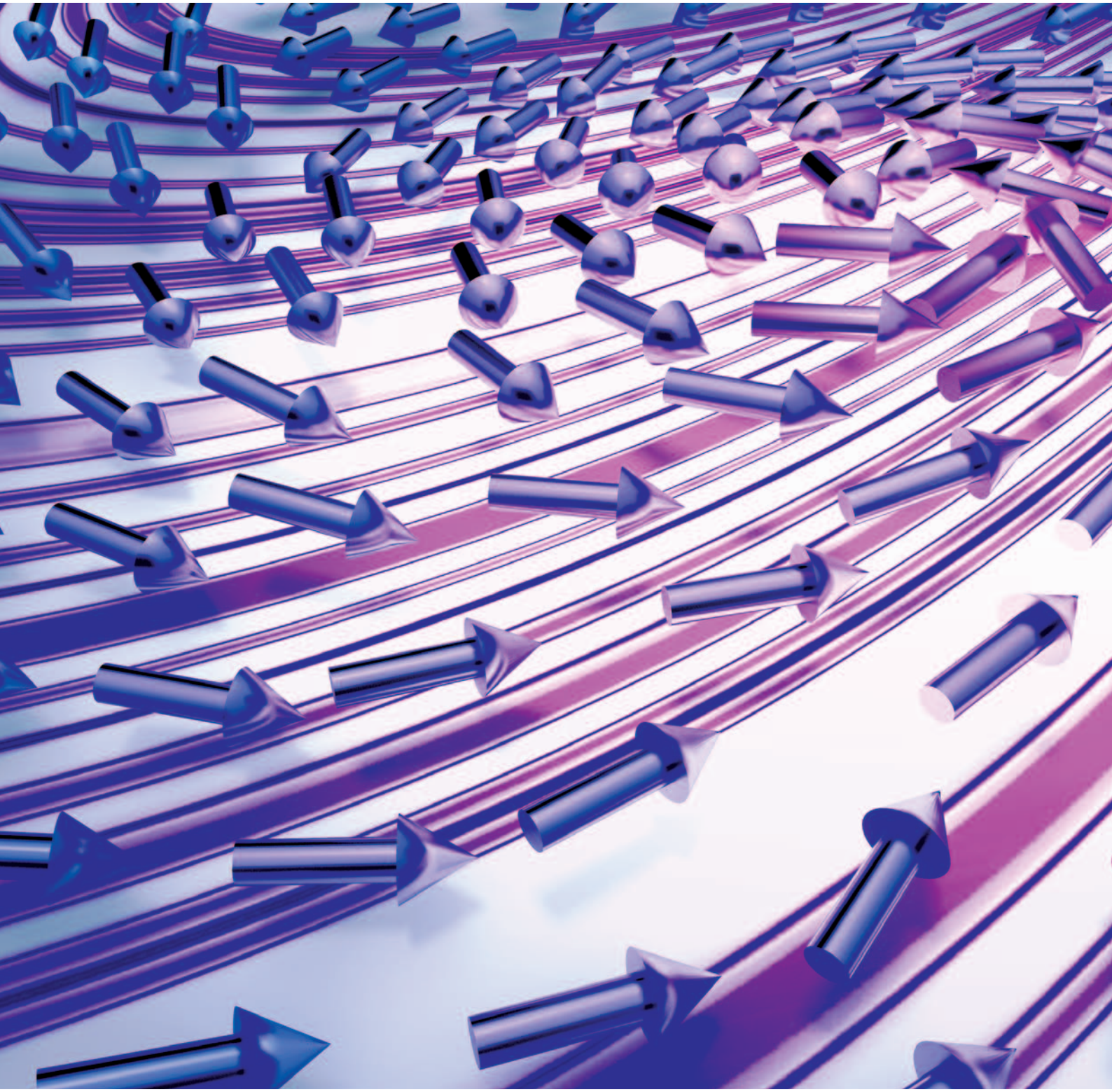
AiM Research

RESEARCH HIGHLIGHTS 2012

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 nine World Premier International Research Center Initiative (WPI) programs established with the support of the Japanese Ministry of Education, Culture, Sport, Science and Technology (MEXT). Since its inauguration in 2007, the 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, Device/Systems — and Mathematics Unit.

Led by distinguished mathematician and Director Motoko Kotani, the institute promotes interdisciplinary research across the different groups while fostering young researchers through 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 AIMR is host to over 130 leading researchers, with around half from abroad, including 32 principal investigators. In addition to the research hub at Tohoku University, the AIMR collaborates with research centers in China, France, Germany, Poland, the UK and the USA. Close ties with other leading overseas institutes 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 AIMR. First published in June 2009, AIM*Research* selects the most important papers from the wealth of research produced by 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 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 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 AIMR.

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AIM*Research* is a publication of the Advanced Institute for Materials Research (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

Integrating mathematics and materials science

As the director of the Advanced Institute for Materials Research (AIMR), Tohoku University, it is my great pleasure to welcome you to the fourth print edition of AIM*Research*: *Research Highlights*. A selection of the AIMR's distinguished research results are published monthly on our website, and this print publication is a collection of those research highlights which appeared in 2012. I hope that this issue will provide you with a comprehensive overview of our research activities, as well as an introduction to some of our researchers, our workshops and our educational opportunities through our In the Spotlight feature articles.

The AIMR was launched in 2007 under the World Premier International Research Center Initiative (WPI) program by the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). True to its name, the program aims to create globally visible research centers within Japan. As one of the WPI research centers, we are taking steps to create an ideal research environment and to become a hub that attracts and circulates the world's best brains in materials science.

Our efforts have succeeded in drawing together an international community dedicated to the advancement of materials science. As of April 2012, overseas researchers made up 55% of all AIMR researchers. With English adopted as the official language and a supportive structure for researchers in both their research and daily lives, we provide an environment in which overseas researchers will thrive and feel at home.

Creating new scientific fields is another important mission of WPI research centers. At the AIMR, we are committed to collaborative and interdisciplinary research beyond conventional ideas, and to this end we are pursuing the following objectives: the elucidation of the fundamental principles underlying the functional properties common to different kinds of materials; the ability to predict new functions and new materials based on these newly established principles; and the creation of "green materials" to contribute to more efficient "energy harvesting" and energy consumption as well as environmental cleanup activities.

Additionally, as the former director, Yoshinori Yamamoto, wrote in the preface to the 2011 AIM*Research* collection, we have established the Mathematics Unit to further promote this interdisciplinary fusion. Since the inauguration of our institute, AIMR materials scientists have observed and controlled atoms and molecules using world-class equipment and have discovered

phenomena for which there are yet no mathematical models. Our collaboration between mathematicians and materials scientists aims to provide new insights for breakthroughs in the understanding of these and other phenomena.

In this, we are at the forefront of a global trend. Although mathematics has a long history of serving as the common language for all scientific fields, direct interaction between mathematics and science and technology has started rather recently and is increasingly recognized as key in this computation age. The AIMR is the world's first organization to have initiated materials science driven by mathematics.

In order to promote the mathematics–materials science collaboration effectively, we have set three target projects: non-equilibrium materials based on mathematical dynamical systems; topological functional materials; and multiscale hierarchical materials based on discrete geometric analysis. These target projects are the result of our efforts to formalize our goals for math–materials science collaborations through joint seminars, Math–Mate Seminars and numerous discussions.

These target projects are now bringing together talented researchers at the AIMR. For active advancement of these projects, project leaders and project subleaders have been appointed in each target project and interdisciplinary teams have been organized including, of course, mathematicians and theorists. (The three target projects and their leadership were the focus of a 2012 In the Spotlight feature article, "Marrying materials with mathematics", appearing on page 35 of this collection.) Research is underway and the project teams have already produced some promising results.

By encouraging talented materials science researchers to

work together in new ways, and by incorporating mathematicians as catalysts, discoveries can progress naturally from basic science to societal applications. I believe that this exciting and challenging avenue of research — integrated mathematics and materials science — will lead to new breakthroughs in materials science at the AIMR.

Motoko Kotani
Director
AIMR

AiM Research

Tohoku University's Advanced Institute for Materials Research (AIMR) promotes fusion research in materials science across disciplinary barriers.

We aim to develop new materials that, rather than simply fulfilling a need, actually change the way we look at the world around us.

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RESEARCH HIGHLIGHTS

The 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 Mathematics Unit further complements the AIMR's research activities.

Thin films

Modulating magnetism

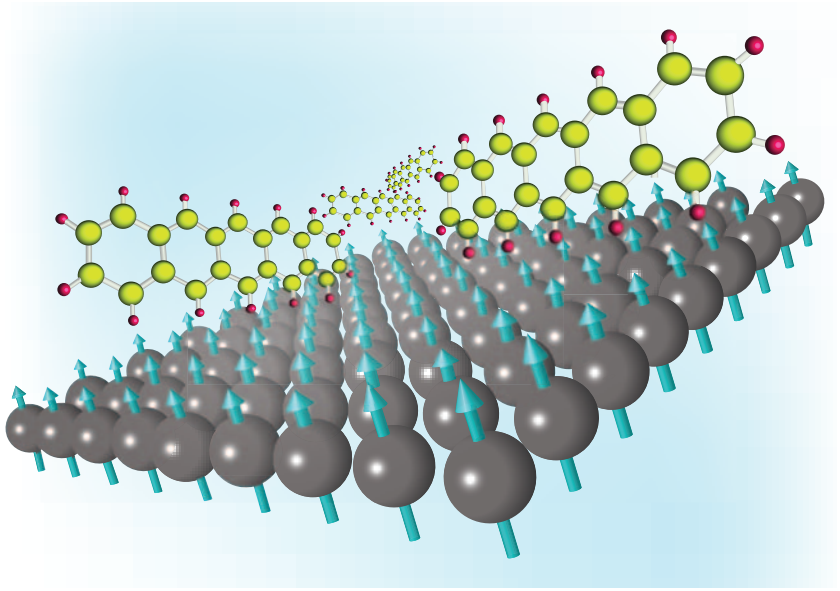
Molecular layers can strongly affect the magnetic properties of cobalt films through interface effects

Thin films of ferromagnetic metals play a pivotal role in a number of spintronics devices by exploiting the spin of electrons as well as their charge. A classic example is a spin valve in which magnetization of the ferromagnetic metal electrode controls the spin of electrical charges.

Perpendicular magnetic anisotropy (PMA) is an essential feature of ferromagnetic thin films which determines the complexity of magnetic switching using an external field. Although molecular layers deposited on ferromagnetic films in organic spin valve devices are known to affect their spin injection and detection efficiency, much less is known about their influence on magnetic properties.

Xianmin Zhang from the AIMR and co-authors at Tohoku University have now demonstrated that capping cobalt thin films with molecular layers can affect their PMA to different degrees depending on the nature of the deposited molecules[1]. The results are important for understanding the fundamental magnetic properties of cobalt films, and are also relevant to spin valves, in which molecular layers used as active elements are placed between electrodes of ferromagnetic metals.

The researchers selected fullerene molecules — hollow, spherical cages composed of sixty carbon atoms — along with the aluminum complex tris(8-hydroxyquinolinato) aluminum, and the linear aromatic molecule pentacene. Molecular layers of varied thickness were applied to cobalt films, and the team measured the magnetization loops of all structures under an external magnetic field positioned either parallel or perpendicular to the film plane.



Schematic representation of a pentacene molecule layer on cobalt film featuring cobalt (gray), carbon (yellow), and hydrogen atoms (red), and spin (denoted with blue arrows).

The data showed a good resemblance between the loops of fullerene and aluminum complex, but a striking difference in the case of pentacene, which exhibited a much higher coercive field of up to 160% more than that of the other two molecules.

Zhang and co-workers believe that the different magnetic behaviour observed is due to a difference in the nature of interactions at the cobalt–molecular layer interfaces, and they intend to conduct further experiments to investigate the origin of these behaviours. As the crystal structure of pentacene deposited on the cobalt film differed from those of the aluminum complex and fullerene, the researchers concluded that both the aluminum complex and fullerene are chemically bound to the cobalt film, whereas pentacene undergoes a process of physical adsorption, a weaker interaction in which the electronic structure of the molecule remains unchanged.

The results are expected to have an important impact on future research. "These findings likely open a new window to further understand the interactions at the interface between ferromagnetic metals and molecules or molecular assemblies, and may contribute to the design of new organic-inorganic hybrid spintronics devices in future," says Zhang.

1. Zhang, X., Mizukami S., Kubota, T., Oogane, M., Naganuma, H., Ando, Y. & Miyazaki, T. Interface effects on perpendicular magnetic anisotropy for molecular-capped cobalt ultrathin films. *Applied Physics Letters* **99**, 162509 (2011).

Structural defects

Know the boundaries

Understanding the basis of atomic defects and impurities offers greater insight into the relationship between the structure and properties of materials

Structural defects play a crucial role in determining the physical and electronic properties of materials, and understanding the nature of these defects is of key importance in correlating the properties of materials with their structure at the atomic level. A thorough understanding of structural defects requires a precise determination of their three-dimensional structure and chemical composition. In polycrystalline materials, this goal is complicated by difficulties in investigating defects occurring at the boundary between adjacent crystals. Now, Zhongchang Wang and Yuichi Ikuhara from the AIMR and other researchers have developed a method for investigating structural defects using a combination of advanced electron microscopy, spectroscopy and first-principles calculations[1].

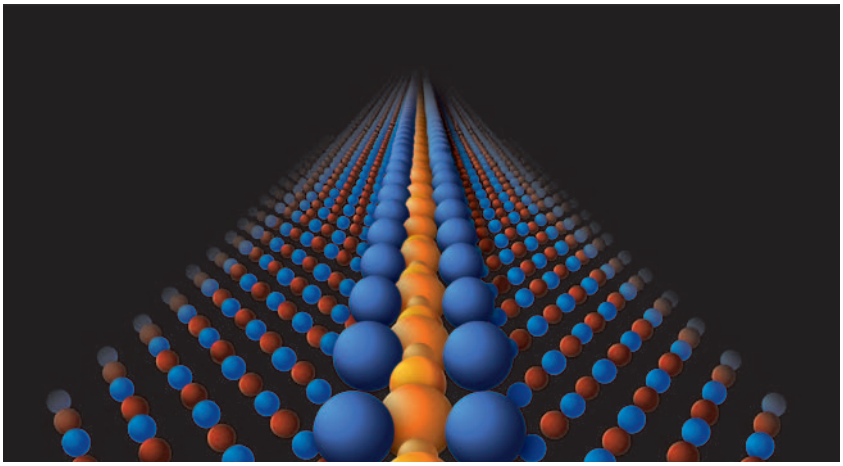


Illustration of an ordered defect superstructure forming at a grain boundary in magnesium oxide. The superstructure consists of oxygen (red); magnesium (small blue spheres); and impurities titanium (large blue spheres), and calcium (orange).

"Natural materials are often polycrystalline and their properties are determined by grain boundaries," explains Ikuhara. Grain boundaries — the interface between two crystallite domains or 'grains' — trap atomic defects such as impurities and vacancies which can induce complex structural changes. However, it is difficult to elucidate the distribution and role of self-trapped grain boundary defects because of their very low concentration, and the lack of chemical information obtained from conventional electron microscopy methods.

To overcome these difficulties, the researchers devised a methodology that combines different scanning transmission electron microscopy techniques, electron energy-loss spectroscopy and high-precision density functional calculations. Furthermore, special care was taken to design an environment for the electron microscope that is free from mechanical vibrations and magnetic fields.

Wang, Ikuhara and colleagues applied the methodology on magnesium oxide, a technologically important material that has been studied for decades, but for which the atomic-scale grain boundary structure has remained unknown. To allow the controlled study of individual grain boundaries, the researchers fabricated a 'bicrystal' consisting of two crystals cut along different crystallographic directions which are joined at their surfaces.

