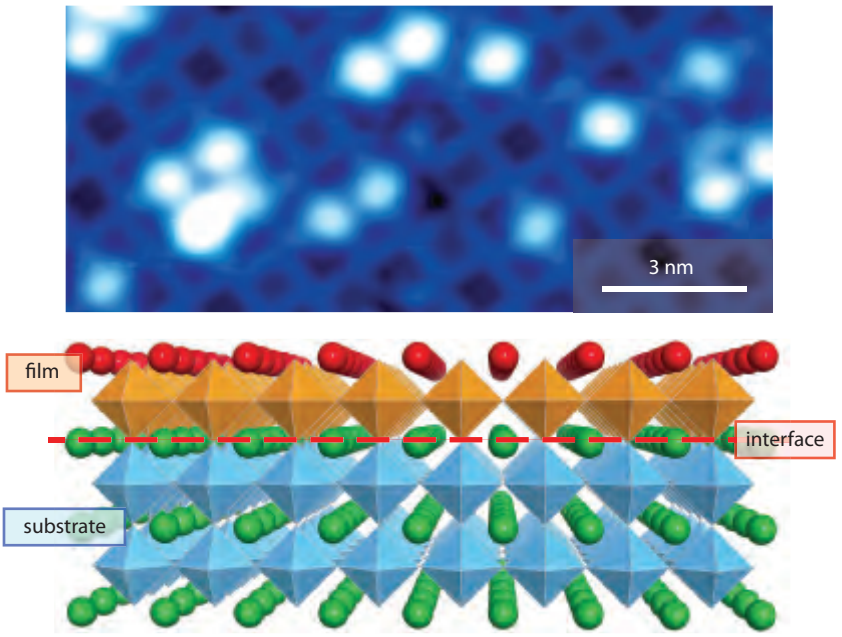
# One atom at a time

Scanning tunneling microscopy reveals unique insights into the atom-by-atom growth of transition metal oxides on substrates

The combination of two similar objects has the potential to create a completely different material. In recent years, the heterostructures of transition metal oxides have demonstrated a range of surprising properties, such as the interface between lanthanum aluminate and strontium titanate. Both materials are insulators in their bulk form, yet also show very high conductivity and under certain conditions can even become superconductive. Given the wide range of compositions these oxides can span, it is expected that more functionalities can be discovered — and possibly used in devices — through judicious combinations. But to achieve this, it is essential to understand and control the morphology and electronic structure of the interfaces at the atomic scale. So far, however, interface formation has been mainly studied at the unit-cell level.

Ryota Shimizu, Taro Hitosugi and colleagues at the WPI-AIMR at Tohoku University and other institutions in Japan have now zoned in on atom-by-atom growth through their construction of a high-resolution scanning tunneling microscopy combined with a pulsed laser deposition system[1]. This device enabled the team to closely investigate the formation of very thin strontium titanate films at atomic resolution[2].

The researchers began their investigation with the homo-epitaxial atom-by-atom growth process of a perovskite material, strontium titanate. Using pulsed laser deposition, they grew a strontium titanate film on a substrate of the same material that has a specific perfectly ordered structure. "We found that this specific surface can be prepared in a wide range of oxygen partial pressures in a reproducible manner. This is why strontium titanate is an ideal substrate to serve as a model, which will then enable us to monitor at the atomic level the growth processes of perovskite oxides more generally," explains Shimizu.






A typical scanning tunneling microscopy image acquired on the strontium titanate surface (top) and a schematic model of an interface composed of perovskite oxides (bottom)

After the films were grown, the team observed the formation of island terraces with an atomic structure identical to that of the substrate. In particular, the results showed atomic-level coherency between the substrate and the thin film, whereby the substrate imposed its morphology on the newly grown film.

The results offer potential growth for other materials as well. "Our team is now conducting growths of other oxide materials, such as strontium oxide, lanthanum aluminate and manganite, to unveil the growth process and interfacial formation between different materials at the atomic scale," says Shimizu. "These investigations may lead to the preparation of new heterostructures, or high quality thin films with exotic multifunctionality."

1. Iwaya, K., Shimizu, R., Hashizume, T. & Hitosugi, T. Systematic analyses of vibration noise of a vibration isolation system for high-resolution scanning tunneling microscopes. *Review of Scientific Instruments* **82**, 083702 (2011).

2. Shimizu, R., Iwaya, K., Ohsawa, T., Shiraki, S., Hasegawa, T., Hashizume, T. & Hitosugi, T. Atomic-scale visualization of initial growth of homoepitaxial $SrTiO_3$ thin film on atomically ordered substrate. *ACS Nano* **5**, 7967 (2011).

