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Editorial

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MESSAGE FROM THE DIRECTOR

Making great progress through mathematics–materials science collaboration

As the director of the Advanced Institute for Materials Research (AIMR), Tohoku University, it is my great pleasure to welcome you to the fifth print edition of *AIMResearch: Research Highlights*. Each month, we publish a selection of the AIMR's distinguished research results on our bilingual website, research.wpi-aimr.tohoku.ac.jp. This publication is a collection of the research highlights and feature articles that appeared online in 2013.

The AIMR was launched in 2007 as one of the inaugural research centers under the World Premier International Research Center Initiative (WPI) program initiated by the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). The program aims to create globally visible research centers within Japan. As such, the AIMR is fostering an ideal research environment

and becoming a hub that attracts and circulates the world's best minds in materials science.

Another objective of the WPI research centers is to create new scientific fields through interdisciplinary fusion. At the end of 2010, the AIMR decided to establish mathematics–materials science collaboration at the institutional level, creating a new materials science that is appropriate for the twenty-first century.

Society currently faces serious environmental and energy problems. To solve these problems efficiently, we have to design and produce functional materials based on theoretical prediction. As mathematics can provide a common language for all scientific disciplines — and has the power to rearrange and integrate the full breadth of materials science — mathematics is our focus.

We spent the two years prior to 2013 rearranging our internal

organization accordingly. We first established the Mathematics Unit consisting of two mathematics laboratories. Then, members of the AIMR reformulated materials research themes from a mathematical viewpoint and set three Target Projects: Non-equilibrium Materials based on Mathematical Dynamical Systems; Topological Functional Materials; and Multi-scale Hierarchical Materials based on Discrete Geometric Analysis.

In setting these projects, we identified the need for interpreters who can bridge the gap between mathematics and materials science. Consequently, we established the Interface Unit that consists of young theoretical researchers in physics, chemistry and applied mathematics. Rather than belonging to a specific laboratory, these independent researchers can freely access any materials scientists and mathematicians at the AIMR. Our

assembly of materials scientists and mathematicians has now completely fused and integrated.

We consulted widely on our approach because the mathematics–materials collaboration is an ambitious challenge that is accompanied by infinite possibilities of producing historical breakthroughs. The challenge is also accompanied by the prospect of discovering problems attractive to both materials scientists and mathematicians.

The AIMR achieved substantial progress as a result of the mathematics–materials science collaboration during 2013. For example, we successfully characterized the atomic structure of icosahedral clusters in bulk metallic glasses. We also revealed atomic-scale competition in energy and geometry for glass formation using computational homology, an advanced mathematical concept but not a tool of conventional

theoretical physics. (This topic was published as a research highlight in 2013 entitled “Metallic glasses: All in order” and appears on page 16 of this collection.)

Globalization also featured as an achievement in 2013. To strengthen cooperation with international satellites, AIMR Joint Research Centers (AJCs) established laboratories at the University of Cambridge, United Kingdom, and the University of California, Santa Barbara (UCSB) in the United States. The AJCs have clear roles in joint research and in increasing the AIMR’s international visibility.

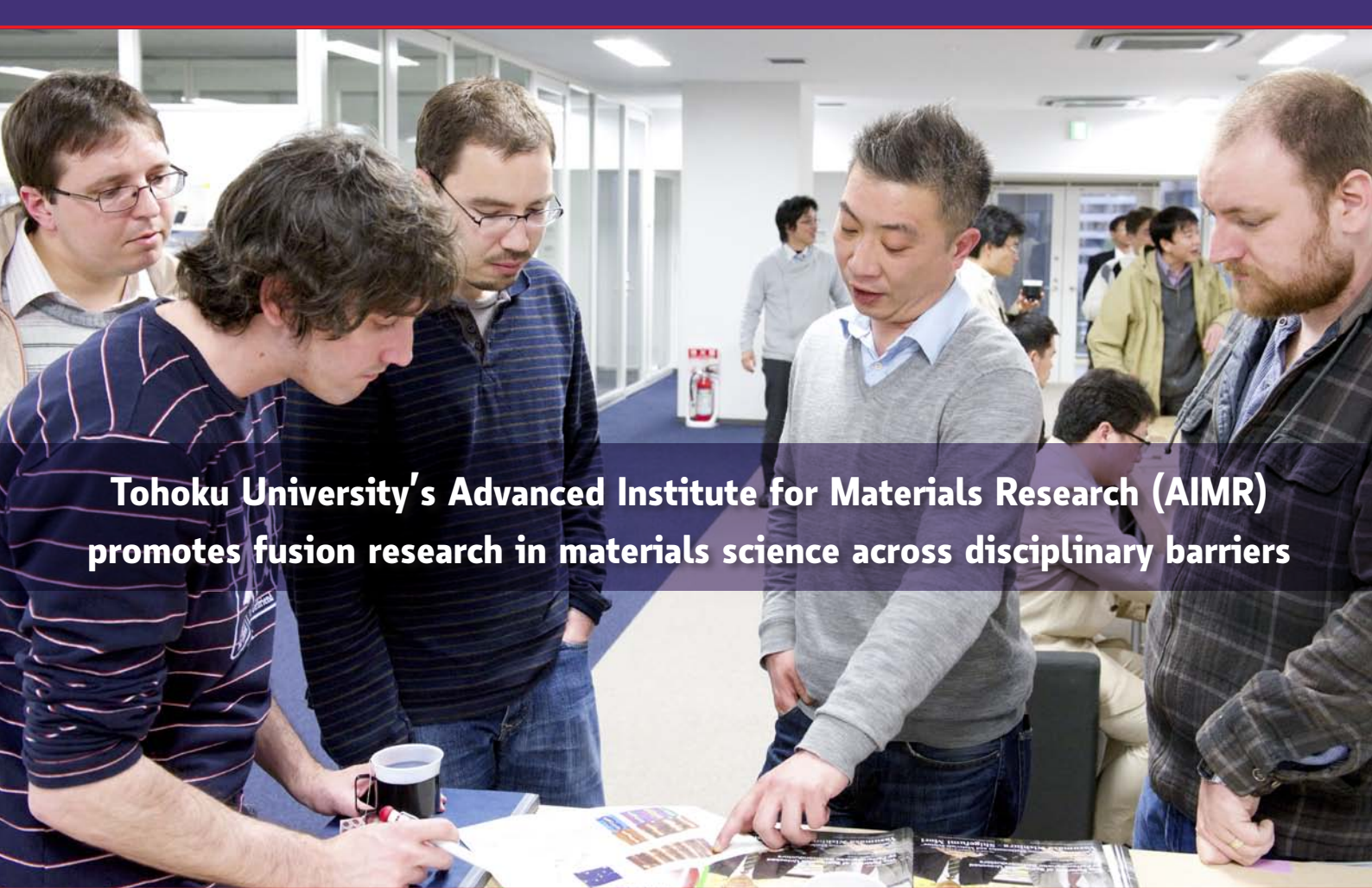
In 2013, we held workshops with UCSB in February and the University of Cambridge in November. The AIMR’s international visibility will also benefit from further reinforcement of our Public Relations & Outreach Office.

In the seven years since its inauguration, the AIMR has produced promising results. This



is largely due to a strong belief in the significance of our approach and the fact that we are supported by solid cooperation between researchers and administrators. As such, I believe that we can deliver ground-breaking research findings in the following years.

Motoko Kotani
Director
AIMR



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

The AIMR is leading the world in facilitating collaboration between materials science and mathematics. In an environment where more than half of the researchers come from abroad, scientists at the AIMR — young and international included — contribute to discussions and joint research projects, enabling the AIMR to achieve world-leading research results.

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Latest research highlights

- Superhard materials: Shear resolution
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- Spintronics: Using nature's symmetries



RESEARCH HIGHLIGHTS

The AIMR advances research in bulk metallic glasses, materials physics, soft materials and device/system 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 complements the AIMR's research activities, and the Interface Unit further supports their integration.