Electron energy loss spectroscopy and transmission electron microscopy measurements revealed that titanium and calcium impurities segregate into the grain boundary. More importantly, these impurities interdisperse into the columns of magnesium oxide atoms, giving rise to a periodic superstructure along an atomically-straight boundary (see image). Comparing the experimental results with the results of the calculations, the researchers were able to pinpoint the structural transformation leading to a stable defect configuration. The analysis further showed that the calcium and titanium are bonded to the oxygen rather than the magnesium atoms.

"This method could in principle be applied to many types of defects in many systems," says Wang. "The main advantage is that the combination of techniques allows extraction of atomic-scale information on point defects in defective regions, and provides insight into the structure-property interplay at the quantum level."

1. Wang, Z., Saito, M., McKenna, K. P., Gu, L., Tsukimoto, S., Shluger, A. L. & Ikuhara, Y. Atom-resolved imaging of ordered defect superstructures at individual grain boundaries. *Nature* **479**, 380 (2011).

Insulators

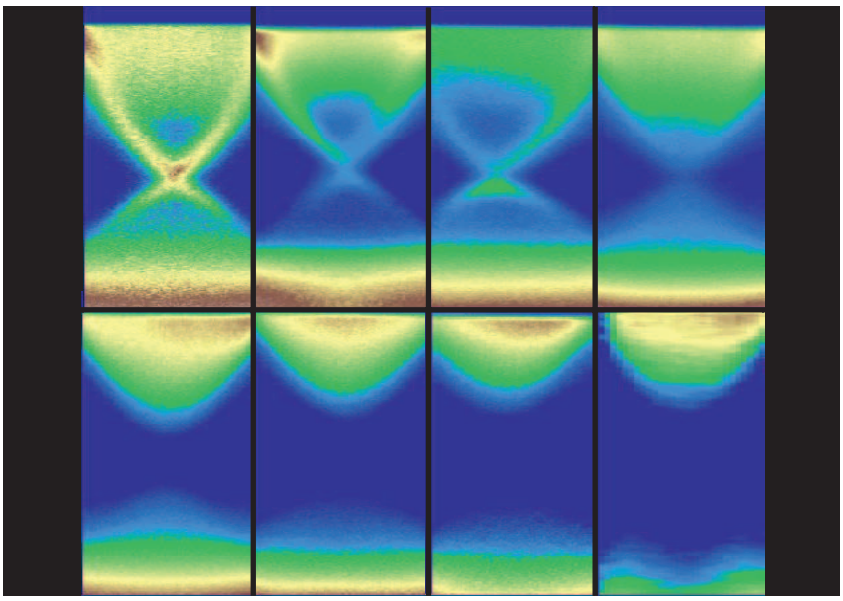
Electrons gaining mass

The potential of electron surface states of topological insulators has now been considerably enhanced by the discovery of surface states with a gap in their energy spectrum

Topological insulators are some of the most promising electronic materials available, because they allow the use of the electron's magnetic property — its spin — for enhanced low-loss computing technology. This advantageous property is based on energy states at the surface, where electrons propagate in a similar way to particles that have no mass. Takashi Takahashi, Seigo Souma and co-workers from the AIMR, with colleagues from Tohoku University's Physics Department and Osaka University, have now made the surprising discovery that in some topological insulators these electrons at the surface state can also show mass, which leads to entirely new effects for spin electronics[1].

The difference between normal electrons and those in the surface states of topological insulators is that the latter show 'time-reversal symmetry', which means, for example, that if the motion of electrons was filmed with a camera, the film would always look the same, whether it is played forwards or backwards. This time-reversal symmetry is at the core of many attractive properties of topological insulators, including their protection against losses. One feature of this symmetry is that the surface energy states show a characteristic X-shape when electron energy is plotted against momentum (see image).

The researchers have now studied how this X-shape evolves in the topological insulator, thallium–bismuth–selenium. The experiments were performed on an angle-resolved photoemission spectrometer at the AIMR, which currently has the highest available energy resolution in the world. During the evolution, selenium atoms are increasingly replaced by sulfur. Because the sulfur analogue, thallium–bismuth–sulfur, is not a topological insulator, the replacement of selenium by sulfur enables the tracking of the transition from a topological insulator to a classical insulator.



From Ref. 1 © 2011 S. Souma

From topological insulator to conventional insulator: the evolution from the topological insulator, thallium–bismuth–selenium (top left), to thallium–bismuth–sulfur (bottom right), shows that the 'X' shape of the surface states is slowly lost, and a gap in the energy states evolves.

With increasing sulfur content, the surface energy states slowly begin to lose their X-shape and a gap opens up in the center of the 'X'. This means that the electrons no longer appear massless. "There are predictions that topological insulators with a gap show a coupling between magnetic and electronic effects, the strength of which is independent of the material," explains Souma. This could be of particular relevance to information storage technologies, because such an effect allows the control of magnetic information with electrical fields.

The present study makes a compelling case for the technological importance of topological insulators, which continue to be one of the most intensively studied materials today. "Our next step will be to study the origin of this energy gap, which remains poorly understood," says Souma, adding that an experimental demonstration of the predicted novel effects will also be important.

1. Sato, T., Segawa, K., Kosaka, K., Souma, S., Nakayama, K., Eto, K., Minami, T., Ando, Y. & Takahashi, T. Unexpected mass acquisition of Dirac fermions at the quantum phase transition of a topological insulator. *Nature Physics* **7**, 840 (2011).

Graphene oxide

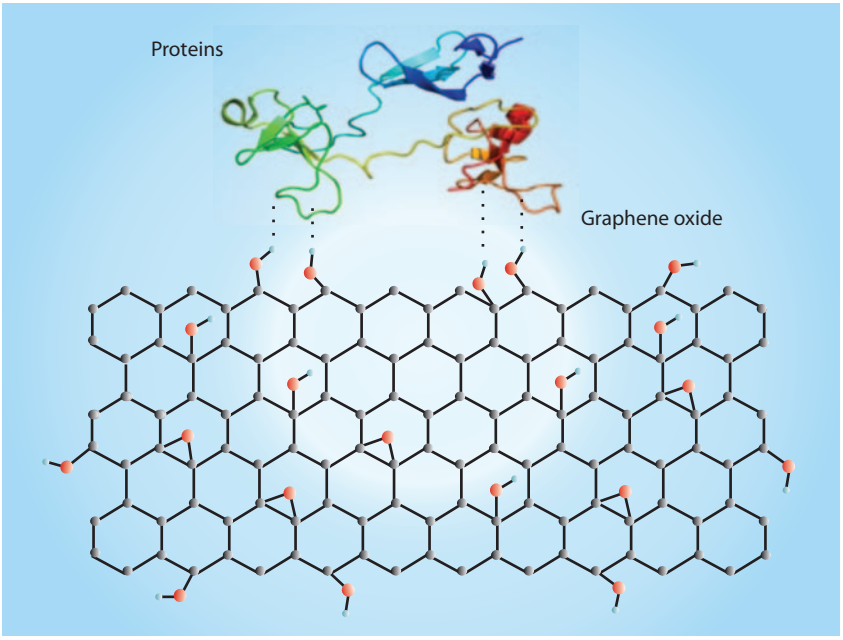
Increased performance through controlled reduction

Optimized cell performance is achieved through controlling the physicochemical properties of graphene oxide, leading to intriguing perspectives for bio-applications

The extraordinary physical properties of graphene — a single layer of carbon atoms arranged in a honeycomb lattice — and its derivatives such as graphene oxide, have excited the interest of scientists and engineers with a view to constructing efficient electronic devices with potentially new functionalities. Graphene-based materials may now also find applications beyond electronics. Haixin Chang, Hongkai Wu and co-workers from the AIMR at Tohoku University and institutions in Beijing and Hong Kong believe that graphene's combination of transparency, flexibility and electrical conductivity could enable a wide range of biological and biomedical applications.

At present it remains unclear whether graphene or graphene oxide can be used *in vivo*, mostly because their toxicity has not yet been established. However, these materials could in theory be used as analysis platforms for proteins and cells *in vitro*, although the complex interplay between these materials' surfaces and cells needs to be better understood before any applications can be realistically considered. In their study of cells attached to multi-layer or 'few-layer' graphene oxide films, Chang, Wu and colleagues have demonstrated a way to optimize cell performance by controlling the films' properties[1].

The most direct way of changing the surface properties of graphene oxide is by varying its reduction state. The team achieved this by reducing pristine films to various extents using thermal reduction — a method through which oxygen-containing groups are progressively removed when heated. Various aspects of cell behavior were tested using three different substrates: non-reduced graphene oxide films, and films that had been reduced for 90 and 260 minutes respectively.



Schematic demonstration of the noncovalent interactions between graphene oxide and cellular proteins.

The researchers first determined the adsorption of various proteins on the films. They observed that the graphene oxide which had been moderately reduced for 90 minutes had the highest adsorption.

This can be explained by considering the combination of conflicting effects arising from the high oxygen content. On the one hand, oxygen promotes hydrogen bonding with the proteins, which increases adsorption. On the other hand, it also induces electrostatic forces and hydrophobic changes, which reduces adsorption.

A similar trend was observed in tests to assess cell adhesion, cell proliferation and cell differentiation. In all cases, the best results were obtained for moderately reduced graphene oxide, which the team ascribes to the stronger protein adsorption obtained in those conditions.

These observations could have serious implications for bio-applications. "The present results open up various possibilities to regulate the biological responses in graphene-based materials by controlling their reduction state," says Chang.

1. Shi, X., Chang, H., Chen, S., Lai, C., Khademhosseini, A. & Wu, H. Regulating cellular behavior on few-layer reduced graphene oxide films with well controlled reduction states. *Advanced Functional Materials* **22**, 751–759 (2011).

Bulk metallic glasses

An unexpected hybrid

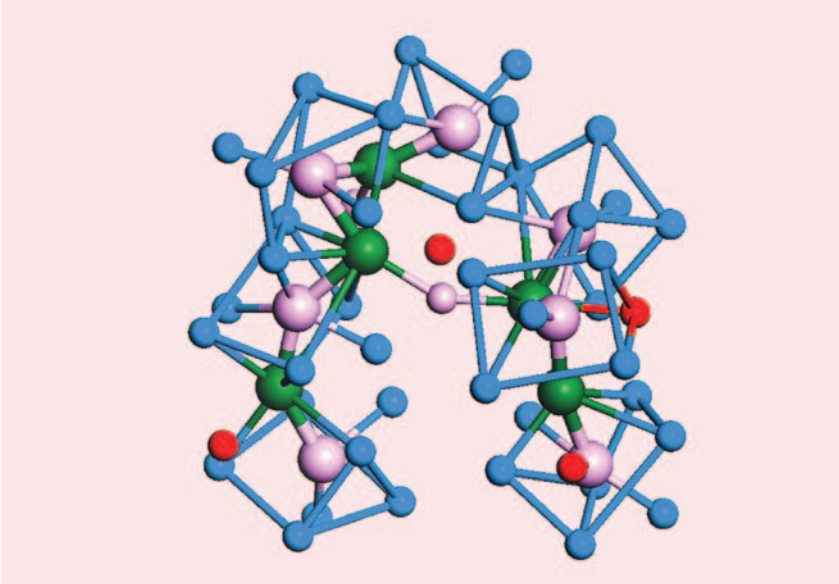
A combined experimental and theoretical study reveals a hybrid structure for metal-metalloid bulk metallic glasses that reconciles previously contradicting observations

The exceptional resilience of bulk metallic glasses (BMGs) combined with their high resistance to corrosion and wear makes BMGs a highly sought-after material in mechanical applications. With a lower thermal conductivity than crystalline metals, BMGs also offer potential applications in thermal management. Divided into two general groups, BMGs are classified as either metal-metal-based glasses or metal-metalloid-based glasses. Fundamentally, however, the atomic structure of metal-metalloid-based glasses is still intriguing and remains a matter of debate among experts in the field.

In metal-metal-based glasses comprising of only metallic elements, their structure maximizes atomic packing. However, the situation is much more complex for metal-metalloid-based glasses, which also comprise atoms such as phosphorus, boron, silicon and carbon that tend to saturate their charge through covalent and coordination bonds. Because the number, direction, and length of these bonds follow specific rules, they inevitably disrupt the dense packing of the metal atoms in metal-metalloid-based glasses.

Until now, it has remained unclear how these contrasting experimental observations can be reconciled. Mingwei Chen, Pengfei Guan and colleagues from the AIMR may have now solved the puzzle by describing a hybrid between a covalent-bond mediated structure and a densely-packed icosahedron structure for a model metal-metalloid BMG, palladium–nickel–phosphorus[1].

"This BMG was actually the first bulk metallic glass reported in the literature, and so far it still has the best glass-forming ability among ternary metal-metalloid alloys," explains Chen.



Atomic structure of the bulk metallic glass, palladium–nickel–phosphorus, comprised of phosphorus (pink); nickel (green); ordered palladium (blue) and disordered palladium (red).

It was therefore a natural choice for the team to focus on unraveling the structure of palladium–nickel–phosphorus. In their analysis, the team performed both X-ray diffraction experiments and *ab initio* molecular dynamics simulations. The results suggest that phosphorus coordinates with both palladium and nickel, while metallic bonding occurs between these two metallic elements.

The researchers propose the structure of palladium–nickel–phosphorus consists of two types of clusters perfectly interconnected, in which tri-capped trigonal prisms centered on phosphorus atoms are linked together by nickel-centered densely-packed icosahedra.

This hybrid structure, which satisfies both the necessity of charge saturation for phosphorus atoms and the dense packing requirement for metal atoms, exhibits the lowest energy achievable in the compounds and is therefore relatively disordered, yet stable.

These findings do not only explain the well-known glass-forming ability of the alloy palladium–nickel–phosphorus, but also hold a wider significance in our understanding of the formation of metal–metalloid glasses. "This may be a universal structural model for metal–metalloid glasses," says Chen. "We have also found the same packing scheme in different alloy systems."

1. Guan, P. F., Fujita, T., Hirata, A., Liu, Y. H. & Chen, M. W. Structural origins of the excellent glass-forming ability of $Pd_{40}Ni_{40}P_{20}$. *Physical Review Letters* **108**, 175501 (2012).

Polymer properties

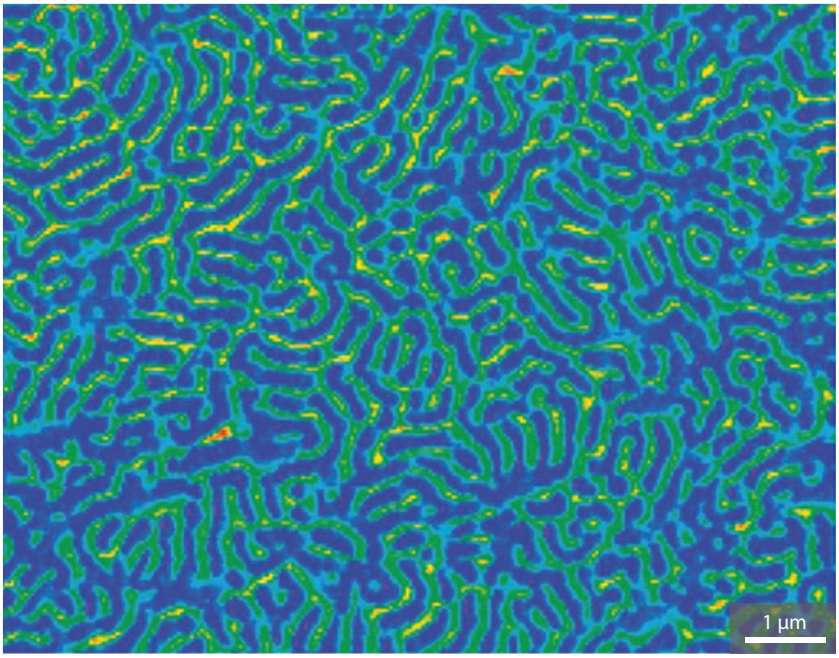
Macromolecular mapmaking

Probing the surface properties of polymers could help to bridge the gap between their macroscale properties and their nanoscale structure

The surfaces of polymers — large molecules comprising repeated structural units — contain special physical properties such as adhesion, wetting, and friction. These properties can be quite different from those of the bulk material, and are difficult to correlate with the polymers' molecular structures. Although modern synthetic strategies offer much control over molecular structure, finding the optimum polymer for a particular device or application remains a challenge. Ken Nakajima, Dong Wang and co-workers[1] from the AIMR at Tohoku University have now succeeded in mapping out the surface properties of a polymer film using atomic force microscopy (AFM).