## Nanoclusters

# Steel that breaks the rules

Atomic imaging of nanoclusters gives greater insight into the remarkable strength and durability of strengthened steel

Following recent events, such as the nuclear accident at the Fukushima nuclear power plant triggered by the 2011 Tohoku earthquake, worldwide pressure is mounting to develop safer nuclear power facilities. The search is on for stronger, more durable materials with which to build structures that are able to endure extremely harsh or toxic environments. Some of the most promising candidates are 'oxide-dispersion-strengthened' (ODS) steels. These ODS steels contain tiny nanoclusters within a steel matrix, and show an outstanding resistance to radiation damage and high temperatures — yet little is known about the internal atomic structures of these nanoclusters.

Using the latest microscopy technology, Mingwei Chen and Akihiko Hirata, together with colleagues at the WPI-AIMR at Tohoku University, Japan and the City University of Hong Kong, have now analyzed the atomic structures of oxide nanoclusters less than 4 nanometers in size found in ODS steels (see image), and have uncovered some surprising results[1].

"We recognized that understanding the atomic structure of the nanoclusters is the most important task in the research of ODS steels," explains Chen. "This underlying crystal structure plays a crucial part in the amazing strength of these materials in harsh environments."

The researchers used Cs-corrected scanning transmission electron microscopy, with a resolution of about 0.1 nanometers, to identify complex atomic structures within the tiny oxide nanoclusters. The high level of magnetism present in the steels represented a challenge. "The magnetic steel matrix makes it difficult to image the clusters," explains Chen. "We minimized the magnetic effect by carefully preparing ultra-thin samples about 5 nanometers thick."

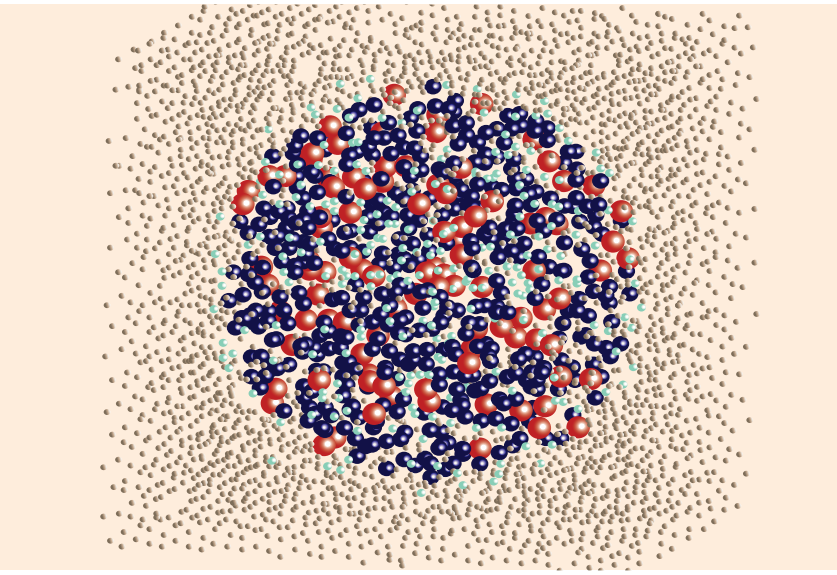




Illustration of an oxide nanocluster in oxide-dispersion-strengthened steel. Defects in the nanocluster crystal structure might increase affinity with the steel matrix, resulting in the material's remarkable strength and durability.

Perhaps the most surprising result from the study is that the nanoclusters have very defective rock salt crystal (NaCl-type) structures, yet are incredibly stable at high temperatures. "This is a pretty interesting phenomenon," states Chen. "We know from thermodynamics that, in perfect crystal structures, lower total energy leads to a more stable phase. However, the nanoclusters in the ODS steels appear to show the opposite."

The data revealed that the atomic structure of small nanoclusters and larger nanoparticles present in the ODS steels both featured NaCl-like structures, but with important differences. "The unstable, coarsened nanoparticles possess a near perfect crystal structure, whereas the stable nanoclusters have a very defective one with a high percentage of vacancies," explains Chen.

The researchers believe that the defective structure might encourage greater affinity between the nanoclusters and the steel matrix, increasing overall stability under high temperatures and neutron radiation. The team intends to further examine other nano-strengthened steels in the near future.

1. Hirata, A., Fujita, T., Wen, Y. R., Schneibel, J. H., Liu, C. T., & Chen, M. W. Atomic structure of nanoclusters in oxide-dispersion-strengthened steels. *Nature Materials* DOI 10.1038/NMAT3150 (2011).