Graphene

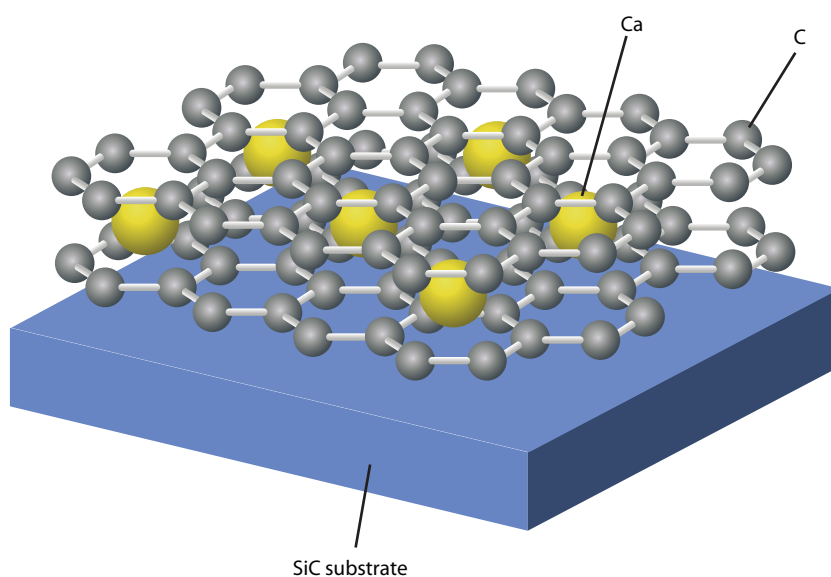
Superconductivity thinned down

Production of the thinnest possible carbon-based superconductor could herald functionalized graphene materials

Graphene has a well-earned reputation as a ‘wonder material’. Isolation of these one-atom-thick sheets of carbon that make up graphite — a material best known for its use in pencils — has opened an avenue for the study and utilization of two-dimensional materials. Bulk graphite has also attracted interest in its own right, especially for its potential practical applications. In particular, the insertion of substances between its graphene layers to form ‘graphite intercalation compounds’ (GICs) has been investigated as a method for the storage of lithium atoms within batteries. Interestingly, some GICs can also conduct electricity without any resistance — an attractive phenomenon known as superconductivity.

Now, by trapping calcium atoms between just two layers of graphene, Katsuki Sugawara and co-workers from the AIMR and the Department of Physics at Tohoku University have constructed a carbon-based superconductor at its two-dimensional limit¹ (see image). Their ‘sandwich’ material offers the advantages of bulk graphite while being as thin as it can possibly be. With the production of this graphene–calcium material, the researchers have constructed the thinnest possible form of the calcium-based GIC C_6Ca .

Among the known superconducting GICs, C_6Ca is arguably the most interesting as it develops superconductivity at a higher temperature than any other. Sugawara and co-workers were able to reduce the thickness of the graphene layer that surrounds the calcium atoms to the absolute minimum. The thin graphene–calcium–graphene material was produced by first introducing lithium



Schematic view of the calcium-based graphite intercalation compound (GIC) C_6Ca . Calcium atoms (Ca, in yellow) are inserted between two sheets of graphene, which are made of carbon atoms (C, in gray). The graphene–calcium sandwich is supported by a silicon carbide (SiC) substrate.

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into a bilayer graphene film supported by a silicon carbide (SiC) substrate — a less challenging task than the direct introduction of calcium, due to the smaller size of the lithium atoms. Subsequently, they replaced the intercalated lithium atoms by depositing calcium onto the graphene–lithium–graphene intermediate, followed by heating. “We had initially developed this method for making millimeter-thick C_6Ca , and have now improved it for use in bilayer-graphene films,” explains Sugawara.

Despite the thinness of the material they created, the scientists were able to successfully perform a number of experiments on it. “The most important result of our study is the characterization of the electronic structure in this

thinnest limit of a GIC,” notes Sugawara. “Our findings should form a basis for understanding superconductivity in GIC systems.” The team now hopes that the same approach will be useful for other GIC applications, including the creation of efficient microbatteries. “This research area should help to gain a fundamental understanding of the physics and chemistry relevant to state-of-the-art batteries using graphite as an electrode,” says Sugawara.

1. Kanetani, K., Sugawara, K., Sato, T., Shimizu, R., Iwaya, K., Hitosugi, T. & Takahashi, T. Ca intercalated bilayer graphene as a thinnest limit of superconducting C_6Ca . *Proceedings of the National Academy of Sciences USA* **109**, 19610–19613 (2012).

Supercapacitors

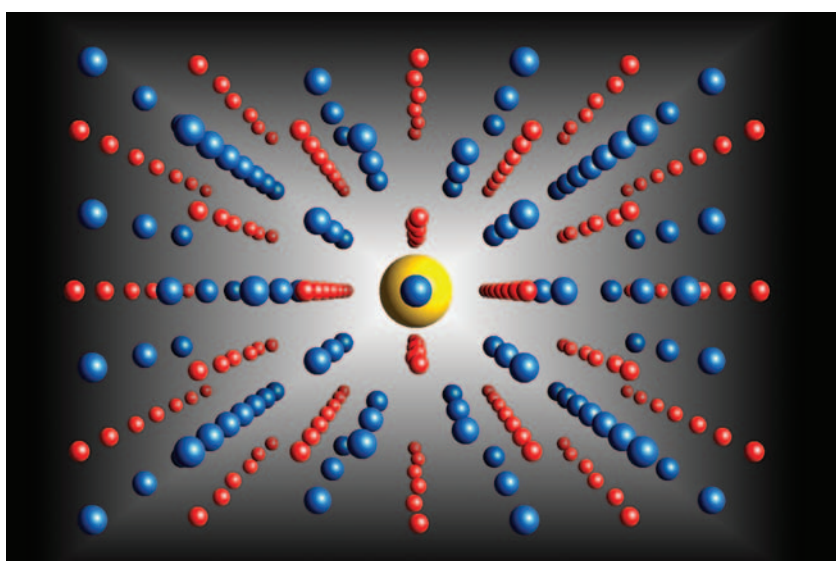
Better with a dash of gold

An innovative deposition technique may help to jumpstart a new generation of high-speed energy storage materials

Supercapacitors aim to surpass batteries by combining immense energy storage with lightening-quick charge times. Manganese oxide (MnO_2) is a promising material for these devices because of its low cost, nontoxic properties and ultrahigh capacitance. However, the compound's intrinsically low conductivity renders electron transport difficult. So far, only nanometer-thin films or low-density nanoparticle dispersions of MnO_2 have displayed the desirable supercapacitance, but unfortunately these structures are too small to deliver adequate power for most applications.

Mingwei Chen, Jianli Kang and colleagues from the AIMR at Tohoku University have now devised a strategy to boost the conductivity of MnO_2 thick films by fashioning them into unconventional nanoporous electrodes that incorporate gold atoms within their oxide lattice¹. First, the team synthesized a porous MnO_2 electrode by electrochemically depositing a nanoscale film with needle-like arrangements onto a gold-polymer substrate. Despite the structure providing plenty of surface sites for energy storage, the electrode's capacitance dropped dramatically when the film's thickness exceeded 350 nanometers, owing to MnO_2 's poor conductivity.

The researchers then bombarded the MnO_2 electrode with gold atoms from a physical vapor deposition system, using a process known as sputtering. Repeating the sequence of MnO_2 electrochemical growth followed by gold 'doping' several times enabled the construction of micrometer-thick electrodes ready for use as supercapacitors. X-ray and electron microscopy analysis revealed that this technique replaces 10% of the MnO_2 with



View of the crystal structure of manganese oxide (MnO_2) (blue and red spheres) doped with an atom of gold (yellow sphere). New findings reveal that this kind of material is ideal for supercapacitors.

© 2013 Mingwei Chen

electron-rich gold dopant atoms that are distributed evenly throughout the oxide (see image). Alternate layering of MnO_2 and gold atoms ensures the dopants are well-integrated within the oxide's lattice and not just physically absorbed, Chen notes. "The electrochemical deposition helps sputtered gold travel to the electrode/electrolyte interface to occupy MnO_2 lattice sites."

The gold-doped MnO_2 was found to have a capacitance 65% higher than that of comparable pure films — the best charge storage ever achieved from thick MnO_2 electrodes. The new material showed outstanding stability and even increased its charge capacity after a few hours' use due to electrochemical dopant redistribution during voltammetric cycling. Collaboration with Kazuto Akagi's research team at the AIMR

uncovered a fundamental theoretical principle behind these findings: gold dopants transfer electrons to manganese and oxygen atoms equally, boosting the entire material's conductivity.

"Manganese oxide is the most promising material for electrochemical supercapacitors," says Chen, adding that "doping is the easiest and best way to improve its conductivity." By implementing an often-considered but rarely realized concept, the team is confident that their doping approach will benefit future commercialization efforts of MnO_2 thick-film devices.

1. Kang, J., Hirata, A., Kang, L., Zhang, X., Hou, Y., Chen, L., Li, C., Fujita, T., Akagi, K. & Chen, M. Enhanced supercapacitor performance of MnO_2 by atomic doping. *Angewandte Chemie International Edition* **52**, 1664–1667 (2013).