Nakajima describes the concept of mapping properties with a simple illustration: "Consider painting a colored ink on a polymer surface — the color will be more easily erased from areas with lower adhesive properties." Polymer properties such as viscoelasticity and adhesion hold great potential in a variety of applications, including automotive manufacturing. "It is clear that this work may be directly applicable in the production of polymer materials for tires, for which adhesive and viscoelastic properties are important. Indeed, we are currently collaborating with several tire companies in Japan," says Nakajima.

In the past, measurements of tensile or shear stress have been used to evaluate adhesive strength and viscoelastic behavior. These methods, however, are a macroscale examination and provide only an average value of properties. In contrast, AFM uses an atomically thin tip attached to a flexible lever to directly probe the properties of the surface at the nanoscale. Here the research team used contact-mode AFM, described by Nakajima as "a nanomassage" in which the polymer's molecular structure consists of a block of poly(ethylene-co-butylene) sandwiched between two blocks of poly(styrene) — a tri-block copolymer. Rather than being homogenously mixed, the polymer molecules in the bulk are arranged so that 'blocks' of similar polymer are close together. At the surface, this is manifested as a pattern of many small polymer 'islands' (see image). "Our AFM technique allows us to prepare a map of how the surface properties vary over the surface," explains Nakajima.



A map of viscoelastic properties of a tri-block copolymer sample.

This technique holds promise in the mapping of mechanical surface properties for other types of block copolymer, provided there is a mechanical difference between the different components. "In the future we hope to characterize the surface properties of other materials such as bulk metallic glasses and biomaterials," says Nakajima. "Ultimately we are hoping to establish a connection between the macroscopic properties of the polymer and a nanoscopic understanding of structure which we can then use to evaluate and design new high performance materials."

1. Wang, D., Liang, X-B., Liu, Y-H., Fujinami, S., Nishi, T. & Nakajima, K. Characterization of surface viscoelasticity and energy dissipation in a polymer film by atomic force microscopy. *Macromolecules* **44**, 8693–8697 (2011).

Topological insulators

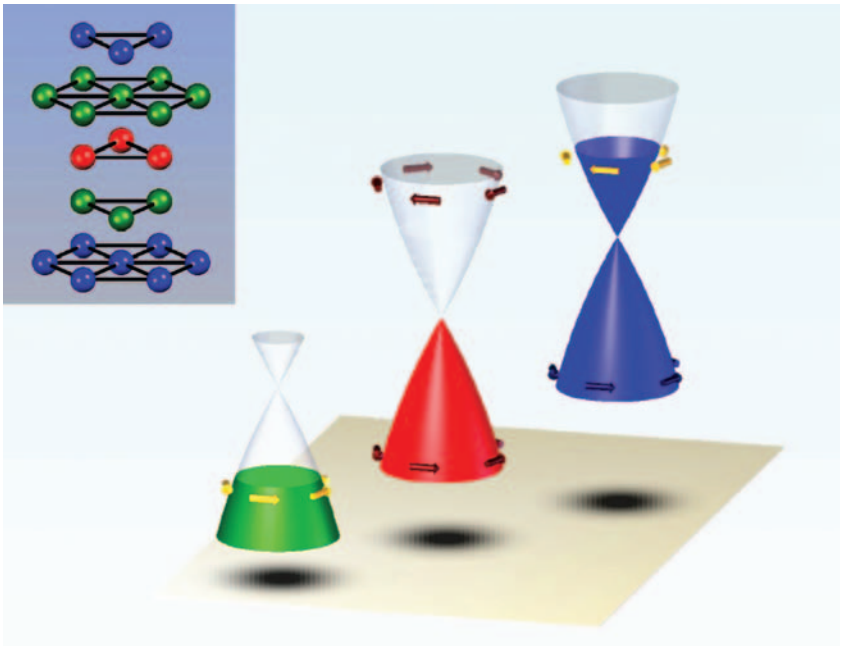
Conduction gets a tune-up

Tuning the composition of a topological insulator material has allowed scientists to control its intriguing surface properties while preventing current from leaking through the bulk

Topological insulators exhibit some of the most fascinating conductive properties of any material. Although the bulk volume of a topological insulator does not pass any current, its surface is highly conductive and the magnetic spin orientations of the surface currents are relatively easy to preserve. This unique behavior has stimulated studies into both the fundamental science behind these properties and applications such as ultralow-power spin transistors. Toshiyuki Arakane, Takashi Takahashi and colleagues at Tohoku University and Osaka University have now developed a topological insulator material that should aid research in this area[1].

The researchers focused on an outstanding problem in the field: the bulk of a topological insulator often has defects through which current can flow. This bulk current can obscure surface currents whose behavior is the intended subject of the experiment. Previous work by other researchers showed that manipulating the elemental composition of a topological insulator can reduce its bulk conductivity while maintaining high surface conductivity.

Arakane and co-workers took this work a step further by showing that manipulating the composition of a topological insulator can keep its bulk conductivity low while also allowing the surface current to be tuned between positive and negative charge carriers. They chose to investigate BSTS — a material made from bismuth, antimony, tellurium and selenium (see image). BSTS is known to have two types of crystal defects: one that contributes positive charge carriers, and one that contributes negative charge carriers. Careful control over the relative amount of each element allowed the researchers to balance these defects, thus minimizing the bulk conductivity.



Tunable Dirac cone in topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$. Controlling the composition ratio of Bi/Sb and Te/Se leads to the change in the filling of Dirac carriers while keeping the bulk insulating nature.

Through angle-resolved photoemission spectroscopy, the researchers revealed that this compositional control can also be used to adjust the energy of the surface charge carriers. They were able to tune the surface carriers to the Dirac energy point, where their concentration fell to zero. Furthermore, they successfully tuned the carrier energy to either below or above the Dirac energy point, thus causing the surface carriers to take on positive or negative character, respectively. In both situations, the bulk conductivity remained low.

According to Arakane, this research should allow a variety of exotic quantum effects to be observed. "We expect to see effects such as the topological magneto-electric effect, the quantum spin Hall effect and excitonic condensation — all of which have been proposed theoretically but not yet observed experimentally due to the bulk carrier problem." Device applications, says Arakane, would benefit from thin-film growth techniques, which will be a future focus of the research group.

1. Arakane, T., Sato, T., Souma, S., Kosaka, K., Nakayama, K., Komatsu, M., Takahashi, T., Ren, Z., Segawa, K. & Ando, Y. Tunable Dirac cone in the topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$. *Nature Communications* **3**, 636 (2012).

Bulk metallic glasses

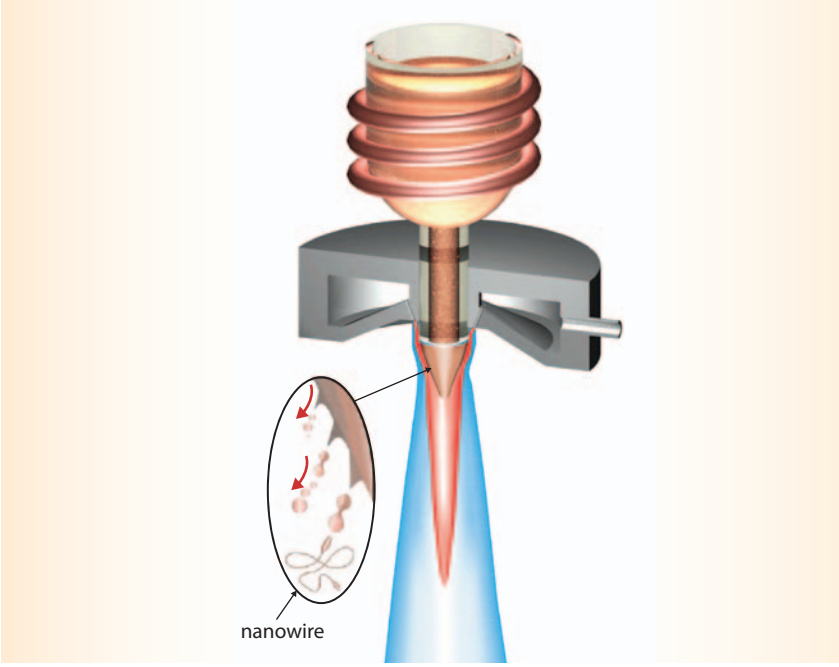
Nanowire gems in the particle dust

A cost-effective method for creating metallic powders helps to accelerate the production of metallic glass nanowires

With their unique properties of exceptional mechanical strength, high elasticity, and resistance to mechanical wear, bulk metallic glasses hold great potential in the design of micromechanical devices and nanoscale catalysts. Although the production of nanoscale metallic glass structures is already underway, the techniques used are too expensive and time-consuming to lend themselves to mass production. Koji Nakayama, Na Chen and colleagues from the AIMR and the Institute for Materials Research at Tohoku University have now discovered a new, cost-effective technique to produce metallic glass nanowires that yields at least a few hundred million nanowires per gram of material[1].

Unlike the structure of crystalline metals, metallic glasses have an amorphous and tightly-packed atomic structure, which makes them tough and resistant to mechanical deterioration. Metallic glasses are produced using a melting process, in which the molten liquid requires a high viscosity, as well as a high "spinnability" — a tendency to form elongated shapes — in order to yield nanowires.

Nakayama and his team found they could create these conditions in a process called gas atomization, commonly used in the production of metallic powders. During this process, molten metal flows from the nozzle of a crucible and meets high-speed gas at the exit, which breaks up the metal stream into a variety of particulate shapes (see image). By supercooling the molten alloy below its melting point, the researchers could increase the viscosity of the melt stream prior to the gas atomization process. Though unremarkable to the naked eye, the atomized products form a metallic lump that contains a tangle of long metallic glass nanowires with diameters of 50–2,000 nanometers.



Gas atomization, a process for making metallic particles, can be used to fabricate metallic glass nanowires. Molten metal flows from a crucible nozzle and interacts with a high-speed gas to break down the metal stream into various particulate shapes, including nanowires (inset).

"The length to diameter of the wire (aspect ratio) increases exponentially with decreasing temperature below the melting point," explains Nakayama, who established a "spinnability rule" to predict how nanowires made from different metallic glasses have an aspect ratio that is dependent on atomization temperature.

The team has so far focused on two metallic glasses — $Zr_{65}Cu_{18}Ni_7Al_{10}$ and $Fe_{76}Si_{9.6}B_{8.4}P_6$ — but plans to make nanowires that contain important catalytic elements like platinum and palladium. "Metallic glass nanowires will have a significant impact on catalyst research," says Nakayama. Since nanowires have a large surface-area-to-volume ratio, they are more catalytically active per gram of material — one of the goals of green chemistry. In future, such metallic glass nanowires may also be formed from magnetic elements, which could have useful applications in the design of miniature devices with a high-frequency impedance response to a changing magnetic field.

1. Nakayama, K. S., Yokoyama, Y., Wada, T., Chen, N. & Inoue, A. Formation of metallic glass nanowires by gas atomization. *Nano Letters* **12**, 2404–2407 (2012).

Oxide materials

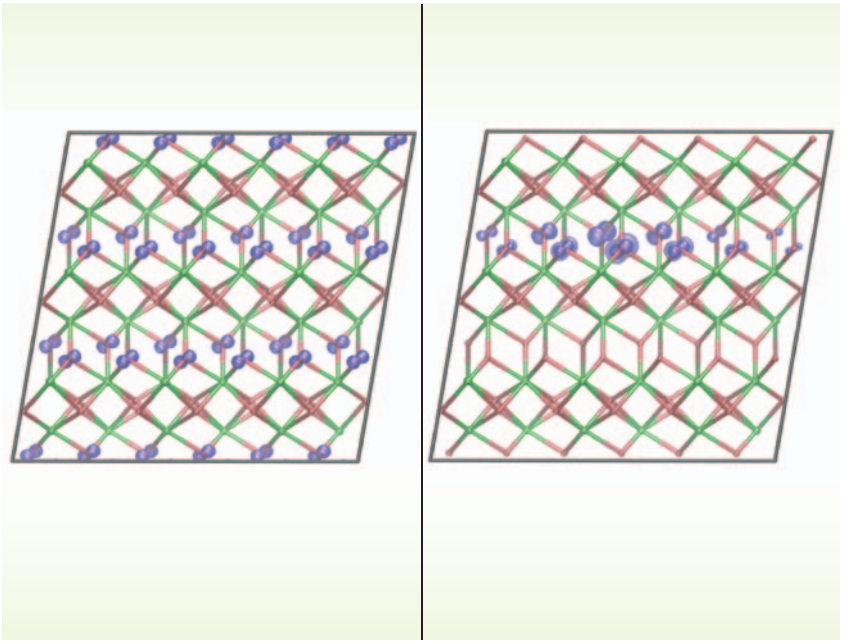
Hidden layers

A new calculational approach predicts that charges trapped in simple and common three-dimensional bulk oxides are restricted to two-dimensional sheets

An important characteristic critical to a variety of technologies is the way in which oxide materials trap charges. For example, hafnium dioxide — used to insulate transistor gate electrodes — can begin to fail if charges become trapped in its bulk. Similarly, the effectiveness of zirconium dioxide as a common catalyst depends on the quantity of trapped charges. Accurately predicting the nature of charge trapping in oxides like these, however, has remained an unmet challenge. Now, Keith McKenna and Alexander Shluger from the AIMR at Tohoku University, along with colleagues from the UK and the USA, have developed a new calculational approach to predict unexpected aspects of charge localization — and thus trapping — in oxides[1].

Calculations of charge trapping generally rely on density functional theory (DFT). The widely used implementations of DFT, however, characterize electrons as interacting with themselves electrostatically — a physically incorrect description. This 'self-interaction error' leads to inaccurate predictions of charge trapping in materials. McKenna, Shluger and colleagues have now carried out calculations using a version of density functional theory that includes cancellation of nonlinearity — that is, a correction to the self-interaction problem. This new insight provides an unprecedented view into how charges are localized in hafnium oxide and zirconium oxide.

Although usually considered to be three-dimensional bulk crystals, the researchers' calculations predicted that charges in these materials behave as if they were constrained to two dimensions. This is because the crystal structure of each material consists of alternating layers, in which oxygen atoms coordinate — or bond — to either three or four metal atoms. When a positive charge is induced in the materials, it induces distortions in the surrounding crystal lattice, and in turn quickly stabilizes the lattice structure (see image). The positive charge together with the lattice distortions are referred to as a polaron.



A positive charge (blue) inside the crystal lattice of hafnium oxide is initially dispersed in three dimensions (left). The charge brings about slight distortions in the crystal lattice which causes it to localize to a two-dimensional sheet (right).

The researchers found that polarons prefer to stay in oxide layers with triply coordinated oxygen atoms. Such two-dimensional behavior has been much studied due to the particular physics it involves, but it has typically been observed only in complex oxides composed of three or more types of atoms, or at interfaces between materials. Its observation in a relatively simple binary oxide, made of only two types of atoms, is unexpected and will lead to a new investigative approach of the particular physics involved. "In addition to the importance of the theoretical methods themselves, our predictions may stimulate new studies of the correlated dynamics and interaction of positive charges in binary oxides," says McKenna.