## Micromirrors

# Metallic glasses begin to shine

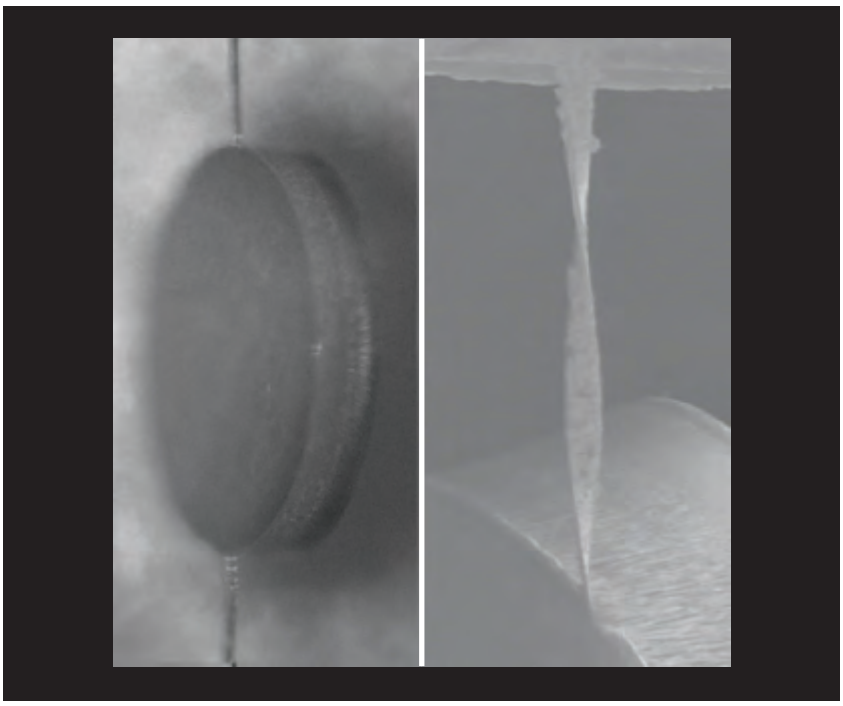
The mechanical strength of metallic glasses makes them ideal components for micromechanical devices, such as rotating mirrors

Silicon is traditionally the material of choice in micromechanical innovations. Complex sculptures are now fabricated onto silicon chips for new types of microscale devices, tiny silicon cantilevers are widely used as acceleration sensors, and micromirrors can be used to scan a light source across a larger area, such as in laser projectors or in endoscopes. The brittleness of silicon, however, limits the possible range of its applications.

Jae-Wung Lee, Yu-Ching Lin and colleagues from the WPI-AIMR in collaboration with researchers from other institutions in Japan and Germany, have now used hard metallic glasses as a tougher alternative to silicon in the development of enhanced micromirrors[1].

Although they look like any other metal, metallic glasses are not very different in structure from ordinary window glass. Unlike crystals, which have an ordered structure, the atoms of metallic glasses are randomly arranged, making them much stronger than silicon, or even some steels. They can bear heavier loads without starting to deform, and are thus ideal for micromechanical devices in which small components are repeatedly subjected to strong forces. Even after many operating cycles, metallic glasses remain largely intact.

The research team constructed a mirror structure by placing a round plate between two torsion bars that form the axis for the mirror's movements (see image). The torsion bars are entirely made of metallic glass, while the plate is a metallic glass film stabilized by a silicon frame. The glasses' composition included substantial iron content to give magnetic properties. "This makes it possible to actuate the mirror by an external magnetic field, which simplifies the design and fabrication process of the micromirror," explains Yu-Ching Lin.





Turning metallic glass mirrors. The mirror surface and torsion axes are fabricated from a single metallic glass film, with the mirror film supported by silicon. The photos show the turning mirror (left) along with a close-up of the torsion axis (right).

The metallic glass has good elasticity and strength, allowing the mirror to reach large tilting angles. When in resonance with an oscillating external magnetic field, the mirrors followed the field and rotated more than 300 times per second without undergoing any damage. Tilt angles of over 70 degrees were demonstrated in this dynamic mode, and in larger static magnetic fields, the mirrors reached up to 270 degrees. However, further development is needed.

"Many compatible micromechanical fabrication techniques for metallic glasses are still missing," says Lin. "Our next attempt is to develop etching technologies for metallic glasses to realize smaller and more versatile patterns." But with such unique mechanical properties, metallic glasses are poised to play a more significant role in micromechanical devices in the future.