Organic spintronics

What matters in the long run

Experiments on fullerene films show that electron spins can be preserved for long distances in optimized organic compounds

An ability to control the spin of the electron would enable the design of spintronic devices that are more efficient than current electronic ones. Research efforts have so far focused on solid-state inorganic materials that can be fabricated to a high purity, easily incorporated into devices and whose composition can be precisely controlled. However, organic materials also pose several advantages, including low processing costs and the opportunity to control their physical properties through careful chemical modification.

Since organic compounds are typically made from light elements — primarily carbon — the spin-orbit interaction, which couples the spin momentum with the angular momentum of the electron, is quite small. This means that the electron spin can be preserved for a long time and electrons can, in principle, travel long distances without flipping their spin. Until recently, the longest distances travelled at room temperature were in the few tens of nanometers and a greater distance had only been observed at a low temperature. Xianmin Zhang and co-workers have now realized devices based on an organic material in which the electrons can travel distances of up to 110 nanometers at room temperature, while preserving their spin¹ (see image).

The researchers constructed their devices from films of fullerene (C_{60}), a molecule which has low spin-orbit interactions as it consists solely of carbon atoms. The absence of hydrogen — common in other organic materials — serves to reduce the hyperfine interactions between electron and nuclear spins that can induce spin-flipping events. Zhang

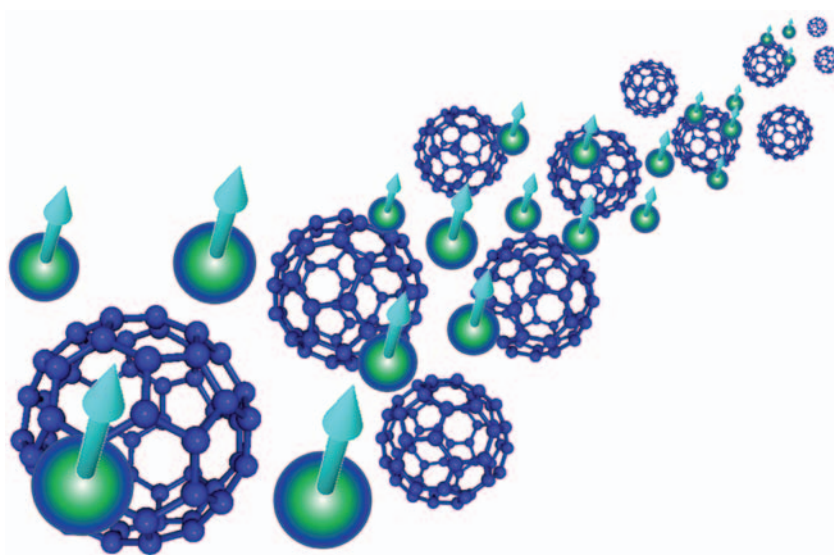


Illustration of the fullerene films in which electrons preserve their spins over long distances. Fullerenes (blue), electrons (green spheres) and electron spins (arrows) are shown.

and colleagues fabricated organic spin valves, in which two ferromagnetic electrodes are placed in contact with an organic layer, and measured their magnetoresistance, which is the difference in electrical resistance when the spin valve's electrodes are magnetized in the same or opposite direction. Magnetoresistance is therefore a measure of the conservation of the electron's spin polarization.

By studying devices composed from various thicknesses of the C_{60} film, the team observed a record value — of up to 110 nanometers in length — for magnetoresistance at room temperature. Zhang explains that it may be possible to further improve on these results as,

according to theory, a spin length of over 400 nanometers can be obtained in crystalline C_{60} — although fabricating films of such a well-ordered material would be quite challenging.

According to Zhang, the significance of the team's results is not limited to C_{60} : an understanding of spin transport in these films could inspire chemists and engineers to design even more efficient compounds and devices.

1. Zhang, X., Mizukami, S., Kubota, T., Ma, Q., Oogane, M., Naganuma, H., Ando, Y. & Miyazaki, T. Observation of a large spin-dependent transport length in organic spin valves at room temperature. *Nature Communications* **4**, 1392 (2013).

Superconductors

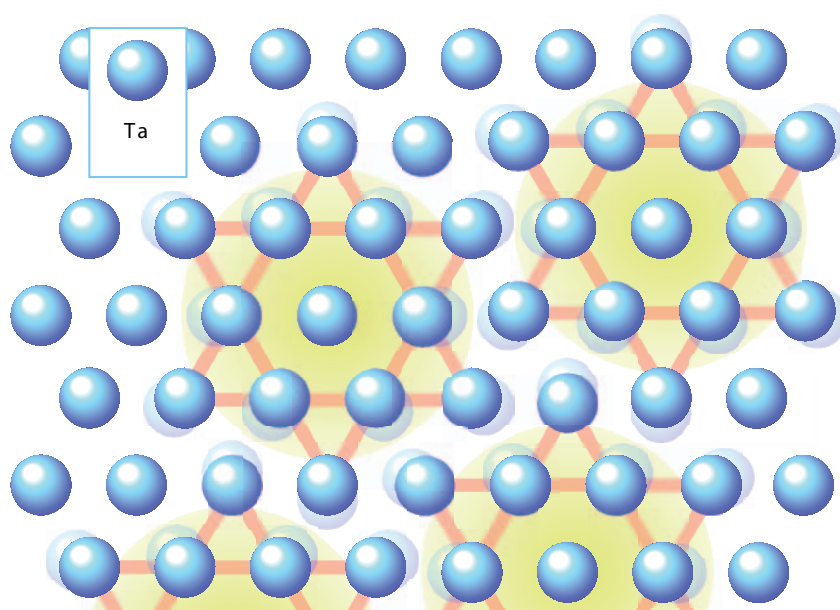
Riding the wave

The coexistence of superconductivity and a wave-like, charge-ordered phase in iron-doped $1T\text{-TaS}_2$ offers a deeper understanding of high-temperature superconductivity

Understanding the origin of superconductivity in high-temperature superconductors remains a major question in physics and is crucial for the development of superconductors that can operate at higher temperatures. However, unraveling the phenomenon is complicated by the fact that electronic properties — such as magnetism — which usually prevent superconductivity, appear to play an important role in the superconducting state at such temperatures. An international team led by Takashi Takahashi and colleagues from the AIMR at Tohoku University has now shown that superconductivity may coexist with these competing states¹.

Superconductivity originates from the existence of pairs of electrons that can roam a crystal without losing energy. In conventional superconductors the formation of such electron pairs is facilitated by oscillations of the atoms in the crystal. However, in high-temperature superconductors other factors including magnetism seem to play a role, despite conventional theory determining that magnetism and superconductivity cannot coexist.

The researchers studied $1T\text{-TaS}_2$, a material consisting of layers of the elements tantalum (Ta) and sulfur (S), as well as its iron-doped derivatives. At lower temperatures the tantalum atoms in $1T\text{-TaS}_2$ arrange into a so-called ‘Star of David’ pattern (see image) and exhibit an insulating behavior in which periodic variations in the density of electrons — known as charge-density waves (CDWs) — arise across the material. Typically, superconductivity and the CDW state are considered to be mutually exclusive. Yet the researchers found that when some of



Tantalum (Ta) atoms organize into a ‘Star of David’ pattern in the charge-density wave (CDW) phase of $1T\text{-TaS}_2$.

the tantalum atoms were replaced with iron, superconductivity could occur.

Takahashi and colleagues used high-resolution angle-resolved photoemission spectroscopy (ARPES) — a technique in which light pushes electrons out of a material — to investigate $1T\text{-TaS}_2$. Measuring the energy and momentum of the ejected electrons provides a direct window into a material’s electronic state. The researchers identified a shallow electron pocket, believed to be characteristic of superconductivity, within $1T\text{-TaS}_2$ in the nearly commensurate CDW (NCCDW) state — a CDW phase that forms at higher temperatures and particular concentrations of iron. “The unique feature of this method is to reveal the electronic states responsible for the CDW state as well as the superconducting state.

This would not be possible with other experimental approaches,” explains team member Ran Ang.

The team was able to show that superconductivity and the CDW state are not separated within $1T\text{-TaS}_2$ crystals but instead coexist, representing an intrinsic property and offering valuable insight into the origin of high-temperature superconductivity. In addition, the ability to control the CDW phase — by switching between the material’s normal metallic and insulating states — has potential for application in electronic devices.

1. Ang, R., Tanaka, Y., Ieki, E., Nakayama, K., Sato, T., Li, L. J., Lu, W. J., Sun, Y. P. & Takahashi, T. Real-space coexistence of the melted Mott state and superconductivity in Fe-substituted $1T\text{-TaS}_2$. *Physical Review Letters* **109**, 176403 (2012).