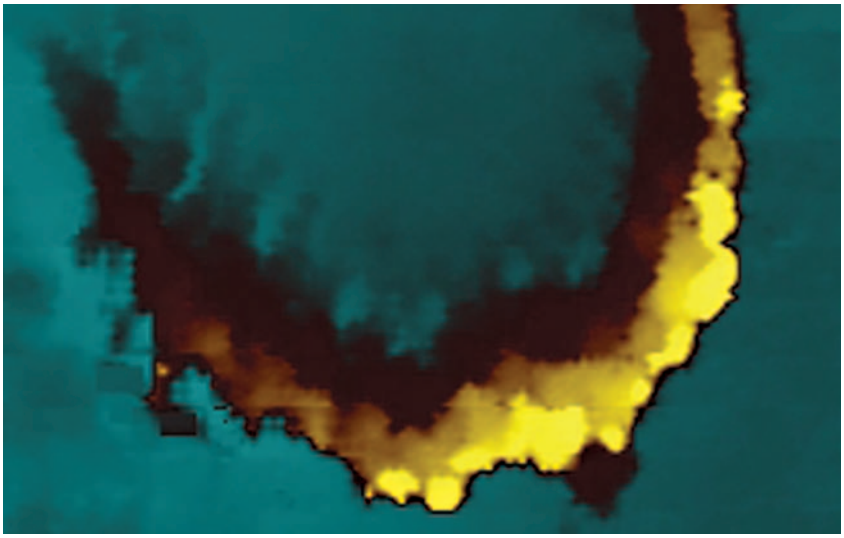
1. McKenna, K. P., Wolf, M. J., Shluger, A. L., Lany, S. & Zunger, A. Two-dimensional polaronic behavior in the binary oxides m-HfO_2 and m-ZrO_2. *Physical Review Letters* **108**, 116403-1–116403-5 (2012).

Cell imaging

Switching it up

A state-of-the-art technique that enables simultaneous topographical and electrochemical imaging of interfaces creates new opportunities for the chemical mapping of living cells

Electroactive and short-lived species that are released and consumed by cells, including neurotransmitters and reactive oxygen-based molecules, are central to cell metabolism, but their detection at cell surfaces and interfaces remains challenging. A research team led by Tomokazu Matsue and Yasufumi Takahashi from the AIMR[1], in collaboration with Yuri Korchev from Imperial College London, has now developed a high-resolution, non-invasive imaging method called voltage-switching mode–scanning electrochemical microscopy (VSM–SECM). The technique, which can be utilized under physiological conditions, provides high-quality topographical and electrochemical images of living cells simultaneously.



Topographical image of hair cells acquired by the VSM–SECM imaging technique.

Many SECM imaging approaches have been developed to determine surface topology and reactivity. However, they usually measure interactive forces by direct contact, through the tip of a tiny electrode that moves across the surface of the substrate being imaged — which can damage cell membranes.

Matsue and colleagues have now used faradaic current, which is generated by the reacting electroactive species, to control the motion of the electrode, and continuously prevent it from touching the substrate surface. Moreover, they fabricated nanometer-sized glass-insulated carbon electrodes that allow for high-resolution imaging.

To initiate one measurement, the team moved the electrode tip towards the surface while monitoring the distance-dependent current created by the hindered diffusion of the electroactive species as they underwent reduction. When the tip current decreased to a level that reflected the desired distance between probe and either the substrate surface or an electroactive molecule, the researchers stopped the probe and recorded its position. At each position, the team switched the voltage applied to the electrode to also determine the species' activity. Repeating this process at several points across the surface yielded simultaneous topographical and electrochemical images.

Similar to ultra-high resolution images, the resulting maps highlighted the small protrusions and wave structures of skin and cardiac cells as well as elongated hair cells (see image). Visualization of cell membrane proteins associated with cancer showed that the protein distribution was uneven and did not match the ultra small features observed from the topological images — demonstrating the usefulness of VSM-SECM for chemical mapping at biological interfaces. Simultaneous topological and electrochemical measurements have also enabled Matsue's team to detect the release of neurotransmitters from neurons. Furthermore, the combination of SECM with fluorescence microscopy clearly showed the extremities of neurons at the synapse.

Currently, the researchers are further exploring neuronal communication using their new method. "We would like to map the neurotransmitter releasing sites," says Matsue. The team is also planning to monitor the release-related changes in neuron topography.

1. Takahashi, Y., Shevchuk, A. I., Novak, P., Babakinejad, B., Macpherson, J., Unwin, P. R., Shiku, H., Gorelik, J., Klenerman, D., Korchev, Y. E. & Matsue, T. Topographical and electrochemical nanoscale imaging of living cells using voltage-switching mode scanning electrochemical microscopy. *Proceedings of the National Academy of Sciences USA* **109**, 11540–11545 (2012).

Spintronics

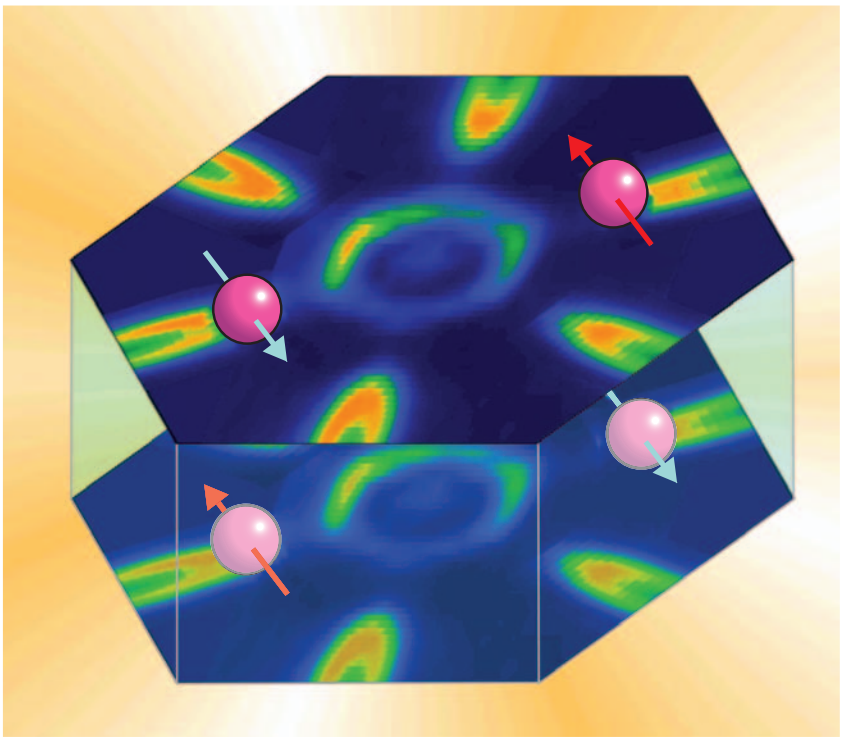
Both sides polarized

The finding that a spin effect — important in spintronics — can be present at both sides of a thin metal film suggests a route to a tunable source of spin-polarized electrons

Spintronics is an emerging technology which exploits the intrinsic angular momentum — or, spin — of electrons for new efficient ways of storing and processing information. In contrast, in conventional electronics only the charge of the electron has a central role. A basic requirement for spintronics devices is the availability of electrons in well-defined, rather than random, spin states. Akari Takayama and colleagues from the AIMR at Tohoku University, together with collaborators from Osaka University, have now found an approach to producing such 'spin-polarized' electrons, with the important feature that the degree of spin polarization can be tuned[1].

Traditionally, the production of spin-polarized electrons involved ferromagnetic materials, in which spins are naturally aligned. For device applications, however, electric fields are often preferred to magnetic ones. A general approach to the electric generation of spin polarization is through 'spin–orbit coupling', which connects the charge of an electron with its spin. One manifestation of spin–orbit coupling is the Rashba effect, in which electrons are polarized when certain types of asymmetries — typically found at the surface of materials — are present.

Takayama and colleagues have studied the Rashba effect in very thin films of the metal bismuth. They deposited films of thickness ranging from 16 to 80 atoms on a silicon surface. To their surprise, they observed in these samples that the spin-polarizing effect was at work not only on the surface, but also at the interface between the metal film and the silicon substrate (see image).



The effect of spin-polarization is seen as expected at the surface of a thin bismuth film (upper plane) but also, surprisingly, at the interface with the underlying silicon substrate (lower plane).

"This result was unexpected, as the simple Rashba picture suggests the existence of spin-polarized electrons only at the top surface of our samples," explains Takayama. Furthermore, the effects on the two sides of the film were found to interfere with each other. As a result of this interaction, the degree of polarization decreased when the sample was made thinner. "This is the most surprising result of our study: spin polarization can actually be tuned by varying the thickness of the film," says Takayama.

The researchers' choice of bismuth for their study was no coincidence. Spin–orbit coupling is particularly strong in materials made from bismuth or other heavy elements, such as gold or antimony. Now that Takayama and colleagues have shown that the degree of polarization is tunable through the thickness of the films used, materials such as bismuth hold even greater promise for future applications in next-generation spintronics devices, for enhancing spin-polarized currents, and for fundamental studies of novel quantum effects.

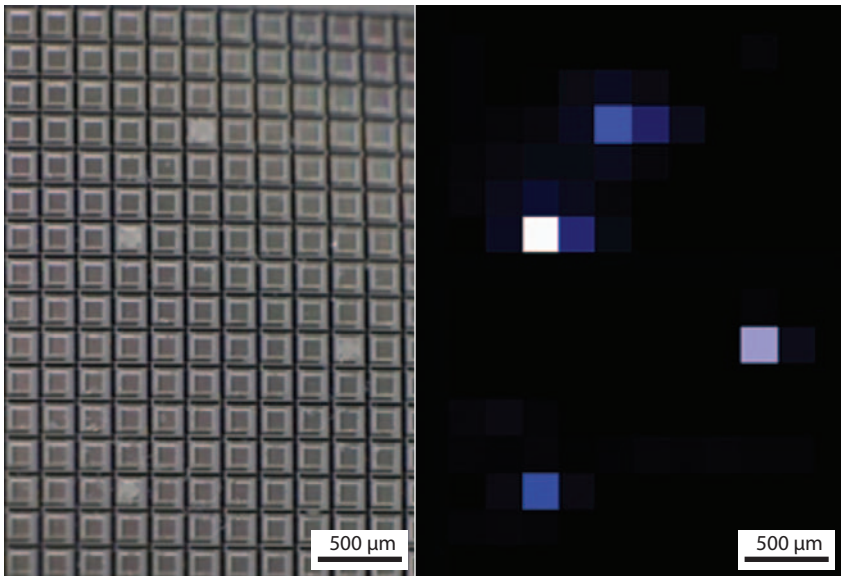
1. Takayama, A., Sato, T., Souma, S., Oguchi, T. & Takahashi, T. Tunable spin polarization in bismuth ultrathin film on Si(111). *Nano Letters* **12**, 1776–1779 (2012).

Lab-on-a-chip

Electrochemical imaging

A high-density electrochemical device has been developed to monitor and image stem cells in three-dimensional embryoid bodies

Traditional methods of culturing cells for biological and biomedical applications use two-dimensional cell cultures, typically growing cells on the base of plastic Petri dishes. In recent years, however, a three-dimensional (3D) environment has emerged as more appropriate for cell culture as it replicates the biological milieu. This is particularly important for embryonic stem cells which can grow into a variety of different tissue structures (such as bone, nerve, cartilage cells) from 3D embryoid bodies. Researchers from the AIMR and the Graduate School of Environmental Studies at Tohoku University have now built an electrochemical device that monitors the activity and differentiation of stem cells in an embryoid body[1].



Optical image (left) of the embryoid bodies sitting on top of individual sensors. The electrochemical image (right) shows the embryoid bodies detected using the lab-on-a-chip device.

Usually, scientists label biomolecules for analysis with fluorescent markers to identify and quantify their presence. But labelling molecules may be toxic or interfere with cellular behavior, and fluorescence levels can be compromised by autofluorescence (signals from unlabeled molecules) or quenching from other non-target materials or liquid turbidity. The electrochemical device developed by Tomokazu Matsue, Kosuke Ino and colleagues does not require these labels, thus removing these problems.

Electrochemical detection has been used before. However, this device has a unique feature. Detection is achieved using an array of 256 electrochemical sensors with only 32 bonding pads for external connection (see image), placed at the base of deep microwells which enables spatially-resolved measurements. "This electrochemical sensor density is the highest in the field of electrochemical lab-on-a-chip devices," the researchers explain.

The research team quantified cellular activity from embryoid bodies on the array by 'redox cycling,' whereby alkaline phosphatase activity (a marker for the differentiation level of embryonic stem cells) was measured by the reduction and oxidation of one of its reaction products. Potentials of electrodes in each sensor were set at levels to initiate redox cycling at a specific location from which the local current signals were collected and measured.

Interestingly, enzymatic activity as measured by the electrode device after a four-day incubation did not increase as expected, suggesting that the stem cells had differentiated. The device will therefore be useful to screen embryoid bodies' differentiation levels, and will provide more quantitative than conventional sorting by morphological analysis.

Furthermore an embryoid body resting on top of the sensor array was imaged without cross-talk from molecular diffusion between sensors due to the microwells. In the next stage of this project, the researchers will explore the limits of this imaging capability.

"We intend to increase the density of the electrochemical sensors even further for electrochemical imaging of a single cell or a single tissue," say the researchers.

1. Ino, K., Nishijo, T., Arai, T., Kanno, Y., Takahashi, Y., Shiku, H. & Matsue, T. Local redox-cycling-based electrochemical chip device with deep microwells for evaluation of embryoid bodies. *Angewandte Chemie International Edition* **51**, 6648–6652 (2012).

Biomaterials

Stimulating patterns

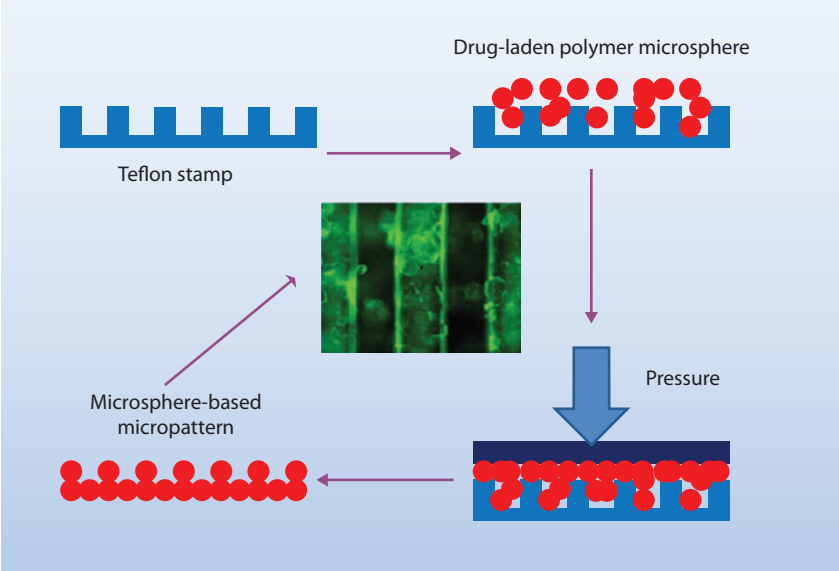
Microscopic patterns made of tiny drug-filled polymer spheres stimulate stem cell growth and differentiation for bone tissue repair

Bone health hinges on the assembly of various cells, including osteoblasts and osteoclasts, into well-defined functional structures that manage bone-specific tasks in the body, such as cell growth, differentiation and protein secretion. However, tumor-induced injuries and other bone-related diseases hinder these self-regulated, sophisticated tasks. To address these conditions it is essential to develop tissue engineering approaches that direct cell behavior.

Xuetao Shi and Hongkai Wu and co-workers from the AIMR at Tohoku University, together with colleagues in Hong Kong and Beijing[1], have now developed patterns that serve as scaffolds for bone regeneration. The patterns consist of polymer microspheres filled with drug or protein molecules that are regularly interspaced.

Prevalent methods for directing cell behavior exploit either chemical and biological signals or topographical cues, but using each of these methods separately has proven ineffective. The former approach can regulate stem cell differentiation into specialized cells but does not properly control cell spatial arrangements, while the latter faces opposite limitations.