1. Lee, J.-W. Lin, Y.-C., Kaushik, N., Sharma, P., Makino, A., Inoue, A., Esashi, M. & Gessner, T. Micromirror with large-tilting angle using Fe-based metallic glass. *Optics Letters* **36**, 3464-3466 (2011).

# IN THE SPOTLIGHT

The WPI-AIMR has grown rapidly since its inauguration in 2007, now with over 120 leading researchers from all over the world, including 31 internationally renowned principal investigators who are charged with pioneering new and innovative breakthroughs in materials science. The institute is also active in developing young, promising researchers with a focus on strong cross-disciplinary collaboration and creativity. AIM*Research* spotlights these talented researchers of the present and future, detailing their daily research activities and scientific ambitions.

INTERVIEW WITH DIRECTOR AND DEPUTY DIRECTOR

Published online 30 January 2012

# Materials research like none other

*Current WPI-AIMR director Yoshinori Yamamoto and deputy director Motoko Kotani reflect on the challenges faced by the institute to date, and share their vision on the institute's next stage of development.*

*The WPI-AIMR recently celebrated its fourth anniversary. What are the most notable research achievements made at the institute since it opened?*

**Yamamoto:** The WPI-AIMR gathers a wide variety of world-class researchers under one roof to carry out cutting-edge research across a range of topics in materials science, and we have published a large number of papers in leading international journals. However, there are some discoveries that particularly stand out. For example, one of our young assistant professors, Seigo Souma, who works in Takashi Takahashi's group, has recently made an extremely important breakthrough in pure research in understanding the mechanism that underpins the phenomenon of high-temperature superconductivity (HTSC). At the WPI-AIMR, we have built the highest resolution Angle-Resolved Photoelectron Spectroscopy (ARPES) set-up in the world, and Souma and his team have used this to establish the important role that electron spin plays in HTSC. Another noteworthy result is the discovery of new materials by Terunobu Miyazaki's group which can be applied to so-called 'normally-off' computers. As you know, conventional computers have to be switched on all the time to work, but as their name suggests, normally-off computers only draw power when it is absolutely necessary for memory operations. It is expected that these normally-off computers will consume up to 70% less power than existing machines.

Current director Yoshinori Yamamoto (left) and deputy director Motoko Kotani (right) discuss the past challenges and achievements of WPI-AIMR and the future direction of the institute.

*Earlier this year the Mathematics Group, under the direction of Professor Kotani, was added to the existing four research divisions at the WPI-AIMR. How is the new group developing and how is it expected to change the way the institute operates?*

**Kotani:** The Mathematics Group is already working actively with colleagues in other groups, such as the Applied Mathematics Forum at Tohoku University. We will soon have three principal investigators, including myself, as well as two associate professors and three assistant professors, and our plan is to eventually add postdoctoral researchers and PhD students who will use mathematics to better explain the theoretical underpinning of the experimental work carried out at the institute. We hope that analyzing materials science at the most fundamental level will allow us to predict the future direction projects should follow to get the best results in the most efficient way possible.

**Yamamoto:** A good example is Seigo Souma's work on HTSC. The standard approach for this application would be to carry out various trial-and-error experiments and gradually move towards more efficient superconductors. However, this can be an unreliable, expensive and time-consuming approach. If we can increase the accuracy of our theoretical models for HTSC, it may help us to focus on higher-performing systems that would otherwise take us much longer to find.

*The WPI-AIMR actively pursues new approaches to create a world-class research environment. What steps have been taken to achieve this and what challenges have you faced along the way?*

**Yamamoto:** Creating the right sort of research environment is probably the biggest challenge we have ever faced. One of the most concrete examples is the magnificent new research facility we are now sitting in. Having all of our researchers here under one roof is vital for carrying out 'fusion' research.

**Kotani:** Our plan for the new building was to feature at the very heart of the design the idea of encouraging free discussion

Current director, Yoshinori Yamamoto

Incoming director, Motoko Kotani

and exchange. This is reflected in the open-plan areas where researchers can meet and talk informally over coffee, but with a whiteboard in reach to aid discussion. In many Japanese universities, this kind of informal meeting area is often considered a waste of valuable space, but for us it is an indispensible part of the research environment. Cultivating a new kind of fusion research culture that can lead to new breakthroughs and also challenge the status quo in Japanese universities is one of the central aims of the WPI program as a whole, and as such it is vital to our success as an institution.

**Yamamoto:** Another big challenge we have faced is how to create an environment that is welcoming to overseas researchers. We have implemented a number of initiatives to help our non-Japanese staff and students. For example, we have adopted English as the official working language within the center to enable easier communication. We are also building a new international house for foreign students and staff.