Microscopy

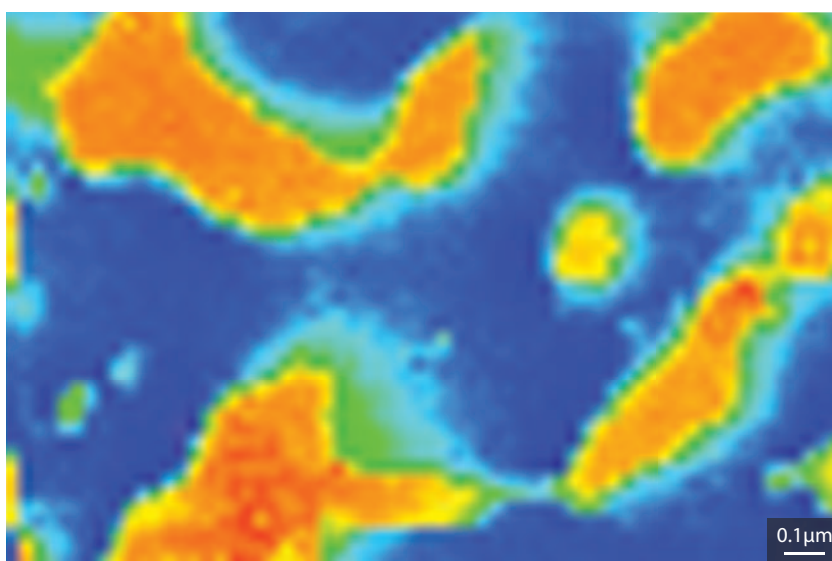
Where rubber meets the probe

A ground-breaking microscope design reveals the nanoscale mechanical properties of rubber surfaces in unprecedented detail

Rubber is an important class of material with applications ranging from high-performance devices to the humble car tire. But characterizing the complex blend of cross-linked polymers and carbon ‘filler’ particles that comprises rubber is far from straightforward. To better investigate its composition, researchers have turned to atomic force microscopy (AFM) — a technique that uses tiny, oscillating silicon probes to measure the physical properties of surfaces.

Conventional AFM instruments are unable to fully investigate the behavior of rubber because their probes cannot vibrate sufficiently fast across different frequencies. Now, Ken Nakajima and colleagues from the AIMR at Tohoku University have solved this problem with a design that uses so-called ‘piezoelectric’ crystal actuators to boost the sensors’ vibrational capabilities¹. While actuators allow the three-dimensional scanning of surfaces, they are designed for large movements, meaning that AFM instruments have a limited frequency range. To obviate this issue, the researchers inserted an additional piezoelectric actuator — small, lightweight and with large resonant frequencies — above the AFM scanner to simultaneously oscillate the sample and probe it up to 20,000 times per second.

The team tested its design on a series of isoprene and styrene-butadiene rubbers. First, they determined mechanical contact parameters by recording how increasing force deformed the materials. They then compared the amplitude and phase of AFM signals from the rubbers to those of a solid mica surface. Repeating the measurements at different frequencies generated ‘viscoelastic’



An atomic force microscopy ‘map’ of the mechanical loss of a rubber surface, which reveals an ‘island–sea’ arrangement of immiscible rubbers. Such maps can be created at different frequencies to fully visualize the surface’s nanoscale features.

parameters that described the rubbers’ dynamic deformation.

Two-dimensional ‘maps’ of the mechanical loss of a mixed rubber surface were created using the AFM scanning functions (see image). These revealed an ‘island’-like arrangement of nanoscale isoprene rubbery regions surrounded by a ‘sea’ of styrene-butadiene rubbery regions. Critically, the immiscible nature of the rubbers only became clear when scanning at a certain range of frequencies.

Nakajima notes that the ability to measure frequency-dependent deformation can eliminate many of the time-consuming tests currently needed to characterize rubber. “In viscoelastic materials, frequency and temperature are believed to be related. Therefore, measurements with narrow frequency

ranges must be performed at multiple temperatures. Our instrument can carry out these measurements with a much wider frequency range at a fixed temperature,” he says.

Furthermore, explains Nakajima, the AFM measurements match many of the frequencies encountered during macroscopic testing. Such direct comparisons of large- and nano-scale phenomena are vital to comprehend multi-component systems. “Our technique can visualize the viscoelastic nature of each component in high resolution, giving valuable feedback for future materials design.”

1. Igarashi, T., Fujinami, S., Nishi, T., Asao, N. & Nakajima, K. Nanorheological mapping of rubbers by atomic force microscopy. *Macromolecules* **46**, 1916–1922 (2013).

Glasses

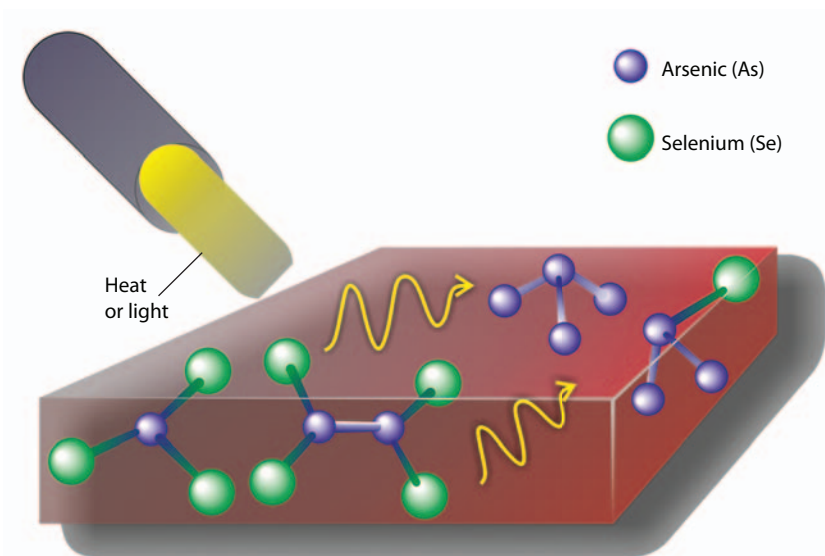
From disorder to disorder

A new type of phase transition in amorphous materials raises fundamental questions about glasses and could lead to faster computer memory

Phase-change materials are of great importance in modern computing due to their use in rewritable optical disks and computer memory. They are particularly suitable for these applications as they can be made to undergo a fast, reversible transition induced by light or electrical pulses. These transitions cause their molecular structure to change from an ordered crystal to an amorphous state resembling that of glass. Materials in these two states have vastly different physical properties, such as their ability to reflect light or conduct electricity, and this phenomenon can be used to encode the 'on' and 'off' states of digital bits.

An international team of researchers, including Jiri Orava from the AIMR at Tohoku University, has now discovered a completely new type of phase transition in which the material switches between two different amorphous states¹. The amorphous-to-amorphous transition is fundamentally different to known amorphous-to-crystalline transitions, and even to previously known amorphous-amorphous transitions, according to Orava.

The researchers studied $\text{As}_{50}\text{Se}_{50}$, which is composed of equal amounts of arsenic (As) and selenium (Se). When freshly deposited as a thin film, the material is amorphous but if heated to high temperatures and slowly cooled it becomes crystalline. However, the team discovered that when only moderately heated, $\text{As}_{50}\text{Se}_{50}$ transitions to a different — and stable — amorphous state. Similarly, when irradiated by laser light, the newly grown material forms another stable amorphous state. These two states can be distinguished by measuring the bonding energy between



Heating, as well as illuminating, a thin film of $\text{As}_{50}\text{Se}_{50}$ causes a reversible transition from one amorphous state to another.

the arsenic and selenium atoms, which provides a unique fingerprint for the atomic configuration.

Transitions between different amorphous states are not unknown, but previously had only been observed in materials subjected to pressure. The change studied here can be induced through heating, suggesting that a further mechanism is responsible for these amorphous-to-amorphous transitions. This mechanism is of particular interest because the material can be reversibly switched between the two amorphous states through successive annealing and laser-exposure cycles. Switching is thought to occur at milli- to microsecond intervals.

Reversible switching between amorphous states resembles previously discovered amorphous-to-crystalline

transitions used in other applications. However, the new system offers the advantage that the switching process requires far less energy. "The changes in atomic arrangement take place with a relatively low cost of energy; no melting is required," comments Orava. Moreover, the new switching paradigm involves far fewer atoms than switching to an ordered crystal, suggesting it could be used to create computer memory devices. Verifying the dynamics of this transition and its benefit for applications remains an aim of future research, says Orava.

1. Kalyva, M., Orava, J., Siokou, A., Pavlista, M., Wagner, T. & Yannopoulos, S. N. Reversible amorphous-to-amorphous transitions in chalcogenide films: Correlating changes in structure and optical properties. *Advanced Functional Materials* **23**, 2052–2059 (2012).