By combining both approaches into microsphere patterns, the researchers have now taken advantage of chemical and physical stimulations at the same time. The patterns induced an aligned growth of cells that simulates the native surfaces of bones and the membrane enveloping their outer surface. "We also used the microspheres to encapsulate and release drug molecules to mimic the *in vivo* bone environment, which contains various beneficial substances such as growth hormones," adds Shi.



Schematic representation of the microsphere pattern manufacturing process.

To create the patterns (see image), Shi's team first mixed an organic solution containing the biocompatible, biodegradable poly(lactic-*co*-glycolic acid) polymer with a drug or protein dissolved in water in the presence of emulsifiers. After depositing the resulting microspheres onto a patterned Teflon mold and adding a solvent to ensure inter-particle cohesion, the researchers covered the mold with a Teflon slide and applied pressure to this lid to obtain the patterned material.

Initial tests showed that patterns with narrow grooves between the microspheres resulted in better cell alignment than wide ones. Moreover, the microspheres efficiently encapsulated and slowly released hydrophilic and hydrophobic molecules, prompting the researchers to simultaneously load multiple drugs into them. Stem cells cultured on these multi-drug-loaded patterns exhibited high levels of bone tissue formation markers, proof of their enhanced differentiation towards osteoblasts.

In addition to bone repair, this combined chemical–topographical strategy can be used to study muscle and blood vessel cells for potential regenerative therapies of cardiac tissues. "Our future work will focus on further developing scaffolds displaying surfaces that mimic native tissue and drug or gene release function for organ and tissue regeneration," says Shi.

1. Shi, X., Chen, S., Zhou, J., Yu, H., Li, L. & Wu, H. Directing osteogenesis of stem cells with drug-laden, polymer-microsphere-based micropatterns generated by Teflon microfluidic chips. *Advanced Functional Materials* **22**, 3799–3807 (2012).

Catalysis

A kink in the golden rules

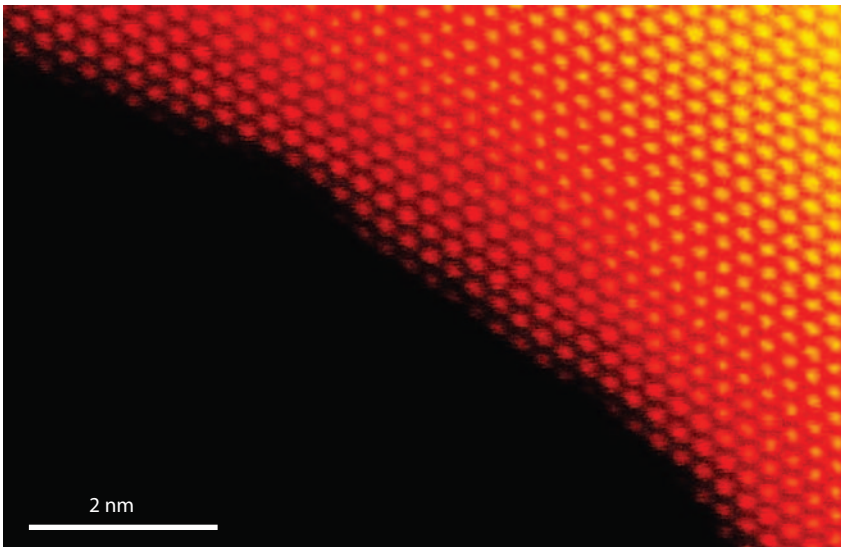
High-resolution imaging of nanoporous gold reveals that 'kinked' surface defects are responsible for its high catalytic activity in carbon monoxide oxidation

Twenty-five years ago, nobody thought that gold would have catalytic activity towards molecular oxygen, because classical thermodynamic principles reject any chemical reaction between gold and oxygen. But the discovery that gold particles smaller than five nanometers could oxidize carbon monoxide (CO) into carbon dioxide (CO_2) at room temperature set off flurries of investigation. Soon, researchers had harnessed this size-dependent catalysis for applications such as decontaminating hydrogen gas in polymer fuel cells. The underlying mechanism for this catalytic activity however remains unclear.

Mingwei Chen, Takeshi Fujita, and co-workers from the AIMR at Tohoku University, in collaboration with researchers from Japan, the US, the UK and China, have captured new evidence that small defects on gold surfaces are active sites for CO oxidation reactions[1]. By developing state-of-the-art techniques to watch surface atomic structures evolve as catalysis occurs, the team also discovered that impurity atoms play critical roles in stabilizing the defect sites — a finding that could boost the longevity and activity of gold catalysts.

Most nanoparticles require an oxide support to hold them in place, making it difficult to pinpoint specific gold catalytic mechanisms. Chen and his team overcame this problem by studying a substance known as nanoporous gold.

Produced by electrochemical de-alloying of a thin gold–silver precursor film, it has a three-dimensional, free-standing architecture of curved nanopores, making it ideal to study gold catalysis without interference from other materials.



A scanning transmission electron microscopy image showing the stepped surface of nanoporous gold.

The researchers turned to spherical-aberration-corrected scanning transmission electron microscopy (Cs-corrected STEM) to identify catalytically active nanoporous gold surface structures. This technique suppresses lattice distortion effects caused by projection lenses, providing sub-atomic resolution capabilities. By carefully controlling gas pressures within a specially-designed specimen holder, the team performed *in situ* characterizations during a CO oxidation reaction in an environmental TEM. "Cs-corrected STEM gives us a great chance to see the true atomic structure of complex materials," says Chen.

The team's high-resolution images revealed that nanoporous gold's surface structure consists of flat, close-packed terraces separated by single-atom steps (see image). Along bent portions of the nanopores, these steps fall out of alignment and become 'kinks' of under-coordinated gold atoms — exceedingly active sites for chemical oxidation. When the researchers exposed the nanoporous gold to a CO/air gas mixture, they observed that the terrace edges dynamically reconstructed into kinked arrangements, a clear sign that these defects play critical catalytic roles. Further experiments revealed that residual silver impurities in nanoporous gold preserved the high density of kinked defects, ensuring high catalytic performance.

Chen notes: "Although many theories have been put forward before, the story of gold catalysis is simpler than anyone ever thought."

1. Fujita, T., Guan, P., McKenna, K., Lang, X., Hirata, A., Zhang, L., Tokunaga, T., Arai, S., Yamamoto, Y., Tanaka, N. *et al.* Atomic origins of the high catalytic activity of nanoporous gold. *Nature Materials* **11**, 775–780 (2012).

Bulk metallic glasses

Taking the color out of polluting dyes

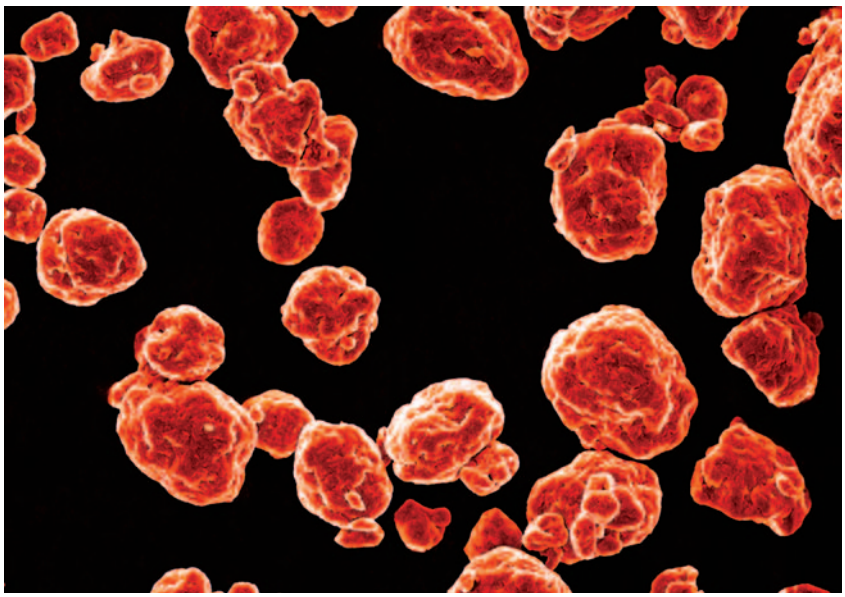
Dye molecules that contaminate effluent streams can be efficiently degraded by metallic glass powders

Synthetic dyes with long-lasting, vivid colors are valuable to both manufacturers and consumers. However, these attributes also make it challenging to clean up these compounds when they slip into wastewater systems and become pollutants. 'Azo' dyes, for example, owe their colors to nitrogen double bonds that resist degradation from bacterial or carbon sorption treatments. Now, Jun-Qiang Wang from the AIMR at Tohoku University[1] and co-workers in Japan and the US have described a way to degrade azo dyes with far greater efficiency than current techniques, using amorphous magnesium–zinc metallic glass powders.

One of the best ways to decompose azo dyes is by using pure, 'zerovalent' metals — in an oxidation state of 0 — such as magnesium or iron to transfer electrons to nitrogen double bonds and crack them apart. However, although zerovalent magnesium is particularly effective at removing organic contaminants from water, it has poor corrosion resistance and is eventually consumed by the aqueous environment. Materials researchers are thus focusing on finding low-cost methods to reduce the corrosion of magnesium while retaining its high reaction efficiency.

Alloying magnesium with another metal can enhance its resistance to corrosion, but only if the atoms are mixed together well. To achieve this, Wang and his co-workers melted magnesium and zinc atoms in a crucible, and then quickly cast them into thin ribbons of metallic glass. The metal atoms pack tightly and homogenously in this glassy state, giving the alloy excellent durability.

Then, to convert the magnesium-zinc ribbons into a form suitable for treating wastewater, the team pulverized them into a fine powder — an unconventional approach that has many advantages, according to Wang.



A high resolution scanning electron microscopy image of a metallic glass powder that efficiently decontaminates dye molecules from wastewater.

"Powders have much larger surface areas compared to ribbons, which enhances their reactivity," he says. "Also, the powdered form may be injected underground to deal with pollutants in groundwater."

Microscopy experiments revealed that the magnesium–zinc powder was well dispersed and did not form aggregates (see image), making it ideal for reacting with synthetic contaminants in an aqueous solution. The powder de-colored a solution of azo dye within 10 minutes — clear evidence that the metallic glass completely degraded stubborn nitrogen double bonds.

Wang notes that in addition to a striking improvement in corrosion resistance, which the researchers attribute to the alloy's amorphous atomic structure, magnesium–zinc metallic glass powders can decontaminate azo dyes with reaction efficiencies 1,000 times greater than that of commercial iron powders.

"These materials can efficiently degrade organic water contaminants in harsh, anaerobic environments at a cheap price, opening up a broad field for metallic glass applications."

1. Wang, J.-Q., Liu, Y.-H., Chen, M.-W., Louzguine-Luzgin, D. V., Inoue, A. & Perepezko, J. H. Excellent capability in degrading azo dyes by MgZn-based metallic glass powders. *Scientific Reports* **2**, 418 (2012).

Tissue engineering

A scaffold for longer-lasting cells

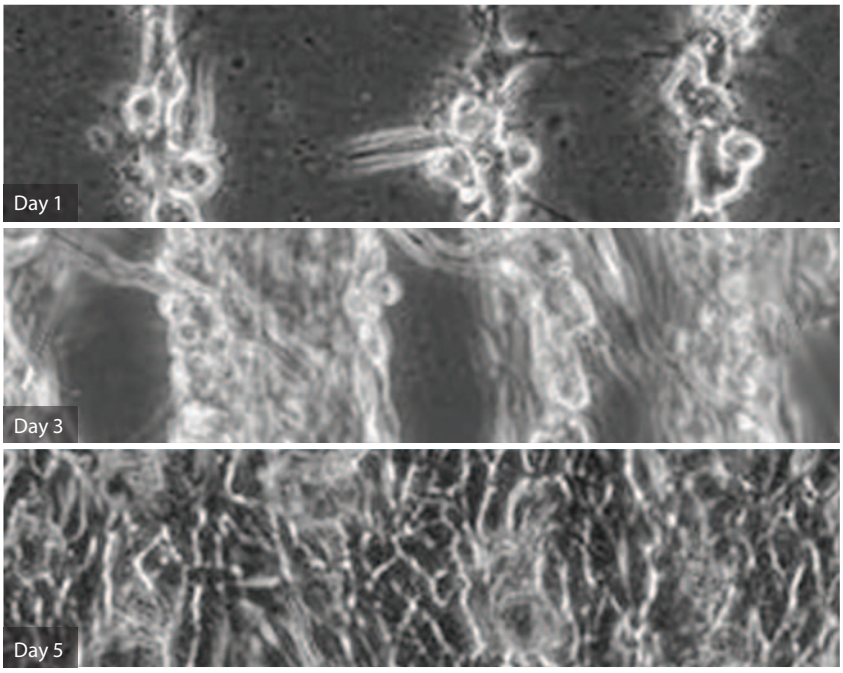
A semi-natural hydrogel scaffold serves to create highly complex artificial tissues with long-term cell viability

Natural tissues are highly organized structures, often formed from multiple cell types precisely positioned to carry out their required roles. Efforts to mimic these structures in order to create artificial tissues — for example, to help heal parts of the body that have sustained damage from injury or disease — is no simple task.

Recently developed techniques such as dielectrophoresis use electric fields to position living cells within a three-dimensional matrix; however, trapping the cells in place while ensuring their long-term viability has proven difficult. A highly biocompatible scaffold material that could solve this problem has now been identified by an international team of researchers led by Ali Khademhosseini and Tomokazu Matsue from the AIMR at Tohoku University[1].

The researchers selected a semi-natural hydrogel material based on gelatin — gelatin methacrylate (GelMA) — to use as a tissue scaffold. Previous studies have shown that GelMA is a suitable material for culturing cells. The researchers also observed that GelMA had the capability to bypass the typical pitfalls of the most commonly used tissue engineering scaffolds. "Owing to its low viscosity and conductivity, we suspected that the GelMA hydrogel could be a promising candidate for cell manipulation using the dielectrophoresis method," says Samad Ahadian, a member of the AIMR team.

Testing GelMA in the laboratory, the researchers confirmed that it was a suitable matrix within which to guide cells into position using dielectrophoresis. Once the cells were in place, the team exposed the scaffold to UV light.



By using a GelMA scaffold, precisely positioned cells are able to grow over several days of culture.

This triggered a chemical cross-linking reaction within the hydrogel, which forms the polymer matrix and traps the cells in place. Using a photomask, the researchers were able to trap one type of cell in one part of the polymer before introducing and trapping a second cell type within the same scaffold.

Crucially, the cells retain long-term viability after the formation of the cross-linked polymer, and readily proliferate over several days (see image). The natural gelatin on which the hydrogel is based is responsible for this high biocompatibility. "The GelMA comprises natural cell-binding motifs that support cell adhesion, migration, and proliferation," explains Ahadian. "The optimized GelMA concentration of 5% ensures that there is plenty of space for the encapsulated cells to obtain the nutrients required and repel wasted products."

The next step will be to produce engineered tissues with differentiated cell types, from neural to muscle cells. According to Ahadian, the potential applications extend beyond damaged tissue repair to include uses in drug screening models or as bio-actuators.

1. Ramón-Azcón, J., Ahadian, S., Obregón, R., Camci-Unal, G., Ostrovidov, S., Hosseini, V., Kaji, H., Ino, K., Shiku H., Khademhosseini, A. & Matsue, T. Gelatin methacrylate as a promising hydrogel for 3D microscale organization and proliferation of dielectrophoretically patterned cells. *Lab on a Chip* **12**, 2959–2969 (2012).