**Kotani:** Currently we are focusing on personalizing administrative support at the WPI-AIMR. Previously it was difficult for our researchers to find out whom to approach for assistance, so now we are ensuring that the roles of support staff will be more clearly delineated and identifiable.

*How was the WPI-AIMR affected by the 2011 Tohoku earthquake and how well is it recovering?*

**Yamamoto:** The earthquake caused widespread devastation and loss of life in the Sendai area and the wider Tohoku region. Immediately after the earthquake, we briefly halted operations to check the damage and ensure the safety of our staff and students. Some of our overseas members returned temporarily to their home countries; however, we were able to reassemble most of the teams within a few weeks after the disaster and return to work, although severe aftershocks continued for several weeks. Whilst the actual buildings of the institute escaped largely unscathed, some of the facilities and equipment were severely damaged.

**Kotani:** Despite the heavy financial burden from the earthquake, we were determined to minimize its effect on our research output. We had to think creatively about how we could best use the equipment that was still intact, for example, by learning to use our equipment in new ways. Some staff took the opportunity to focus on analyzing existing data and writing up papers while they were waiting for equipment to be repaired or replaced. As a center, we felt a very strong sense of responsibility to people in the Tohoku region to play our part in the rebuilding effort, and the best way we could do that was to continue our research.

*Next year the WPI-AIMR will have new leadership as Professor Kotani takes over as director of the institute. What plans does the WPI-AIMR have for expansion in the next 5 years?*

**Yamamoto:** The institute will probably remain at its current size of about 200 members. However, we still have to focus on developing the WPI-AIMR so that it can influence our university and others in Japan. Institutions in East Asia need to rethink their approach to learning and research in order to compete with those in the USA and Europe. To address this issue, we aim to set up institutions that will help transform the research culture of Japanese universities.

**Kotani:** Our overarching research theme at WPI-AIMR will be "Building the future through materials". We will also increasingly use mathematics to improve the accuracy and reliability of our theoretical models, and to improve the predictability and efficiency of our experimental work. Through this WPI-AIMR will become an unprecedented model of research institute which combines mathematics and materials sciences. Going forward, I want the WPI-AIMR to become a center like no other in the world, one that attracts the very best and most ambitious researchers from across the globe to develop new materials that, rather than simply fulfilling a need, actually change the way we look at the world around us. ■

The new WPI-AIMR Main Building

ROUNDTABLE INTERVIEW

Published online 26 September 2011

# Tearing down the walls of research

*Researchers at the WPI-AIMR share their perspectives on the benefits of cross-disciplinary collaboration and discuss some of the latest advances in the design of novel hybrid metal catalysts and green technology applications.*

As the technologies of the future become more elaborate and more reliant on the convergence of multiple, often wildly dissimilar fields of research, substantiating such cross-disciplinary collaboration as an integral part of the research culture has become more important than ever. Bringing together researchers from vastly different scientific backgrounds to work together effectively on the type of 'fusion' research that can lead to the next great innovation, however, requires more than casual collaboration.

When it was established in 2007, the WPI-AIMR at Tohoku University set out specifically to nurture fusion research on innovative functional materials by adopting an organizational and research structure that makes interdisciplinary collaboration a natural part of the work environment. After four years and a total of 44 fusion research projects, the institute's reputation for innovative, cross-disciplinary materials-oriented research extends across the globe, attracting some of the world's leading researchers in materials science.

From left to right: Naoki Asao, Takeshi Fujita, Hongwen Liu, Koji Nakayama

## Close-knit network of researchers

The WPI-AIMR is now home to 119 researchers, about half of whom are from countries other than Japan, and many resolved to join the institute specifically because of its emphasis on innovative interdisciplinary research. "The fusion research we are carrying out here is creating completely new research fields, so it is much more than just simple collaboration," says Naoki Asao, a professor at the WPI-AIMR's Soft Materials Group since 2009. Asao carries out fusion research aimed at developing nanostructured hybrid metal catalysts. "Before coming to the WPI-AIMR, I had never heard of nanoporous materials during my career in synthetic chemistry," he says. The opportunity to collaborate with Mingwei Chen, principal investigator of the Bulk Metallic Glasses (BMG) Group, however, has enabled Asao to hone his expertise in the production of nanoporous gold based on a process known as dealloying. The procedure involves treating a gold–silver alloy with nitric acid that selectively removes silver, leaving behind a nanoporous gold structure. Due to its remarkably high specific surface area, nanoporous gold is a material of emerging interest for the development of novel catalytic and sensor applications.