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Molecular electronics

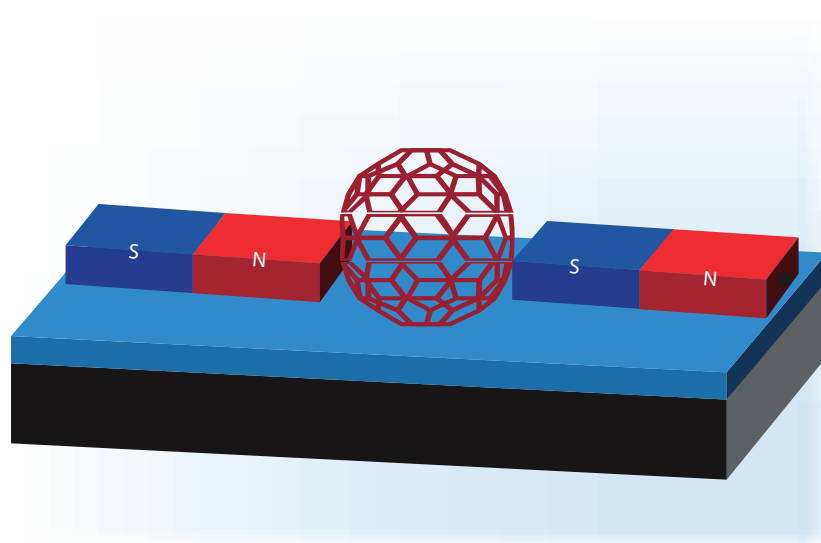
In the right place

Precise alignment of the electronic states in metal contacts and organic molecules is needed to optimize performance in molecular electronic devices

A fundamental discrepancy exists between the basic building blocks that underpin modern engineering and those found in natural organisms: while computers and electronic circuits are based on inorganic materials, such as silicon, biological processes revolve around organic molecules. Increasingly, researchers are striving to combine the two to fabricate complex artificial devices from organic molecules. Ikutaro Hamada, Masaru Tsukada and co-workers from the AIMR at Tohoku University and the University of Tokyo have now shown how the right choice of metal electrodes and operational conditions can enhance electronic performance¹.

Molecular electronic devices are particularly interesting for a number of spintronic applications, which exploit the electron's magnetic property, known as 'spin'. "The realization of spintronic devices consisting of single molecules promises highly functional sensing, logic (computing) and information-storage devices," says Hamada, a member of the research team. Until now, however, spin-based effects have not been strong enough to use in practical applications.

While the performance of a molecular electronic device would be chiefly dictated by the organic molecule, contact between the molecule and the adjacent metallic electrodes also plays a key role. The researchers fabricated devices featuring two magnetic nickel electrodes separated by only 1 nanometer — far enough apart to accommodate the fullerene (C_{60}) molecule (see image). To create this precisely sized gap, they used an electromigration-based



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An illustration of the molecular electronic device's geometry, with a fullerene (C_{60}) molecule (red, center) embedded within magnetic nickel electrodes. N and S represent the north and south poles, respectively, of the device's magnetic contacts.

process to move nickel atoms out of the electrodes, slowly closing the space between them.

The team then studied the effect of the electrodes' electronic levels on the properties of the spintronic device by measuring the change in electrical resistance when they applied different external magnetic fields, a property known as magnetoresistance. By varying the voltage applied, the researchers could tune the device to observe a change in resistance of up to -80%. Theoretical calculations revealed that hybridization at the nickel- C_{60} interface may be responsible for the observation of this unusual negative value and, in addition, magnetoresistance was maximal when the applied voltages led to the perfect alignment of the

electron spins in the C_{60} molecule and the nickel electrodes.

These findings demonstrate that molecular electronic devices should be envisaged as a whole since it is crucial to realize an appropriate combination of metallic contacts and organic molecules. Hamada is confident that the team's approach is applicable to a range of related devices. "Using the theory developed in the present work, I believe that it is possible to predict the properties of spintronic devices made from other molecules and electrodes."

1. Yoshida, K., Hamada, I., Sakata, I., Umeno, A., Tsukada, M. & Hirakawa, K. Gate-tunable large negative tunnel magnetoresistance in Ni- C_{60} -Ni single molecule transistors. *Nano Letters* **13**, 481–485 (2013).

Fuel cells

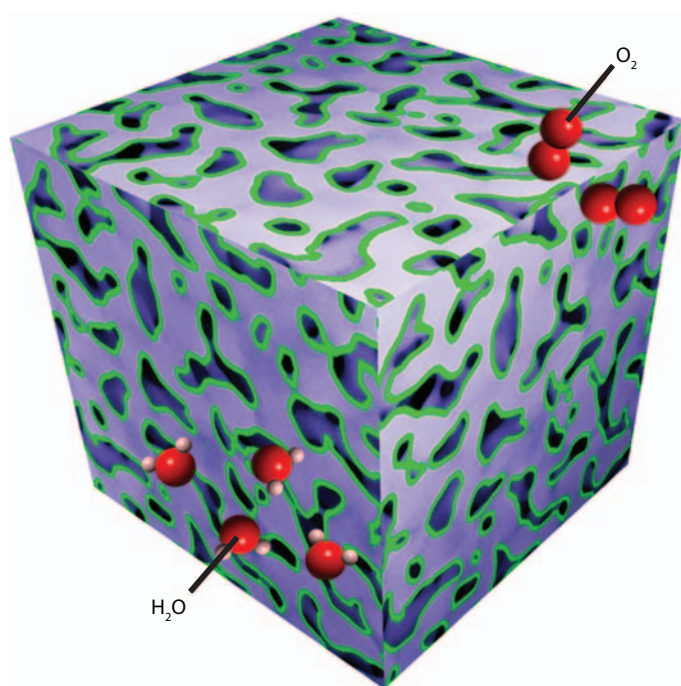
Improved cathodic catalysts

An electrochemical dealloying method allows the preparation of highly active and tunable platinum–copper catalysts for the oxygen reduction reaction

The development of cheap and efficient fuel cells — devices that convert chemical energy into electricity — is a key component of the push toward cleaner energy sources. Instead of burning fuel to produce heat, fuel cells extract energy as electrons, which can then be fed into an electrical circuit. In the most basic example — the proton exchange membrane fuel cell (PEMFC) — hydrogen gas is oxidized to protons and electrons at one electrode. These electrons then pass to the other electrode, via an electrical circuit, where they reduce oxygen. Lastly, the resulting oxide anions combine with the protons, which have moved through a membrane, to form water — completing the same conversion as occurs when hydrogen is burnt as a fuel.

Although commercially available fuel cell systems use platinum absorbed onto carbon to catalyze the oxygen reduction reaction (ORR), the rate of the reaction is still low, meaning that a large amount of expensive and scarce platinum is required to achieve an efficient reaction. Now, Mingwei Chen and Xingbo Ge from the AIMR at Tohoku University and co-workers have created a cheap and active ORR platinum–copper catalyst¹. Their system consists of a nanoporous platinum–copper alloy core covered by a thin skin of pure platinum (see image).

Previous research revealed that the precise ratio of platinum to copper in the core of these nanoparticulate catalysts is particularly important for their function. “Controlling the composition of bimetallic particles at the nanoscale is extremely difficult,” says Chen. “Our electrochemical dealloying can selectively dissolve the copper from



An illustration of the nanoporous platinum–copper catalyst developed for use in the oxygen reduction reaction of fuel cells.

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an alloy and is much easier to control.” The dealloying process itself is governed by the voltage that is applied, allowing the final composition of the catalyst to be tuned and, in turn, the optimum catalyst to be identified.

Chen and his co-workers showed that while the catalytic activity of their material can be attributed to the thin layer of pure platinum at its surface, this property can be honed by changing the composition of the catalyst’s alloy core. This is due to the way in which the atoms in the thin layer of platinum bind to the core. Correspondingly, by adjusting the platinum–copper ratio of the core, the

team was able to produce a nanoporous material that outperforms commercial platinum on carbon catalysts.

“We are now using our dealloying method to prepare other bimetallic catalysts for energy-related applications,” says Chen. “In addition, we are planning industrial collaborations to promote the practical applications of these catalysts.”

1. Ge, X., Chen, L., Kang, J., Fujita T., Hirata, A., Zhang, W., Jiang, J. & Chen, M. A core-shell nanoporous Pt–Cu catalyst with tunable composition and high catalytic activity. *Advanced Functional Materials* **23**, 4156–4162 (2013).