Bulk metallic glasses

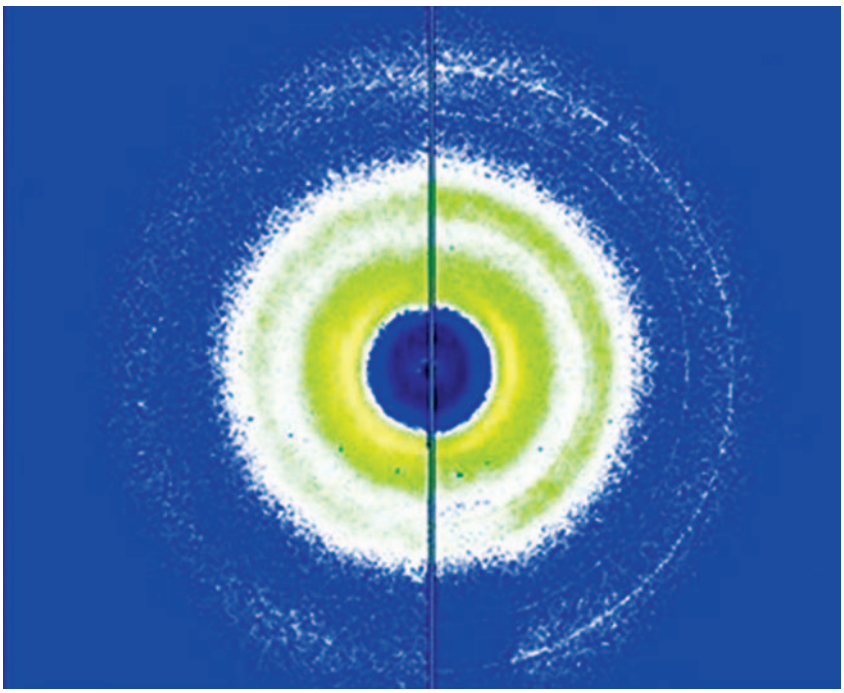
Glasses that bend the rules

The partial crystallization of disordered metals under bending has now been explained

Metals normally have a crystalline structure — that is, the atoms in the material are typically ordered in a repeating pattern. In contrast, atoms in metallic glasses are arranged in no particular long-range order. This disorder endows metallic glasses with a high resilience against deformation, as they lack the natural fault lines along which crystals tend to break. However, crystalline regions have been found to form in some — but not all — metallic glasses when the material is bent. Until now, the reason why these crystalline regions form has remained unclear.

AIMR researchers at Tohoku University together with an international team led by Alain Reza Yavari have now undertaken a combined experimental and theoretical study, and present a model that explains this behavior[1]. The researchers used an X-ray microscope to examine a ribbon of the metallic glass, $Pd_{40}Cu_{30}Ni_{10}P_{20}$. As the ribbon was bent, crystalline regions appeared on the side where pressure was applied. This behavior had previously been observed, however the researchers' use of a high-resolution X-ray microscope enabled a closer, more detailed look at the crystallization process.

The study revealed that compression alone is not sufficient for crystallization to occur. Yavari and co-workers found that a wide supercooled-liquid region is also required to bring about crystallization. This supercooled-liquid region is the range between the temperature at which a glassy metal becomes liquid when heated and the crystallization temperature (typically, far above room temperature). In $Pd_{40}Cu_{30}Ni_{10}P_{20}$, the material studied by Yavari and co-workers, this region spans about 100 °C. In other metallic glasses, the temperature window is much smaller, or does not exist at all. Thus, in those systems, the phenomenon of crystallization under bending does not develop; instead, cracking and mechanical failure occur.



A diffraction image obtained with an X-ray microscope. This image provides researchers with detailed information about the properties of a bent metallic-glass ribbon.

Yavari and his team's findings may have the potential for wider application to a broad range of materials. "In our study, the experimental results fit the theoretical predictions very well. This gives us confidence in our model, which suggests that similar processes should be observable for other chemical compositions," explains Yavari. The model provides important fundamental insights into the properties of disordered metals, but the findings may hold practical significance too. "It is not fully understood how metallic glasses respond to deformations," says Yavari. "Crystallization phenomena, such as the one we described, lead to a hardening of the material, which may in fact prevent metallic glasses from failing under compression."

1. Yavari, A. R., Georgarakis, K., Antonowicz, J., Stoica, M., Nishiyama, N., Vaughan, G., Chen, M. & Pons, M. Crystallization during bending of a Pd-based metallic glass detected by X-ray microscopy. *Physical Review Letters* **109**, 085501 (2012).

Spin electronics

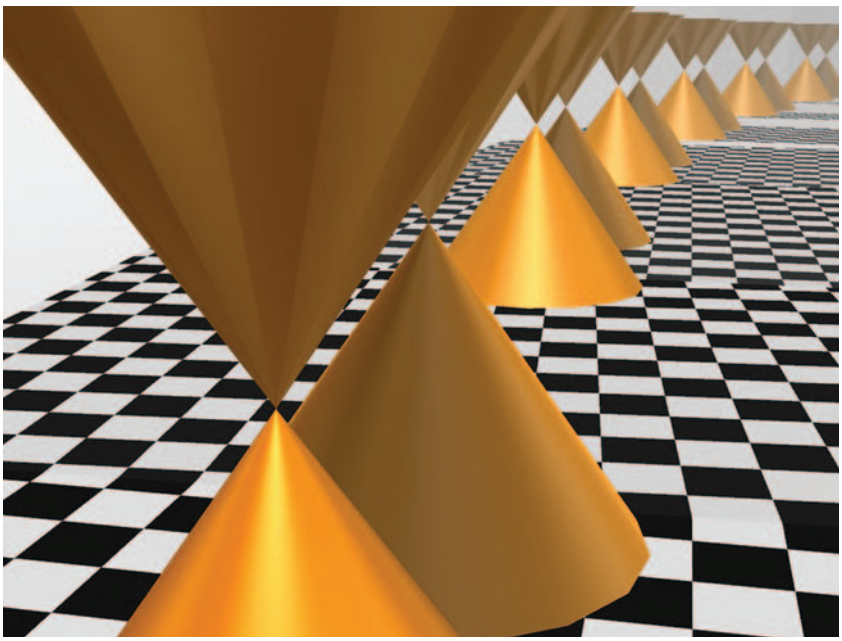
Mirror, mirror on the wall

The discovery of topological insulators whose properties are based on both time-reversal and crystal symmetries offers a new approach to electronic devices

Topology is the study of the fundamental relationships between the properties of different objects. It can explain, for example, why a coffee mug shares similarities with a donut (both have a hole in their structure, and either shape can be morphed to the other), but not a football. Although topology is often viewed within a geometric context, its implications extend much further. Most recently, attention has focused upon the interesting properties of topological insulators.

Topological insulators consist of an insulating bulk with conducting surfaces. This unique topology arises from the time-reversal symmetry of a material's electronic states, in which 'time-reversal' refers to the reversal of motion through time. "So far, all known topological insulators are based on time-reversal symmetry," explains Seigo Souma from the AIMR at Tohoku University. However, together with colleagues from the Physics Department at Tohoku University and Osaka University, the research group has now discovered an interesting class of crystalline tin telluride-based topological insulators whose properties arise from a combination of both time-reversal and crystal symmetry[1].

In time-reversal symmetry, events occur in the same way irrespective of whether time progresses forward or backward. For topological insulators this means that some electronic currents can flow with minimal loss, which has considerable practical applications for low-energy devices. The possession of an additional symmetry, such as crystal symmetry, can help to support similar behavior — as is the case for crystalline tin telluride, whose symmetry is based on the mirroring of its crystal structure as well as its time-reversal one. The electronic states at the surface of the material assume a recognizable 'double cone' shape — a tell-tale sign for topological insulators (see image).



Unlike conventional topological insulators, the electronic states of those made from crystalline tin telluride assume a 'double cone' shape.

"The discovery of crystalline tin telluride marks a new way of finding topological insulators," explains Souma. However, the finding did not come easily and required observation of the topological state in samples carefully prepared to minimize crystal impurities, as well as accurate measurement of electronic states, which was achieved with high-resolution angle-resolved photoemission spectroscopy — a method that determines the energy of photo-emitted electrons.

In the future, the team plans to directly characterize crystalline tin telluride's electronic properties to determine if they differ from conventional topological insulators, a process that should aid the fabrication of functional devices. Moreover, Souma expects this study to be an initial step towards the discovery of further topologies where insulators based on other symmetries could exist, with potentially significant implications for the development of electronic devices.

1. Tanaka, Y., Ren, Z., Sato, T., Nakayama, K., Souma, S., Takahashi, T., Segawa, K. & Ando, Y. Experimental realization of a topological crystalline insulator in SnTe. *Nature Physics* **8**, 800–803 (2012).

Oxide materials

A see-through superconductor

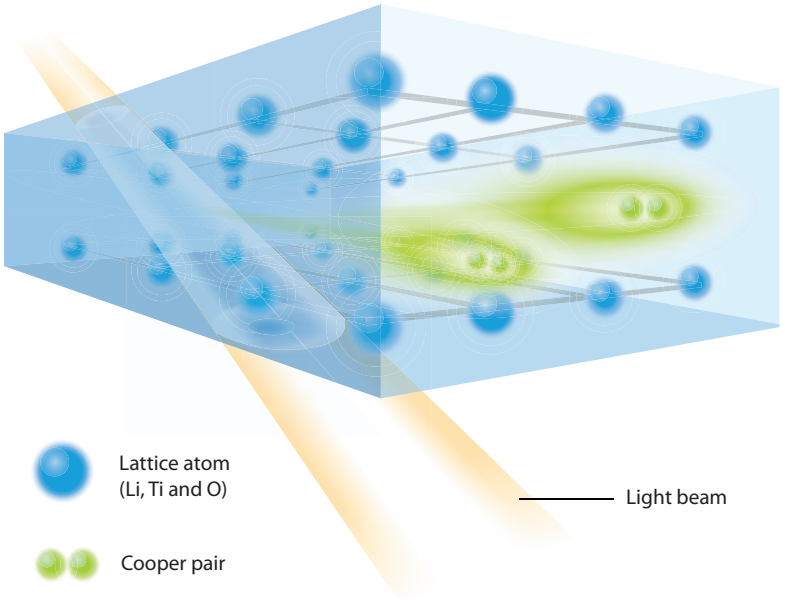
A study of the growth conditions of oxide thin films leads to the production of a transparent superconductor with a record transition temperature

Oxide alloys exhibit intriguing physical properties, such as superconductivity and magnetism, which make them promising components for a wide range of devices including transistors and batteries. Control of the stoichiometry of these materials is an essential requirement for achieving high performance. Now, Taro Hitosugi, Takeo Ohsawa and co-workers at the AIMR have studied the growth of two interesting spinel lithium titanate oxides[1]. Their careful observations have allowed them to optimize the stoichiometry of these materials, leading to the production of superconducting thin films which also have a high level of transparency.

High-quality oxide films are usually produced by a method known as pulsed laser deposition (PLD). The technique involves hitting a structurally and compositionally low-quality oxide alloy with high intensity laser pulses, so that it vaporizes and subsequently re-deposits onto a substrate. Hitosugi and co-workers were particularly interested in $LiTi_2O_4$, a spinel oxide known to exhibit superconductivity below 13.7 K, and its close relative $Li_4Ti_5O_{12}$, which is commonly used as an electrode in lithium-ion batteries.

Previously the researchers observed that the films obtained by PLD tend to have much lower lithium content than their precursor materials. They also noticed that the oxygen pressure during growth plays an important role in the resulting film's composition.

The team selected $Li_4Ti_5O_{12}$ as a target for PLD and fabricated various films at different oxygen pressures in a growth chamber. At high oxygen pressure a $Li_4Ti_5O_{12}$ film was obtained — but at low oxygen pressure the lithium content became depleted, resulting in the deposition of $LiTi_2O_4$ instead. This means that, depending upon the oxygen pressure, the thin film growth occurs through two different mechanisms which influence the lithium/titanium ratio and, in turn, the structure and composition of the material deposited.



A schematic illustration of a transparent superconductor showing light passing through the superconducting material.

The PLD-grown oxide films are of an exceptionally high quality, as exemplified by the high electrical conductivity, $3x10^3$ S/cm, of the $LiTi_2O_4$ film at room temperature. A transparency of up to 70% makes them particularly promising for use in touch screen displays and flat panel displays, as well as for the realization of transparent electrodes for solar cells. In addition, they exhibit a superconducting temperature of 13 K — a record high for such a thin film. The films could also hold potential for quantum information applications where superconducting qubits are coupled with photons. As this temperature is higher than that of liquid helium (approximately 4 K), this offers the advantage of using relatively simple cryogenic techniques to reach 13 K, boosting application-oriented research using transparent superconductors.

1. Kumatani, A., Ohsawa, T., Shimizu, R., Takagi, Y., Shiraki, S. & Hitosugi, T. Growth processes of lithium titanate thin films deposited by using pulsed laser deposition. *Applied Physics Letters* **101**, 123103 (2012).

Ultra-hard ceramics

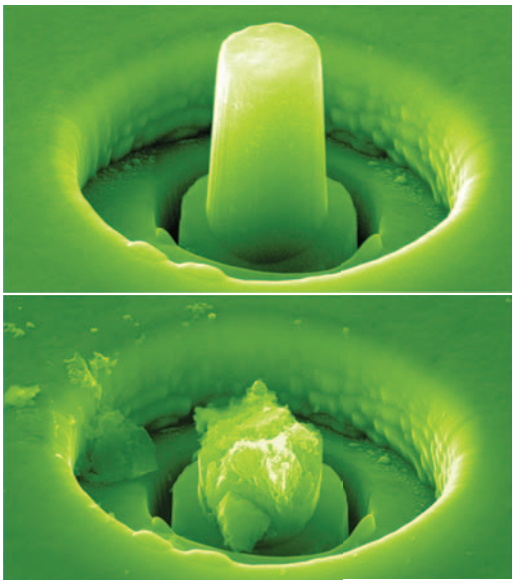
Open up and toughen up

Introducing porosity inside super-strong boron carbide ceramics enables these materials to bend, rather than break, during mechanical deformation

Despite being hard enough to repel bullets, boron carbide ceramics suffer from a critical brittleness that leads them to fracture at low stress levels. However, an international team of researchers led by Mingwei Chen from the AIMR at Tohoku University[1] has now discovered a way to enhance the durability of boron carbide by synthesizing it into a 'nanocrystalline' ceramic with plastic deformation capabilities. Surprisingly, this increased toughness arises from the distribution of small pores and amorphous interfaces — factors that normally weaken ceramic materials.

Commonly, ceramics are made through the process of sintering which heats compressed powders to a temperature just below their melting point. Although this produces a very hard substance, it also generates a variety of crystal grain structures, which may act as fracture initiation points. Chen and his co-workers decided to take a different approach to synthesis: under a lower sintering temperature, they used intense pressures to fuse the boron carbide crystallites into uniform grain sizes, with the expectation that this would reduce brittleness.

High-resolution electron microscopy and X-ray diffraction characterization of the nanocrystalline boron carbide allowed the team to observe the fine-grained structure of the ceramic. They were amazed to spot tiny, irregularly-shaped holes — nanopores — throughout, as well as thin, amorphous carbon layers coating the crystal and nanopore surfaces. Chen explains that these flaws probably appear because they cannot be completely driven away by the reduced temperatures during sintering.



A micropillar carved from nanocrystalline boron carbide ceramic deforms plastically instead of fracturing during compression, owing to a distribution of nanopores.

Mechanical experiments revealed this new ceramic to be tougher than any boron carbide seen before — able to withstand indentation pressures of up to 75% higher than those of conventional materials. Re-examination of the deformed ceramic showed that while the crystal grains remained intact, the nanopore population had severely diminished. This led the team to postulate that the pores and carbon layers help to lubricate the crystal grains, enabling them to slide during compression and therefore tolerate greater pressures.

By carving individual micropillars from the nanocrystalline boron carbide ceramic (see image), the researchers were able to see the effects of indentation first-hand. At high compression pressures, the micropillars bent plastically like a metal instead of shattering — an unprecedented observation for this type of hard material. "This new plastic deformation mode can effectively dissipate the energy of crack tips — preventing crack growth," says co-author and PhD student Madhav Reddy.

According to the researchers, the enhanced toughness of the nanocrystalline boron carbide should benefit applications ranging from cutting tools to body armor. They are currently exploring if their strengthening strategy can be expanded to other hard ceramics, such as silicon carbide.