Most fusion research projects at the WPI-AIMR benefit from seed funding for one year, and the institute is rare in its provision of financial funding for such short projects. "This type of financial support allows younger researchers to concentrate on their projects without expending vast amounts of time and energy applying for research grants, thereby simplifying the whole procedure," says Hongwen Liu, an assistant professor in the Materials Physics Group. Liu is currently developing plasmonic substrates that increase the

efficiency of opto-electrical conversion. "I feel very fortunate to be working in an environment where the barriers that normally exist between fields are broken down, which allows younger researchers like myself to work on truly cutting-edge projects," she says.

Fusion research enables researchers not only to learn about new scientific developments outside of their respective fields, but also to gain a fresh perspective on their own work. "When I joined the WPI-AIMR's BMG Group after completing my PhD in nanotechnology, I had to approach metallic glasses from a physics point of view," says Koji Nakayama, an associate professor of the BMG Group. Nakayama conducts research on the controlled fabrication of metallic glass nanofibers based on noble metals, which are characterized by exceptionally high damage tolerance. "In many ways, my time at the WPI-AIMR from the very start has been one ongoing fusion project," he says.

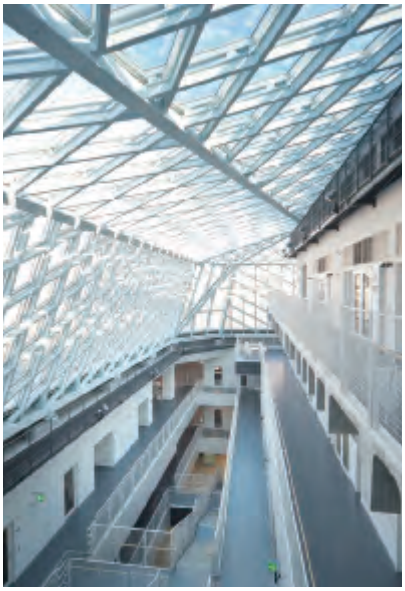
The WPI-AIMR's emphasis on maintaining open channels of communication encourages researchers to learn from others and lend a helping hand to colleagues and young researchers in particular. Takeshi Fujita, an associate professor in the BMG Group, notes, "A postgraduate student working on soft matter recently asked me about using nanoporous gold as a cell substrate. I was happy to assist because manufacturing nanoporous gold is my specialty."

To facilitate the exchange of ideas among its researchers, the WPI-AIMR hosts seminars on a regular basis, and every week holds a 'Tea Time' event designed to spark lively scientific discussion in an informal setting. "These events not only encourage us to learn about what other people are doing, but also open our minds to other research fields," says Liu. "If I ever go back to China, I would like to hold similar events for the benefit of my students and colleagues."

## Taking the green approach

With increasing demand for clean energy, the WPI-AIMR is intensifying its focus on developing innovative 'green' materials, such as reusable catalysts, solar cells and sustainable engineering solutions based on organic chemistry. Nakayama explains, "Green activities in Japan used to be concerned with how we can save the environment, but now they are more focused on how renewable energy devices such as solar cells with improved efficiency can be developed through materials science."

Researchers at WPI-AIMR's 'Tea Time' event in August



The recently opened WPI-AIMR Main Building

Advances in nanotechnology, for example, are rapidly driving the development of next-generation charge-storage devices that improve on the performance of traditional lithium-ion batteries. Fujita, who has been investigating the electrical storage capabilities of supercapacitors using transition metal compounds, says, "We are aiming to develop a new type of battery that can be charged quickly using solar cells and which in the future may be compatible for use in mobile phones and electric cars."

The WPI-AIMR's commitment to developing new forms of green innovation with a global outlook was reinforced by the 'Cutting-edge Functional Materials for Green Innovation' workshop held in February 2011, which attracted many internationally renowned materials scientists from the Asia-Pacific, Europe and North America.

By bridging the disciplines of materials science, physics, chemistry, biotechnology and engineering, the WPI-AIMR not only provides a unique environment that nurtures the development of breakthrough technologies, but also continues to promote international joint research projects and multidisciplinary exchange through its satellite centers and network of 19 overseas collaborative research institutions. ■

INTERNATIONAL WORKSHOP

Published online 25 April 2011

# Green innovation in the limelight

*The 4th WPI-AIMR Annual Workshop was held in Sendai, Japan on 21–24 February 2011 drawing an international audience.*

The WPI-AIMR Annual Workshop, held on 21–24 February 2011 in Sendai, Japan, amid brilliant late winter sunshine, is a central part of academic life at the WPI-AIMR, providing a forum for members of the institute to meet as a body with other top-level researchers from around the world to discuss the state-of-the-art of materials science, establish research contacts and plan for the future.