Organic electronics

It's all in the twist

A small molecular bending effect helps flexible light-emitting transistors to outshine other optoelectronic technologies

Organic light-emitting field-effect transistors (OLETs) are innovative devices that combine brilliant light production with fast electronic switching. With the potential for application in flexible low-cost displays and all-organic lasers, OLET development has so far been hampered by a fundamental materials-based challenge: the molecular interactions that boost the mobility of charge carriers — a key transistor parameter — generally stifle light emission. In joint experimental¹ and theoretical² studies, a multidisciplinary research team led by Tienan Jin, Susumu Ikeda, Hiroyuki Tamura and Katsumi Tanigaki from the AIMR at Tohoku University has found a way to preserve electron mobility and generate higher luminescence efficiency in OLETs using short chains of oxygenated aromatic molecules that form unusual bent structures in the crystal state.

Previously, the researchers synthesized a promising organic semiconductor known as BP2T by linking phenyl rings and thiophene — a pentagonal aromatic molecule containing a sulfur atom — into chains called oligomers. But despite BP2T's impressive bipolar amplification characteristics, it only converted 38% of incoming photons into luminescent emissions — a quantum yield too low for OLET applications.

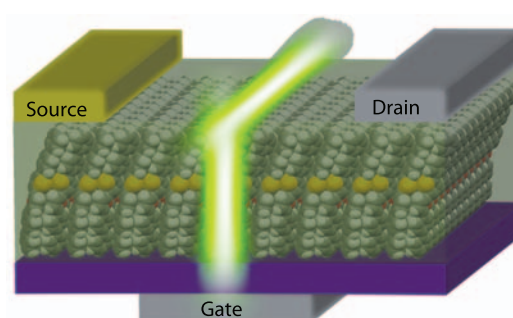
The team hypothesized that substituting thiophene's sulfur atom with oxygen, which turns the molecule into a furan ring, might enhance BP2T's performance. As oxygen atoms are smaller than sulfur, this change should favor the growth of more tightly packed crystal structures — ideal for moving charge quickly. Furthermore, notes Jin, oligomerized furans have

a strong track record of brightening luminescent materials.

When the researchers synthesized the new furan-containing compound, BPFT, and incorporated it into an OLET (see image), they saw their strategy pay off — the luminescent quantum yield jumped significantly to 51%. Next, the team used X-ray crystallography to peer into BPFT's molecular structure. Instead of being packed flatly like most aromatic molecules, the furan oligomers had a distinct structural kink resulting in alternation between flat and bent alignments in the solid state.

Theoretical simulations revealed that BPFT's bending critically enhanced the OLET's photoluminescence. According to Tamura, this particular packing arrangement 'breaks' the equilibrium inherent to aromatic solids, causing asymmetric electronic dipoles to form during the transition to a photo-excited state. These dipoles then generate luminescent emissions that are forbidden in totally symmetric complexes.

The researchers note that high-performance OLETs are rarely discovered



A new aromatic compound that packs into 'bent' solid-state crystals can produce fast organic transistors that emit bright luminescent light.

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because diverse expertise is required to synthesize, fabricate and model organic semiconductor devices. Collaboration between different research groups proved crucial to identifying and tailoring the BPFT structure, they add. "These results could not have been accomplished without long-term discussion and complete fusion within our team," say Jin and Tamura.

1. Oniwa, K., Kanagasekaran, T., Jin, T., Akhtaruzzaman, Md., Yamamoto, Y., Tamura, H., Hamada, I., Shimotani, H., Asao, N., Ikeda, S. & Tanigaki, K. Single crystal biphenyl end-capped furan-incorporated oligomers: Influence of unusual packing structure on carrier mobility and luminescence. *Journal of Materials Chemistry C* **1**, 4163–4170 (2013).
2. Tamura, H., Hamada, I., Shang, H., Oniwa, K., Akhtaruzzaman, Md., Jin, T., Asao, N., Yamamoto, Y., Kanagasekaran, T., Shimotani, H. *et al.* Theoretical analysis on the optoelectronic properties of single crystals of thiophene-furan-phenylene co-oligomers: efficient photoluminescence due to molecular bending. *The Journal of Physical Chemistry C* **117**, 8072–8078 (2013).

Metallic glasses

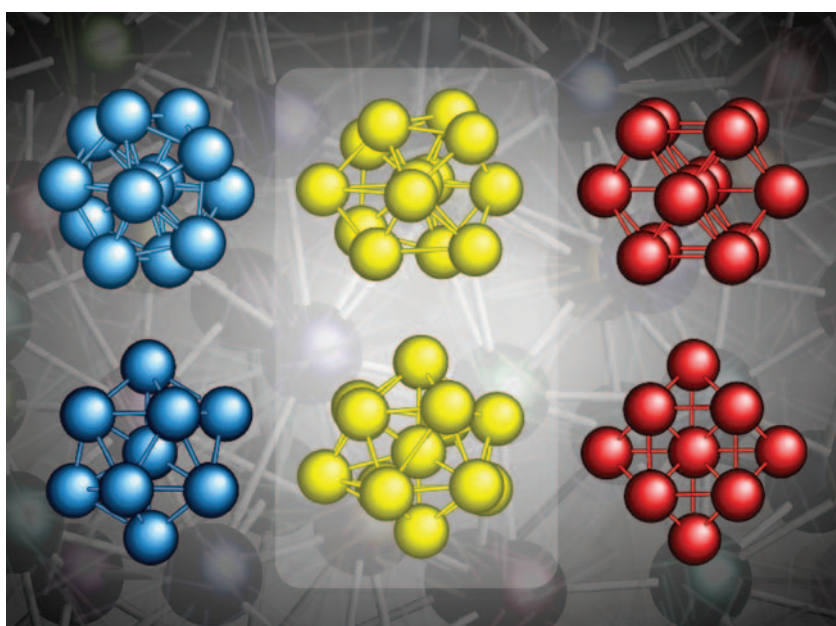
All in order

The local atomic order of metallic glasses has been solved by electron-beam imaging at the atomic scale

Most of the glasses that we encounter everyday are transparent and appear to be rather ordinary. A closer look, however, reveals an intriguing composition: glasses are basically frozen liquids, meaning that their atoms are randomly arranged. Researchers from the AIMR at Tohoku University and international collaborators have now shown that, surprisingly, the atoms of some glasses containing metallic components also display a local order that is based on icosahedral geometric structures¹. “We provide the first direct experimental evidence of the existence of icosahedral order in metallic glasses,” explains Mingwei Chen, who led the research team to this discovery, which confirms previous theoretical predictions.

Atoms in metals behave like perfect spheres, forming perfect crystals with atomic arrangements in the form of face-centered cubic (fcc) or body-centered cubic (bcc) structures, for example. Some metallic compounds can also form glasses when cooled fast enough after melting. Scientists were unsure as to why some metals form glasses instead of crystallizing and assumed that upon fast cooling, atoms in the metal are prevented from forming a crystal when they arrange into icosahedra. Such arrangements are similar in appearance to fcc crystal structures but importantly cannot form large-scale, periodic structures (see image).

To study the structure of metallic glasses, Chen, Akihiko Hirata and colleagues used an angstrom-beam electron diffraction technique in which a tiny beam of electrons is guided onto a sample of glass that is only a few atoms wide. As the electrons pass through the



The assumed icosahedral local atomic structure of metallic glasses (left, blue), the face-centered cubic (fcc) structure of the corresponding metal crystal (right, red) and the actual distorted icosahedral arrangement of metallic glasses (center, yellow). The top and bottom rows show the same structures from a different angle.

glass, they are reflected by the atoms and subsequently hit a screen that records the pattern of their reflection. With the help of computer analysis, the positions of the atoms in the sample can be determined from these patterns.

While the researchers were able to confirm the icosahedral atomic structure of metallic glasses, they also found that the icosahedra were not perfectly formed, as previously assumed. Interestingly, this slight distortion occurs in a way that makes the icosahedra appear even closer in structure to the fcc arrangement.

Beyond the discovery of local order in metallic glasses, the angstrom-beam electron diffraction technique itself is a

powerful way of studying compounds on the atomic scale, comments Chen. “We have just reached the starting point to understand the true relationship between structure and properties of disordered materials. We now have a reliable experimental method to directly investigate local atomic structure, and in the present case to show the correlation between atomic-scale structure and glass formation, and perhaps even the structural origin of the glass transition.”

1. Hirata, A., Kang, L. J., Fujita, T., Klumov, B., Matsue, K., Kotani, M., Yavari, A. R. & Chen, M. W. Geometric frustration of icosahedron in metallic glasses. *Science* **341**, 376–379 (2013).

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Spintronics

Current generation

A detailed, quantitative analysis of spin current reveals the importance of effects that are often overlooked in spintronic devices

The field of spintronics relies on exploiting the spin of the electron in the same way that electronics is dependent on the electron's charge. Spintronics holds exciting promise for the generation of ever smaller devices, and an important step in their realization is the introduction of spin current to non-magnetic materials.