1. Reddy, K. M., Guo, J. J., Shinoda, Y., Fujita, T., Hirata, A., Singh, J. P., McCauley, J. W. & Chen, M. W. Enhanced mechanical properties of nanocrystalline boron carbide by nanoporosity and interface phases. *Nature Communications* **3**, 1052 (2012).

Catalysis

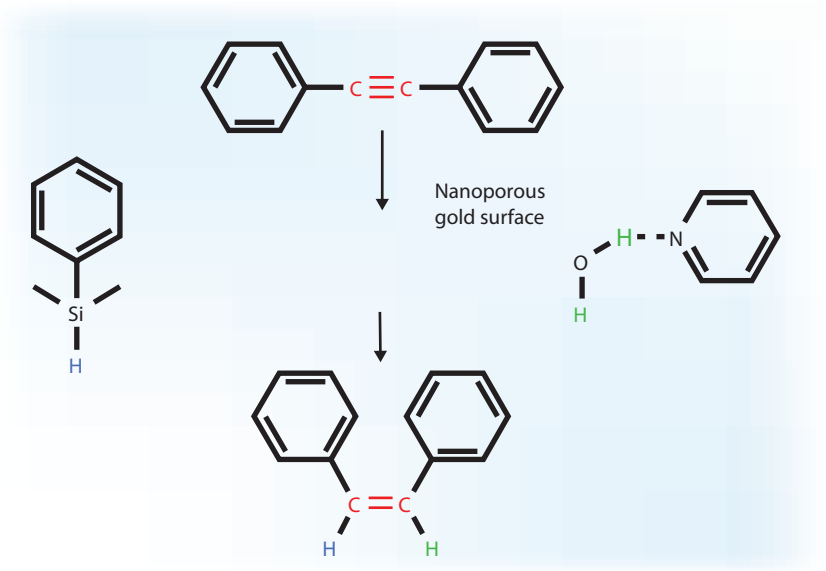
Going for gold

Porous gold catalyst proves useful in the selective reduction of carbon-carbon triple bonds to double bonds

Nanoporous gold catalysts have recently gained popularity due to their long lifetime and green credentials. As heterogeneous catalysts — in the solid state and dispersed throughout the reaction mixture — they are convenient to handle, in contrast to homogeneous ones which are dissolved within the reaction medium. They have proved to be efficient in highly selective oxidation reactions, such as the conversion of an alcohol group (consisting of a C–OH moiety with a single carbon–oxygen bond) to a carbonyl group (a double-bonded carbon–oxygen moiety). Until recently, however, nanoporous gold was thought to be inactive for reductive hydrogenation reactions.

Tienan Jin and co-workers from the AIMR at Tohoku University, in collaboration with researchers from Japan and China, have now shown that this catalyst can be used in the selective hydrogenation of alkynes to alkenes, where carbon–carbon triple bonds are reduced to double bonds (see image)[1]. Interestingly, the reaction is both chemoselective and Z-selective. This means that in addition to it not progressing all the way to a single bond, the two hydrogen atoms added to the alkyne moiety are always placed on the same side of the bond, forming what is known as a Z-alkene. "The accomplishment of perfect Z-selectivity and chemoselectivity has previously been unsuccessful in both homogeneous and heterogeneous catalytic processes," says Jin.

By replacing homogeneous palladium and platinum catalysts with the heterogeneous nanoporous gold, it has been possible to obtain higher yields of the desired alkenes. "Heterogeneous catalysts are also more robust than their homogeneous analogues and have a longer lifetime," explains Jin. "Additionally, they can be easily recovered by filtration and reused several times."



Alkynes can be efficiently reduced to alkenes on a nanoporous gold surface in the presence of organosilane, water and an amine.

To produce the catalyst, a thin gold–silver film, featuring three-dimensionally curved nanopores, was subjected to electrochemical dealloying. Control experiments using deuterium-labeled species revealed that organosilane and water, the hydrogen sources in the reaction, each contributed a hydrogen. An appropriate amine additive, such as pyridine, was also required to prevent the formation of molecular hydrogen.

Jin's team tested the nanoporous gold-catalyzed reaction on numerous alkynes, with both terminal (at the end of the molecule) and internal triple bonds. All showed complete conversion and almost all provided yields of above 90%.

"It is expected that nanoporous gold will not only be used in the selective reduction of various functional groups, but will also open opportunities for applications in more complicated heterogeneous catalytic methodologies for clean chemical synthesis," comments Jin. "In preliminary experiments, we have already succeeded in the application of the present catalyst systems to the selective hydrogenation of heteroaromatic compounds and carbonyl moiety."

1. Yan, M., Jin, T., Ishikawa, Y., Minato, T., Fujita, T., Chen, L.-Y., Bao, M., Asao, N., Chen, M-W. & Yamamoto, Y. Nanoporous gold catalyst for highly selective semihydrogenation of alkynes: remarkable effect of amine additives. *Journal of the American Chemical Society* **134**, 17536–17542 (2012).

IN THE SPOTLIGHT

The AIMR has grown rapidly since its inauguration in 2007, now with over 130 leading researchers from all over the world, including 32 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.

INTERNATIONAL WORKSHOP

Published online date 26 March 2012

A calculated approach to materials science research

The 2012 WPI-AIMR Annual Workshop held in Sendai, Japan on 20–24 February 2012 showed a maturing institute that is recovering well from the effects of the 2011 Great East Japan Earthquake

The WPI-AIMR Annual Workshop is a focal point of the intellectual life of the AIMR, and brings together members of the institute from across the world to discuss the latest developments in materials science and the work of the AIMR.

The 5th Annual Workshop, the first since the Great East Japan Earthquake that struck the region on 11 March 2011, causing widespread damage and loss of life, was held at the Sendai International Center from 20–24 February under the theme of "Cutting-edge Functional Materials for Green Innovation" and attracted 267 participants from 10 countries. As the research institution closest to the epicenter of the Great East Japan Earthquake, Tohoku University sustained heavy damage to much of its equipment. However, the university was able to resume most of its pre-earthquake activities in less than half a year due to the committed efforts of staff and students, supported by central government and municipal authorities and the determination of the local community to overcome the disaster. As part of the national effort of reconstruction and regeneration, a new International Research Institute of Disaster Science will be opened in 2012 at Tohoku University.

Current director, Yoshinori Yamamoto, February 2012

The 2012 Annual Workshop was also the first to be held since the opening of the Mathematics Unit as the fifth research group of the AIMR in March 2011, and the interaction between mathematics and materials science was given a central place in the workshop's program. The key role that mathematics is intended to play in the scientific direction of the AIMR in the next five years was mentioned by the current WPI director, Yoshinori Yamamoto in his welcoming address to delegates on the first full day of the workshop. "We strongly expect mathematics to accelerate 'fusion' and interdisciplinary research between the four existing research groups," said Yamamoto. "This is because mathematics is able to address fundamental issues from a wide range of research areas … we believe that interdisciplinary and fusion research catalyzed by mathematics will lead to an entirely new kind of materials science," he added.

Yamamoto, who has led the WPI-AIMR since its opening in 2007, will step down as director in April 2012 to be succeeded by Motoko Kotani, an internationally recognized mathematician and winner of the Saruhashi Prize, given to outstanding Japanese women scientists, which she received in 2005 for her work on Discrete Geometric Analysis of Crystal Lattices. Kotani is the current deputy director of the AIMR and head of the Mathematics Unit, and will become the first female director of a WPI center when she leads the AIMR from April 2012.

Incoming director, Motoko Kotani, February 2012

The theme of mathematics-guided materials science research was also emphasized by Akihisa Inoue, the president of Tohoku University, in his opening speech to the assembled delegates. Inoue began by praising the work of the AIMR, which, since its establishment, had "made tremendous efforts to advance research activities that fuse fields and create new disciplines while reforming and educating its research environment." Inoue also welcomed the challenges and opportunities

offered by the "new mathematical viewpoint" which he foresaw promoting "interdisciplinary and fusion research which will create a new materials science as well as developing innovative functional materials" and making a major contribution to the continuing development of the AIMR as a "unique and leading hub of the materials sciences in the world." The enhanced international character of the AIMR also won praise from the university president, who noted that 61 of the 127 researchers at the institute are non-Japanese nationals, and commended the role played by the 15 WPI-AIMR overseas partners and the three satellite institutions at the University of Cambridge; the University of California, Santa Barbara and the Institute of Chemistry at the Chinese Academy of Sciences.

Inoue also discussed the key role of the AIMR at Tohoku University, and noted that through the Tohoku University Action Plan (the Inoue Plan) the university promises to strengthen the organization of the AIMR to aid its development as an international research network. Furthermore he indicated that the university intends to extend its "maximum and continuing support" to the center after the completion of the WPI program to "establish an advanced institute of materials science as a world-leading center of intellect based on the achievements of AIMR."

The new focus on mathematics-guided materials science at the AIMR was also reflected in the academic program of the workshop, which began with a Mathematics–Materials plenary session chaired by Kotani and featured lectures on quantum mechanics, the theory of aperiodic solids and network formation and ion conduction in ionomer membranes. These were followed on the first day by sessions on bulk metallic glasses, materials physics and soft materials and over the course of the workshop by sessions covering other key aspects of the work of the AIMR, including systems and devices, soft materials, biodevices and materials chemistry. In total 39 lectures divided into 13 plenary and parallel sessions were presented during the three-day workshop, as well as a two-day poster session, which drew close to 90 contributions from AIMR researchers in Japan and overseas on a wide range of cutting-edge materials science research.

The 5th WPI-AIMR Annual Workshop was concluded on 24 February with a closing address from the director-in-waiting, Motoko Kotani. In this address, Kotani spoke of her vision of the AIMR as an institute driven by bottom-up fusion research guided by a mathematical understanding of the fundamental aspects of materials science, and indicated a number of areas as key topics for study, including non-equilibrium materials based on mathematical dynamical systems, topological functional materials, and multi-scale hierarchical materials based on discrete geometric analysis. Kotani ended her address by thanking the organizers, speakers and participants before inviting all present to join the next WPI-AIMR Annual Workshop to be held on 18–23 February 2013. ■

More than 260 participants from 10 countries took part in the 2012 WPI-AIMR Annual Workshop

DIRECTOR'S INTERVIEW

Published online on 28 May 2012

A new director, a new direction

The AIMR was established in 2007 as one of the inaugural research institutes of the World Premier International Research Center Initiative (WPI). In April 2012 the institute entered its sixth year of operation, with mathematician Motoko Kotani succeeding organic chemist Yoshinori Yamamoto as its second director

Motoko Kotani, director of the AIMR

The AIMR was founded in 2007 as one of the original WPI centers under an initiative of the Ministry of Education, Culture, Sports, Science and Technology of Japan and administered by the Japan Society for the Promotion of Science. In just a few years the institute has established itself as a leading center of materials research in Japan and is building a growing international reputation. Now entering its sixth year, the AIMR is about to embark on a new phase of development with a unique and ambitious mathematics-oriented approach to materials science research. Motoko Kotani, an internationally acclaimed mathematician and the institute's newly appointed director, talks to AIM*Research* about the successes of the past and her vision for the future of the AIMR.

AIM*Research: The AIMR recently celebrated its fifth anniversary. As its new director, how do you see the institute developing over the next five years?*

Researchers at the AIMR have produced exciting world-class research across a wide range of fields. Based on a long record of excellence in materials research at Tohoku University, the AIMR has taken a leading role in making important scientific breakthroughs in the fields of bulk metallic glasses and spintronics, as well as developing the areas of nanoporous materials and microelectromechanical engineering (MEMS). Using such achievements as a base, the AIMR is now looking to make the leap to the next level of research activity. The recent establishment of a mathematics unit will play a central role in this process. Until now, each of the research groups at the AIMR has concentrated on discovering new materials in their own unique fields of expertise, and they have been very successful in doing so. We now wish to discover new scientific principles based on a fundamental understanding of materials through fusion research. Mathematics will guide materials scientists in this approach by simplifying and giving uniform formulation for complex phenomena.

AIM*Research: You mention the increased use of mathematics in the work of the AIMR. How does the AIMR plan to integrate mathematics and materials science?*

Bringing together materials science and mathematics is a unique and rather ambitious idea. Initially we will focus on using an integrated mathematics approach to investigate three target materials that have found recent research success: namely non-equilibrium materials based on mathematical dynamical systems; topological functional materials; and multiscale hierarchical materials based on discrete geometric analysis. These are all wide-ranging themes, and it will take some time to investigate each of them thoroughly. Although we have formed a number of study groups to identify immediate, mid- and long-term goals for each theme, achieving substantial progress may take five or ten years, or perhaps even longer.

AIMResearch: One of the goals of the AIMR is to become a research center that is visible on the world stage. To what extent has this been achieved and how will the AIMR continue to develop its international presence?

Becoming internationally visible is a common goal of all centers in the WPI program, and we're doing pretty well in that respect. Surveys carried out by the Japan Society for the Promotion of Science indicate that name recognition of both the WPI program and the individual WPI centers is growing, and citation analysis shows that the number of WPI papers in the top 1% of cited research as a proportion of their total output is the second-highest in the world. The AIMR contribution to this achievement has been substantial; many of the papers we publish in top-level international journals go on to be highly cited. We appealed for international collaborators during development of the three new mathematics-driven materials research objectives I mentioned previously. Even though we set only a short window for applications, we had a very good response from scientists outside Japan who were interested in working with us. The AIMR also has 22 overseas partner universities including three satellite centers at the University of Cambridge, the University of California, Santa Barbara and the Chinese Academy of Sciences. We are in the process of creating joint laboratories with these institutions and are setting up more satellite centers to increase our international collaborations and broaden our global reach.

AIMResearch: The AIMR has the highest proportion of non-Japanese researchers among all six WPI centers. What is the secret to your success in this area?

All of our 'principle investigators' (PI) are extremely active in the international arena, which brings the work of our institute to the attention of a global audience. Another important factor is the longstanding pedigree of Tohoku University in materials research. Both of these factors are extremely helpful in attracting high-quality PhD students and postdoctoral researchers to the AIMR. We are proactive in recruiting outstanding scientists from overseas to participate in the work of the AIMR, and this helps us to attract more overseas students. Currently there are three types of foreign PIs: those who move here permanently to establish Japan as their main base of research; those who set up a sizable laboratory at the AIMR and spend several months a year here while maintaining a group in their home country; and those based at one of our partner universities abroad who send postdoctoral students to work on collaborative projects at the AIMR and thus form a bridge between the two institutions. Foreign PIs living abroad typically visit Japan once or twice a year to meet with their Japanese counterparts and discuss project progress. The joint laboratories at our satellite centers play an important role in facilitating academic exchange visits between the AIMR in Japan and partner institutions in foreign countries.

AIMResearch: One of the aims of the WPI movement is to change the academic culture of the center's home institution. In this context, what influence has the AIMR exerted on Tohoku University?

Tohoku University understands the special approach that we take towards research at the AIMR. We have been given a lot of freedom to develop the kind of academic and organizational style that suits us as an institute. As a result we have implemented a number of new initiatives, such as introducing a merit-based pay system, allowing staff to hold dual affiliations — which is rather unusual in Japanese institutes — and have taken a number of innovative measures to make our research and pastoral support services more flexible and responsive to the needs of our staff and students. Our intention is to see how this knowledge can be applied to the working practices of Tohoku University as a whole. To that end we will supply the university with an extensive dossier of our experiences at the AIMR. We anticipate that many of the initiatives and protocols established over the past five years will be taken up by other parts of Tohoku University, such as the Disaster Control Research Center and the recently established Medical Megabank. We hope that the work of the AIMR will have a major impact not only on the Japanese university system, but also on the entire field of materials science. ■

In April 2012 the AIMR entered its sixth year of operation

ROUNDTABLE INTERVIEW

Published online on 30 July 2012

Bringing mathematics to life

Ambitious plans by the AIMR to develop a new approach to materials science research driven by mathematics offers the prospect of great advances for materials scientists and mathematicians alike

Since its inception in 2007, the AIMR, as one of the inaugural research institutes of the World Premier International Research Center Initiative (WPI), has pursued a program of innovative cross-disciplinary research that brings together techniques and know-how from a range of materials science-related fields. This approach — dubbed 'fusion research' — has attracted the attention of the material science community and already led to several important discoveries in the field. Now entering its sixth year of operation, the AIMR has embarked on a new research trajectory, with the introduction of an ambitious program of mathematics-driven materials research.