In 2011, the workshop — the fourth since the establishment of the WPI-AIMR at Tohoku University — was convened at the Sendai International Center under the banner of 'Cutting-edge Functional Materials for Green Innovation', drawing more than 220 participants from 41 organizations in 10 countries, including many senior and internationally renowned materials scientists from the Asia-Pacific, Europe and North America.

Speaking to AIM*Research* on the eve of the workshop, WPI-AIMR director Yoshinori Yamamoto looked forward to a lively and constructive meeting and outlined his plans for the forward development of the institute, including the further development of links with leading international institutions such as the University of Cambridge in the UK and advancing the agenda of green innovation at the WPI-AIMR. Yamamoto maintained this theme in his welcoming address to the workshop participants, recalling the progress made by the institute's researchers in further developing fusion research and placing green innovation squarely at the heart of the work of the institute.


Georg Bednorz

"There is no doubt that creating new functional materials for green innovation leading to the development of green materials needs the approach of fusion research," he said. Following this, in his opening remarks Tohoku University president Akihisa Inoue congratulated the WPI-AIMR on their "tremendous efforts in advancing fusion research to create new research disciplines" and noted the importance in this endeavor of the network developed between the WPI-AIMR and its 22 partner institutions, which includes three satellite centers located around the world. This international outlook is manifested by the large number of non-Japanese researchers at the WPI-AIMR — just over half of the current total of 128 come from outside of Japan.

Inoue also spoke of his high expectations for the key part that the WPI-AIMR will play in realizing his eponymous development plan for Tohoku University, which he introduced in 2007. Describing the institute as a "locomotive for reinforcing the research foundations of Tohoku University as a research-intensive university," Inoue praised the WPI-AIMR strategy of developing green innovation for the benefit of society, calling the initiative "timely." This message was reinforced by Toshio Kuroki, the WPI program director, in his welcoming address to the conference, calling upon the WPI-AIMR to become "a frontrunner for materials science research by creating new materials for a future society."

Sendai International Center

## Special lectures

Following the opening session, the academic program of the conference commenced with a special first session composed of three lectures on a diverse series of cutting-edge topics delivered by a trio of particularly highly acclaimed materials science researchers. In the first of these, Georg Bednorz from IBM Research Zürich, who shared the 1987 Nobel Prize in Physics, addressed the conference on the latest developments in superconductivity. Bednorz noted that 2011 is the 100th anniversary of the discovery of the phenomenon of superconductivity, and went on to describe recent developments in high-temperature superconductivity, an area that has witnessed a dramatic rise in importance in the last quarter century to the point

Peter Grünberg

that it has now become a key technology for ensuring reliable, environmentally friendly and efficient energy use.

A neat counterpoint to the opening lecture was given by the 2007 Physics Nobel Laureate Peter Grünberg from the Jülich Research Centre in Germany, who spoke on the use of giant magnetoresistance and its potential to address problems of world energy. This was the second contribution made by Grünberg, who had earlier entertained participants as part of a musical ensemble that played a selection of Japanese and Austrian folk melodies at the pre-conference wine mixer on the previous night. The special session was rounded off by carbon nanotube pioneer Sumio Iijima, Professor of Meijo University as well as WPI-AIMR Adjunct Professor, who reported on the current state-of-the-art in the industrial production and applications of carbon nanotubes and graphene. The theme of the closing lecture was on one of the most pressing issues in materials science research and took on even greater significance in the context of the awarding of the 2010 Nobel Prize in Physics for pioneering work in the field of graphene research.

### Plenary lectures

The academic program also boasted 20 plenary lectures given by leading international materials scientists, including members of WPI-AIMR overseas satellite centers, as well as other presentations delivered in six parallel sessions. As in previous years, the lecture program was supplemented by a poster session that drew over 80 contributions on a wide variety of topics over the first two days of the meeting. The research presented during the three days of the 4th WPI-AIMR Annual Workshop encompassed a diverse range of topics including bulk metallic glasses, materials physics, soft materials and device/system construction. In so doing it reflected the wide-ranging research remit of the center and further reinforced the workshop as a key event in the annual WPI-AIMR calendar. ■

Sumio Iijima

## FEATURED RESEARCHERS

Published online 25 July 2011

# Fusion research abounds with infinite possibilities

*Recently appointed WPI-AIMR deputy director Motoko Kotani plans to use the power of mathematics to accelerate fusion research between the institute's various research groups.*

In any walk of life, communication matters, and science is no exception. So when one of the leading experts in the world in mathematics — a field that has the power to generate closer communication among scientists from different backgrounds — is brought in to enhance fusion research, good things are bound to happen.