In solids, the spin and momentum of an electron are coupled, leading to a reciprocal conversion between charge and spin currents that can be described by a phenomenon known as the spin Hall effect. Whereas the 'direct spin Hall effect' converts current into an accumulation of spins, the 'inverse spin Hall effect' converts spin flow into charge current. Interestingly, both effects have been observed in metals and semiconductors.

The inverse spin Hall effect is often determined through the measurement of spin currents. Through a quantitative study, Lin Chen, Fumihiro Matsukura and Hideo Ohno from the AIMR at Tohoku University have now unambiguously shown that other — galvanomagnetic — effects must be taken into account when investigating spin currents¹.

Galvanomagnetic effects are observed when an external magnetic field is applied to a current-carrying conductor or semiconductor material. To demonstrate their presence, Chen, Matsukura and Ohno prepared a sample comprising a ferromagnetic layer, gallium manganese arsenide ((Ga,Mn)As), on a semiconducting substrate, gallium arsenide (p-GaAs).

The researchers generated a spin current in the (Ga,Mn)As and injected it

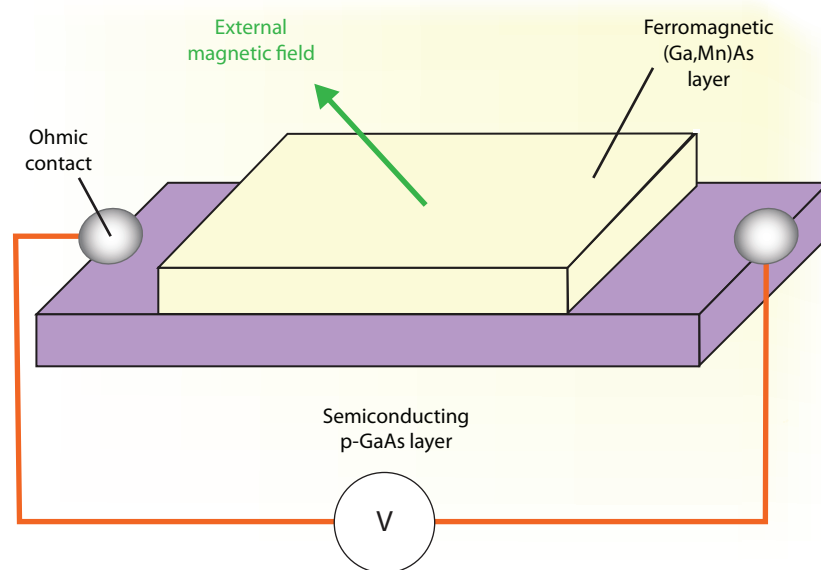


Illustration of the system devised to carry out the direct-current voltage measurements.

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into the p-GaAs layer using a method known as 'spin pumping'. They then measured the resulting direct-current voltage in the p-GaAs layer. The study was carried out under ferromagnetic resonance (FMR) conditions, allowing the magnetization of the ferromagnetic layer to be characterized by FMR spectroscopy. In particular, the team examined the influences of the magnitude and angle of the external magnetic field.

Analysis of the results revealed that the expected inverse spin Hall effect was accompanied by a galvanomagnetic phenomenon — the 'planar Hall effect' — in the ferromagnetic (Ga,Mn)As layer. "It is especially difficult to distinguish the inverse spin Hall effect from the planar Hall effect, as they both produce lines of the same

symmetry and width in FMR spectra. The difference lies in the angular dependence," explain the researchers. "These findings indicate the critical importance of separating the origins of the direct-current voltage."

The next step will be to show that this strategy is not just applicable to materials like (Ga,Mn)As that demonstrate significant galvanomagnetic effects. "This method should help further our understanding of the physics of spin current and the development of new functional spintronic devices," says Matsukura.

1. Chen, L., Matsukura, F. & Ohno, H. Direct-current voltages in (Ga,Mn)As structures induced by ferromagnetic resonance. *Nature Communications* **4**, 2055 (2013).

Batteries

A crash course in nanofabrication

A collaborative study reveals that atomic collisions play critical roles during laser-driven assembly of electroactive thin films

Developing high-capacity lithium ion batteries is an important research problem in materials science, and the realization of high-quality thin films of lithium metal oxides is a step toward this goal. Pulsed laser deposition (PLD) is a promising method of creating such films. In this technique, atoms from a lithium-containing source are vaporized using high-powered bursts of light, and the resulting 'plume' of plasma-phase atoms subsequently lands on a designated surface as a nanometer-thin coating.

However, when depositing films of electroactive materials such as lithium, the composition of the final thin film often differs from that anticipated. This 'non-stoichiometric' behavior makes it hard to predict the final result of particular fabrication strategies. Although the causes of the non-stoichiometry may be attributed to the volatile and chemically reactive nature of lithium atoms, quantitative explanations of this phenomenon have been lacking. Daniel Packwood, Susumu Shiraki and Taro Hitosugi from the AIMR at Tohoku University¹ have made a discovery that should significantly improve the quality of PLD lithium-based thin films thanks to a model that describes collisions between high-energy atoms during the deposition process.

During experimental trials, the researchers noticed that adding background pressures of oxygen gas to the PLD chamber could change the proportion of lithium in the thin film structures. Intrigued by this result, they investigated this behavior — and the role of oxygen — with a theoretical model of the scattering process as a series of two-dimensional, head-on collisions between classical particles (see image).



A representation of the combined mathematical and materials study into the deposition of electroactive thin films. The simulated trajectory of a lithium atom at an oxygen pressure of 10^{-6} torr (black line) is superimposed over a plot of a lithium plasma plume after expanding for 5 microseconds at an oxygen pressure of 10^{-2} torr (background).

After synthesizing several prototypical lithium–manganese oxide thin films at different oxygen pressures, Packwood, Shiraki and Hitosugi compared the films' chemical composition to the predictions of their new model. The results were striking: the theory correctly mirrored the experimental results and revealed that the presence of oxygen gas caused lithium ions to scatter in erratic trajectories, often violently. Heavier manganese atoms pushed through oxygen practically unimpeded. According to the team, these findings indicate that lighter atoms will always show deficiencies when background gas pressures rise above a certain threshold — thus, source materials must be chosen carefully to achieve desired lithium compositions.

Packwood notes that the model works well because it captures the physics behind the critical energy exchange occurring during atomic scattering. This ensures reasonable thermal equilibrium in the model and predictions of spatial distribution that have proven experimentally valid. The team expects that their analysis can guide the fabrication of higher-quality interfaces that would lead to lithium ion batteries with higher charge–discharge rates by reducing the effects of electrical resistance.

1. Packwood, D. M., Shiraki, S. & Hitosugi, T. Effects of atomic collisions on the stoichiometry of thin films prepared by pulsed laser deposition. *Physical Review Letters* **111**, 036101 (2013).

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Biomaterials

Getting cells in line

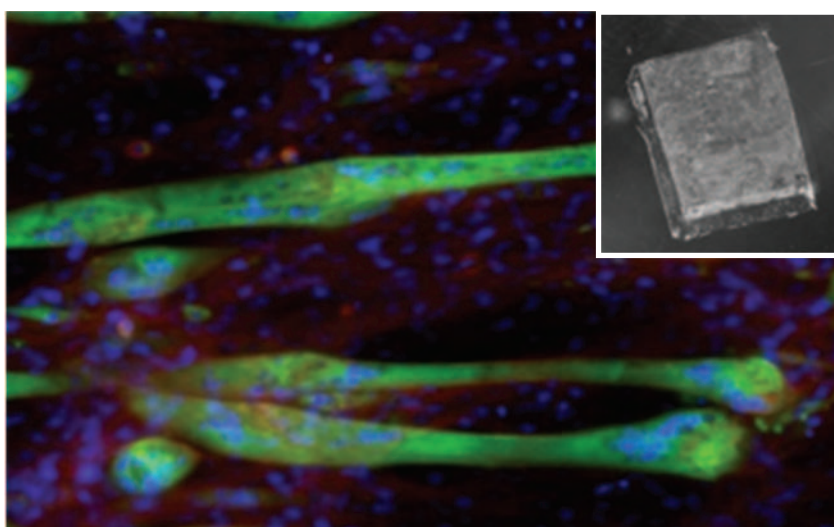
A flexible artificial extracellular matrix is paving the way for new approaches to regenerative medicine

Biomaterial supports that promote the orderly growth and differentiation of cells are crucial for tissue engineering and repair. However, reproducing the structural and biological properties of the extracellular matrix, which governs cell organization in the body, remains a challenge for materials scientists. Now, Toshinori Fujie and Ali Khademhosseini from the AIMR at Tohoku University and co-workers from Japan, South Korea and the United States have devised a free-standing ultrathin polymer film that mimics the inherent ability of this matrix to direct cells. The resulting ‘nanomembrane’ exhibits nano- and microscale features, similar to those of natural tissue¹.