The new approach is thought to be the first of its kind in the world, and is based on harnessing the power of mathematics to answer fundamental questions in material science to open up new areas of investigation in the field and to guide AIMR scientists in the most promising research directions. Although this bold initiative has the potential to deliver important new advances, challenges remain in applying the approach to concrete research goals.

Left to right: Takeshi Fujita, Natsuhiko Yoshinaga and Daisuke Hojo

Natsuhiko Yoshinaga, Mathematics Unit

To gain insight into some of the challenges and future directions of research at the institute, AIM*Research* talked to three young AIMR faculty members charged with the task of developing mathematics-driven materials science as part of their current research programs.

Merging ideas

Natsuhiko Yoshinaga is an assistant professor in the AIMR Mathematics Unit and a specialist in the mathematics of soft condensed materials. He is optimistic about the prospect of merging materials science and mathematics, while also recognizing the potential challenges that lie ahead. "The new approach is very interesting because it brings together two quite radically different styles," he says. "Traditionally, materials science research is largely empirical and involves a great deal of trial-and-error. By contrast, mathematics is all about setting clearly-defined parameters, then building and testing theories. Mathematics can help materials science research by providing mathematical tools to help make sense of experimental results."

Bridging differences in the two distinctive research cultures is considered to be key to the success of the new strategy, and careful selection of research goals is crucial. To this end, initial efforts will focus on three research areas: non-equilibrium materials based on mathematical dynamical systems; topological functional materials; and multiscale hierarchical materials based on discrete geometric analysis that the AIMR has

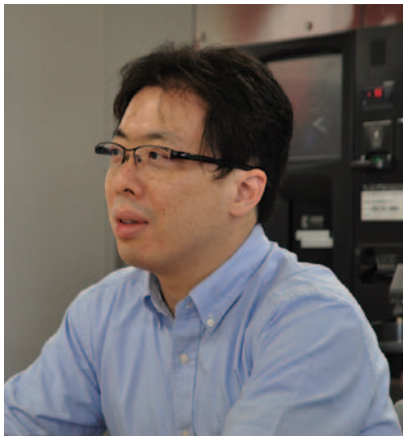
identified as being particularly suited to the mathematics-driven approach.

Some existing research themes at the AIMR are more likely to bear early fruit than others. Takeshi Fujita, associate professor of the Bulk Metallic Glasses (BMG) Group, shares his views on how mathematics can add value to his area of specialty: "Bulk Metallic Glasses are a good candidate for mathematics-driven research," he explains. "Our work already involves a lot of calculation — for example, when investigating the effect of packing patterns on the properties of new materials. We expect that working with our colleagues in the Mathematics Unit will help to identify the most promising research leads and increase the speed at which we can realize new advances."

Assistant professor Daisuke Hojo, a soft materials specialist in the Soft Materials Group at the AIMR, also sees great potential for the new approach. "We are currently researching the dispersive behavior of nanoparticles smaller than ten nanometers in non-polar solvents and building three-dimensional models of these systems," he explains. "We want to use mathematics in our group to investigate how distribution of electric charges in the particles changes with structure. We are also examining the effect of different dispersion models on structure based on mathematical calculations."

Brainstorm Friday

In addition to singling out specific problems in materials science for mathematics-driven treatment, the AIMR is spurring further integration of the two disciplines by encouraging "cultural exchange" between members of the mathematics group and other researchers at the institute through free discussion. As part of this initiative, researchers give informal talks on their research fields at a monthly event known as the "Friday Seminar" to colleagues from across the AIMR, as well as members of the Interface Unit, a group of theorists in physics and chemistry, set up as a bridge between mathematics and experimental materials scientists. Such activities offer an important way of connecting researchers with the wider mathematics community at Tohoku University and the Applied Mathematics Forum, an informal grouping of Tohoku University mathematicians.



Takeshi Fujita, Bulk Metallic Glasses Group

Seminars focus on introducing fundamental principles in each field as well as presenting new research results, with the aim of helping colleagues from other groups at the AIMR to gain a deeper understanding of the general background to a research field. The sessions are purposely interactive, and joining in discussions and asking questions are positively encouraged.

In addition to discussion seminars and the weekly "Friday Tea Time" poster sessions for which the AIMR is well-known, researchers are encouraged to interact informally as much as possible. "Brainstorming is a very important way to help mutual understanding of the different ways in which materials scientists and mathematicians see the world," says Hojo. "In our group, we meet with colleagues from the Mathematics Unit once a week to chat about what we've been doing, often without any formal focus. This kind of free discussion can lead to potentially interesting new ideas for experiments, or ways of improving our theoretical models."

Yoshinaga adds, "Being able to interact with researchers from a different discipline on a daily basis is very stimulating. More often than not, we don't have a fixed mathematical solution for problems in materials science, and so we need to work closely with our colleagues to develop a new approach or a different model. Some of the materials science research carried out here links in with really cutting-edge pure mathematics. Although we have only been working together for a short time, we have made a number of interesting advances in mathematics as well."

Daisuke Hojo, Soft Materials Group

Speeding progress, opening doors

The collaborative spirit that underlies fusion research at the AIMR has been a key theme from the very beginning, and now, with the addition of mathematics, this approach is being taken to the next level. Greater interaction between fields also opens up the possibility for researchers to publish papers in journals traditionally regarded as being out of their areas of specialty, leading to the exposure of their work to a more diverse audience.

"It is important to select research themes carefully," says Fujita, "but if we get that right, then application of the mathematics-driven approach should accelerate progress and increase our scientific output, as well as opening up brand new research fields."

By melding materials science with mathematics in this way, the AIMR continues its tradition of innovative fusion research directed at establishing new research frontiers, building on multidisciplinary exchanges, and ultimately developing breakthrough technologies for the benefit of the scientific community and human society. ■

SUMMER SCHOOL

Published online on 27 August 2012

Young researchers delve deeper into materials science

23–29 July 2012: The AIMR hosted an English-based Summer School program for international graduate students in Sendai, Japan

Students, supervisors and staff at the ASSM2012

The AIMR at Tohoku University recently welcomed 30 graduate level students from around the world – representing 13 different nationalities – to Sendai, Japan to learn from top materials science researchers at the 2012 WPI-AIMR Summer School of Materials Science (ASSM2012).

This one-week English-based summer school program, held over 23–29 July 2012, is a recent international initiative organized by the AIMR that will likely have an integral role in the institute's continued efforts to develop the world's next generation of leading researchers. It offered up-and-coming scientists and outstanding graduate students in fields such as physics, chemistry, materials science, electrical engineering, precision engineering and mechanical engineering a glimpse into materials science research and technology at the AIMR, hands-on experience using the institute's cutting-edge experiment equipment, and the opportunity to build a global network with AIMR researchers and other students.

Originally scheduled to be launched last year, the program was cancelled due to the Great East Japan Earthquake, but received almost 200 applications this year from Master's and PhD students all over the world wishing to attend. A selection committee made up of AIMR researchers carefully selected participants based on their academic background and motivation for joining the program.

With a theme of "Advanced Materials to Build a Better Future," the program consisted of morning lecture sessions given by the principal investigators of each of the AIMR's four main research groups (Soft Materials, Materials Physics, Device/Systems Construction and Bulk Metallic Glasses), followed by afternoon laboratory sessions in which pairs of students performed various experiments under the supervision of AIMR researchers.

AIMR Director Motoko Kotani officially commenced the summer school on the afternoon of 23 July with an opening address, in which she explained the aim of ASSM2012 is to offer students "a fruitful and productive opportunity to experience high-level and advanced research," and emphasized the importance of bringing young scholars together to build networks for future research. "These networks will be indispensable for humans as they tackle many complicated obstacles, which are unprecedented in the history of the human race. I believe the foundation of the AIMR networks is composed of the networks formed among students and researchers."

Spending the next four days with some of the world's top materials science researchers gave the students a valuable opportunity to do just that. Professor Kazue Kurihara, principal investigator of the Soft Materials Group and current president of the International Association of Colloid and Interface Scientists, delivered the first lecture of the week on Tuesday morning by discussing the measurement of surface forces for nanomaterials science and technology.

After each lecture, students proceeded to four-hour laboratory sessions on topics that ranged from making nano-sponge metals to fabricating hydrogels for cell encapsulation and drug delivery. This balance of classroom instruction from leading researchers with laboratory time using advanced equipment exposed the students to many fascinating aspects of materials science and introduced them to the research goals and achievements of the AIMR.

AIMR researchers supervised summer school participants in various laboratory sessions

Students presented their work over the last two days of the ASSM2012

The following days featured more lectures from renowned researchers. Professor Katsumi Tanigaki of the Materials Physics Group spoke on the functions of nanomaterials and their industry applications, while Professor Terunobu Miyazaki of the Device/Systems Construction Group discussed the importance of magnetic materials and how magnetism can be understood intuitively. Tanigaki is a former research leader at NEC known for his contributions to superconductivity research, and Miyazaki is the pioneer of tunneling magnetoresistance (TMR) and the 2009 recipient of the Oliver E. Buckley Condensed Matter Prize of the American Physical Society, considered the most prestigious award in the field of condensed matter science.

The final lecture of the course was given by Professor Alain Reza Yavari of the Bulk Metal Glasses Group, who in 2011 received the Award for Scientific Excellence from the French National Center for Scientific Research (CNRS). One of the highest ranking researchers at CNRS, his lecture covered metallic glasses from bulk metallic glasses down to a microscopic scale.

After the lecture and laboratory sessions wrapped up on Friday afternoon, the students prepared for a full weekend of discussions and presentations to conclude the intense week of learning, but not before experiencing a slice of Japanese culture by painting *kokeshi* (traditional handmade Japanese dolls) at the Zao Royal Hotel.

A closing ceremony was held after the final presentations and discussions on Sunday afternoon, where students were presented with certificates of successful completion of the course. It marked the end of a productive week for the students and AIMR researchers, one that helped the AIMR and Tohoku University to carry out their commitment to supporting the development of young researchers around the world. ■

Director Kotani (right) presented students with certificates marking their successful completion of the summer school program

ROUNDTABLE INTERVIEW

Published online on 26 November 2012

Marrying materials with mathematics

By bringing different areas of materials science together and now building bridges with mathematics, the AIMR is stepping out in a truly original direction. Where to? A definite answer is not expected for another several years, but clues are already emerging

Since its launch in 2007, the AIMR has unwaveringly encouraged materials scientists with different backgrounds, expertise and research interests to work together. "This approach stems from the idea that it is not sufficient to gather a collection of excellent researchers to achieve truly original research," explains Masaru Tsukada, the AIMR's administrative director. "Much can be learnt from crossing frontiers," says Mingwei Chen, the Target Project (TP) leader of the Non-equilibrium Materials project. Entering the second 5-year phase of its development, the AIMR is building on its ongoing 'fusion research' by taking another significant step: incorporating mathematics.

Integrative and targeted

The AIMR has established three 'target projects' (TPs) that combine materials science research expertise with topics of interest to mathematicians — namely, Non-equilibrium Materials Based on Mathematical Dynamical Systems, Topological Functional Materials and Multi-scale Hierarchical Materials Based on Discrete Geometrical Analysis.

Chen explains that a good understanding of non-equilibrium phenomena relies on mathematic dynamics. Tadafumi Adschiri, the TP leader of Multi-scale

Masaru Tsukada, the administrative director of the AIMR

Hierarchical Materials, agrees: "What we are embarking on with our mathematician colleagues is the analysis of the materials' properties — from our characterization, but from a mathematics point of view." A longer-term goal is to close the loop back from mathematics to materials, and use the models to predict which materials should be synthesized for specific uses.

Hierarchical materials are also particularly intriguing for mathematicians, as understanding the behavior of atoms does not easily translate into an understanding of a material's properties. Taro Hitosugi, sub-leader of the Multi-scale Hierarchical Materials project, elaborates: "As the atoms aggregate into clusters and extended materials, different properties emerge — in the same way that cells form organs, and organs form human bodies. What we are now trying to do, together with mathematicians, is to establish a link between the atoms (discrete points) and the bulk material (a continuum)."

This mathematics-driven approach may lead to a conceptual revolution of the research interests of topological functional materials. Katsumi Tanigaki, the TP leader of the Topological Functional Materials project, works on semiconductors, for which inorganic materials such as silicon have traditionally been used. With flexible semiconductor devices being touted as the next technological target, inorganic-based semiconductors may no longer be the best choice. "For big changes we need new ideas, both from theory and experiments," says Tanigaki. "We are now trying to use organic-based semiconductors for spintronics as well as electroluminescent devices in place of inorganic semiconductors, and we have had some success. The theory part is where we'll work with mathematicians."

"The AIMR's mathematics-driven strategy provides an important framework which guides the projects in a particular direction," Tanigaki continues. "This is a challenging approach that may well enable us to find something very original and exciting. Marrying materials with mathematics like this is a brand-new area."

Interfacing between disciplines

In the target projects, the traditional approach to collaboration is reversed: the mathematicians and materials scientists first team up together, then search for a common interest and identify a project that can benefit both parties.

Even when a suitable project has been identified, challenges can arise. Specialist terminology, for example, varies across the disciplines, which can hinder communication. To address this, the AIMR hosts a series of informal, interdisciplinary team meetings where researchers can learn more about each other's discipline and research interests. When each member presents their own research, common interests and novel research avenues emerge. In the Multi-Scale Hierarchical Materials project, for example, Hitosugi is fascinated by interfaces at the atomic level whereas other project members are interested in the continuum of bulk properties. "These differences, and how to get passed them, is the essence of the target program," he says. "It is a good chance for us to go in a totally new direction."

The AIMR has also enlisted the help of 'interface researchers', theoretical physicists and chemists who do not belong to any specific research laboratory, but can freely collaborate with any group. According to Adschiri, they play the most important role in bridging the gap between disciplines. Tsukada explains: "They can communicate efficiently with both parties, thus efficiently conveying messages and connecting people." New to the AIMR, these independent researchers are already facilitating communication.

Blurring borders

Concomitantly, working on the target projects has started to influence the researchers' methods in their own, more 'conventional' research. Tanigaki notes that this unusual collaboration is already impacting the way his team works — before they characterized materials and looked for ways to improve them, but now they employ modeling as well. He adds: "What interests mathematicians in topological materials are the topology and geometry aspects, not whether it is inorganic or organic, and working with this in mind is very interesting."

Chen is also excited that he has been able to expand his work, modeling a variety of glasses and working towards establishing some universal rules. "By broadening our interests we have also started to work on porosity — a pretty intriguing new direction," he says. Such interdisciplinary research provides invigorating challenges, especially for younger researchers who are still establishing their own research progression.

"We are waiting for that big result that will be our success story," says Tanigaki. As such major achievements usually take years or decades of research, the AIMR's 5-year mathematics-focused initiative presents AIMR researchers with another challenge as they aim to produce results in a compressed timeframe. Each year the TPs are required to achieve fixed goals, and the AIMR monitors their progress in reaching these annual targets. In these early stages, it is encouraging that some milestones have already been reached and joint papers between materials scientists and mathematicians have been published.

"All researchers agree that the AIMR is embarking on a bold strategy and it is difficult to forecast the results," summarizes Chen. Tsukada agrees that it is a very ambitious project, something that the program committee members of the World Premier International Research Center Initiative (WPI) recognize. "It is a challenge, but we believe it will lead to some utterly original and excellent research," says Tsukada. ■

Left to right: Masaru Tsukada, Mingwei Chen, Taro Hitosugi and Katsumi Tanigaki

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