On 1 May 2011, Motoko Kotani, who is a special advisor to Tohoku University president Akihisa Inoue, officially started her tenure as deputy director of the WPI-AIMR. Kotani heads up the newly created Mathematics Unit and has been charged with overseeing research carried out at the WPI-AIMR. This will include the important task of furthering fusion research between the four research groups that make up the institute: the Bulk Metallic Glasses Group, Materials Physics Group, Soft Materials Group and Device/System Group.

Motoko Kotani

An internationally renowned mathematician, Kotani received the prestigious Saruhashi Prize — given to female Japanese scientists for achieving outstanding research results — in 2005 for her research on Discrete Geometric Analysis on Crystal Lattices. When talking about mathematics, Kotani's face becomes animated and her voice takes on a strong, persuasive tone. "Mathematics is appealing because it can break things down to their very essence," she says.

It is this strength that Kotani wants to use to bring researchers from different backgrounds together to work on cross-disciplinary research themes. This can sometimes be a challenge because the principal investigators in each research group speak a distinctive scientific language that is not necessarily easy for others to understand. "That is where we mathematicians come in. We can try to understand the background principles between each scientific field, and then simplify them to create a universal language that is understood by everybody," explains Kotani. "Simple ideas have the ability to inspire others to develop their own thoughts, which is how real fusion research is conducted."

## Opening up communication

Communication is another key element for promoting collaboration. Kotani plans to have researchers in each group conduct introductory seminars and survey talks that give their colleagues a basic understanding of what their field of research is essentially about, rather than the kind of presentations where researchers simply announce their latest findings. Without such activities, Kotani believes that researchers will find it hard to bridge what can be expansive scientific divides.


Kotani brings a wealth of international experience to her role and knows the value of close-knit collaboration. In 1993–1994, she spent a year at the Max Planck Institute in Germany, and in 2000–2001, she spent a year in Paris at the prestigious Institut des Hautes Études Scientifiques (IHÉS), an institute predominantly staffed by overseas researchers who mainly come from a mathematics background, as well as some theoretical physicists and biologists. The spirit of cooperation prevalent at the IHÉS allows researchers to bounce ideas off each other and make breakthroughs in their research—something from which Kotani herself benefited. "At the WPI-AIMR, I would like to create an ideal research environment similar to the one at IHÉS where researchers can freely immerse themselves in their work," says Kotani.

## Supporting women in research

Another goal that Kotani feels passionately about is helping her fellow female researchers. From 2006 to 2008, she was the project leader in the Tohoku Women's Hurdling Project — an initiative established by the Japanese government to 'develop models that support women researchers'. The establishment of such a program is very much in keeping with the strong tradition of promoting female involvement in science at Tohoku University, which in 1913 was the first university in Japan to admit women as undergraduate students.

Today, the university provides researchers with family assistance, including kindergarten and babysitting services. Such facilities are particularly important for female researchers from overseas, who may lack the ability to communicate effectively in Japanese and thus find help on their own. Kotani says she will do her utmost to create a system that allows female researchers to concentrate on their research but also spend time with their family — essential for allowing them to relax and formulate 'wild' ideas. "If you have to worry about your family, you cannot concentrate on your research," she notes.

Establishing an environment in which female researchers find it pleasant to work is also crucial. "If you create an atmosphere that is comfortable for female scientists, it is comfortable for everybody," says Kotani, who is eager to stress that her goal, and that of the university as a whole, is to make the university a top-notch research university that is attractive to men and women alike.

Such ambitions extend not just to researchers from inside Japan but also to those from other countries. Kotani is quick to point out that the WPI-AIMR has much to offer researchers from overseas, including a wealth of opportunities to interact with preeminent scientists from a wide spectrum of disciplines, creating an environment where stimulating ideas are often exchanged. The possibilities for fusion research at the WPI-AIMR, Kotani notes, are practically endless. "We want researchers to think of one and one as not being equal to two — but to infinity," she says. ■


The new WPI-AIMR Main Building incorporates a part of the original building which formerly housed the Department of Metallurgy in the School of Engineering. It promotes collaborative research by bringing together researchers from materials science, physics, chemistry, biotechnology, engineering, and mathematics under one roof.


Advanced Institute for Materials Research
Tohoku University