Numerous synthetic extracellular matrices have previously been developed, including hydrogels and elastomers. Unfortunately, unlike their natural counterparts, the size and components of such materials hinder the hierarchical assembly of cells into complex tissue structures.

Using microfabrication techniques, the researchers manufactured their film from nanometer-sized polymer fibers containing cell-adhesive domains, which allowed them to replicate the basement membrane of tissues — a dense, sheet-like structure that serves as a cellular scaffold.

First, they prepared an ultrathin polystyrene film on a glass surface pre-coated with a sacrificial polymer layer. Next, using a microscopic stamp, the researchers patterned the surface of the film with features made from a fibronectin-carbon nanotube composite to functionalize it for cell alignment and adhesion. After cell culture, they then dissolved the



Differentiated muscle cells (green and blue) assembled on the ultrathin polymer film nanomembrane. The free-standing micropatterned nanomembrane is shown inset.

initial polymer layer to release the cell-patterned nanomembrane.

In vitro cell studies showed that the micropatterning facilitated the alignment of muscle progenitor cells, known as myoblasts, on the nanomembrane. The fibrous nanotubes also enhanced the elongation and differentiation of these cells into functional myofibers. “These results suggest that the film’s surface is a useful platform for studying cell–substrate interactions,” says Fujie.

The researchers were able to produce films of various thicknesses — ranging from tens to hundreds of nanometers — by tuning the polystyrene concentration. Analyses of the thickness dependence of the mechanical properties revealed that, in addition to the free-standing films being highly flexible, the thinner films displayed greater flexibility. These unique properties allowed the team to

transform the myoblast-coated films into tubular assemblies — without damaging the cells — by rolling them around a soft silicone tube, showcasing the potential of using the nanomembranes as scaffolds in complex tissue architectures.

The team is currently investigating how they can apply these findings to the development of flexible biodevices and tissue regeneration. “The system will be useful for mimicking blood vessels or investigating tissue responses to various drugs and toxic chemicals using lab-on-a-chip devices,” says Fujie.

1. Fujie, T., Ahadian, S., Liu, H., Chang, H., Ostrovidov, S., Wu, H., Bae, H., Nakajima, K., Kaji, H. & Khademhosseini, A. Engineered nanomembranes for directing cellular organization toward flexible biodevices. *Nano Letters* **13**, 3185–3192 (2013).

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Raman spectroscopy

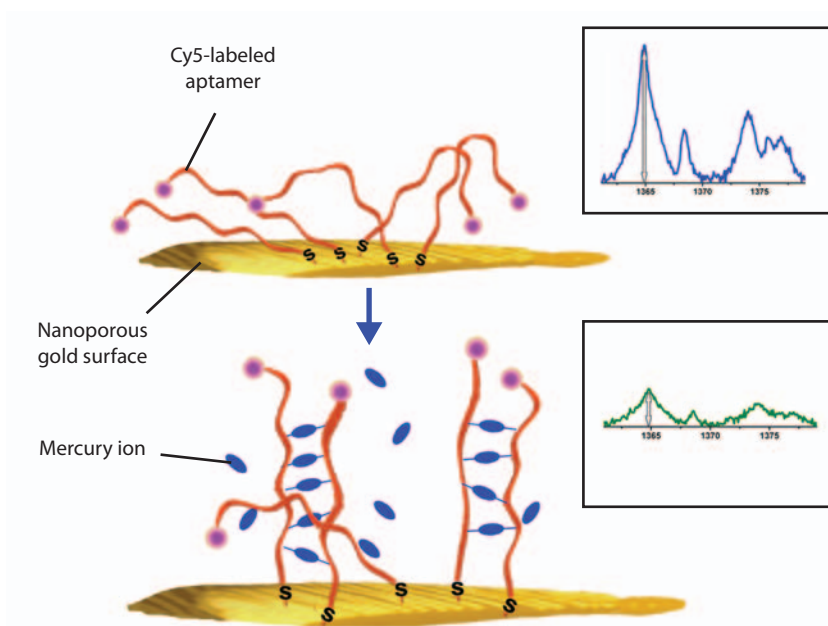
Pairing up for mercury detection

An extremely sensitive nanoporous gold-based optical sensor improves the detection of mercury ions in drinking water

Mercury enters drinking water from a number of sources, including the erosion of natural deposits, wastewater discharged from oil refineries and runoff from landfill and agricultural land. As its accumulation in humans can cause irreversible damage to the brain and central nervous system, the levels in water are closely monitored.

“Although many methods have been reported, developing a quantitative approach capable of detecting sub-part-per-trillion levels of mercury ions with high selectivity is still challenging,” explains Ling Zhang from the AIMR at Tohoku University. Zhang, Mingwei Chen, Qi-Kun Xue and co-workers have now designed a nanoporous gold-based optical sensor that is around 1,000 times more sensitive than conventional optical methods¹. “This is the most sensitive optical sensor for mercury ion detection in water known so far,” Xue says. “The US Environmental Protection Agency’s limit for mercury ions in drinking water is 10 nanomoles per liter, and the detection limit of our sensor is 10,000 times lower.”

The team’s sensor utilizes the technique of surface-enhanced resonance Raman scattering (SERRS). Like Raman spectroscopy, SERRS relies on the fact that every molecule scatters light differently — an effect that can be weak and difficult to detect. To overcome this issue, the Raman signal is amplified in two ways. First, a roughened metal surface — in this case nanoporous gold — is used. A laser excites the gold’s surface plasmons, which increases the surrounding electric field. As Raman scattering intensities are proportional to this electric field, the signal is therefore



Within the sensor, mercury ions cause aptamers to bind together in pairs, pulling the cyanine 5 (Cy5) fluorescent tags away from the gold surface and therefore changing the intensity of the Raman signal (inset graphs).

amplified. Second, the excitation wavelength of the laser is matched to the absorbance of the molecule being analyzed. Thus, the laser light is absorbed, further amplifying the signal.

In the researchers’ study, the fluorochrome reporter molecule cyanine 5 (Cy5) is detected, rather than the mercury ion itself. Their sensor comprises flexible, single-stranded aptamers that are tagged with Cy5 and immobilized on the gold surface. Mercury ions, when present, bind to adjacent aptamers, pairing them to produce relatively rigid duplex-like structures (see image). This pulls the Cy5 tags up and away from the gold, resulting in a measurable reduction in the SERRS signal.

At higher mercury concentrations, a greater number of aptamers are bound together, which further reduces the SERRS signal.

“Having successfully detected mercury ions in river water and underground water,” says Chen, “we are now working on the design and fabrication of a microchip that can be used in conjunction with a portable Raman spectrometer for real-world *in situ* detection.” The team is also looking to tweak the aptamers to test for other heavy metal ions.

1. Zhang, L., Chang, H., Hirata, A., Wu, H., Xue, Q.-K. & Chen, M. Nanoporous gold based optical sensor for sub-ppt detection of mercury ions. *ACS Nano* 7, 4595–4600 (2013).

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Graphene oxide

Responding to infrared light

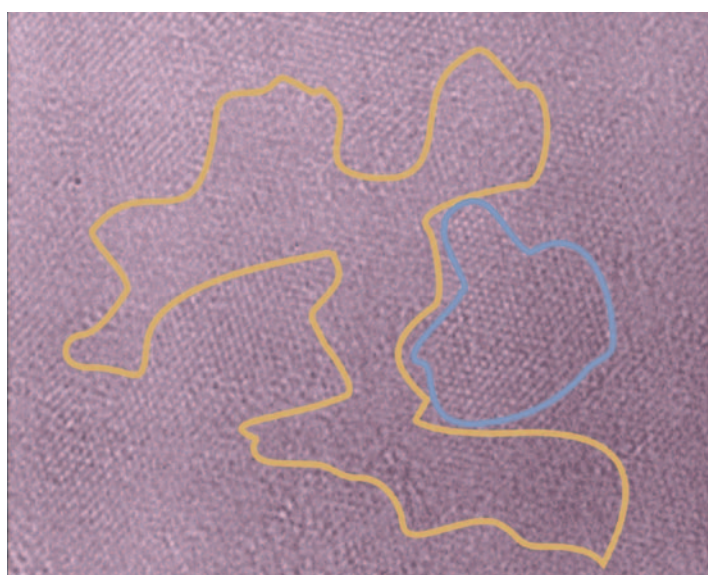
Efficient infrared photodetectors can be fabricated by controlling the atomic structure and number of defects in graphene oxide

Photodetectors, especially those that sense the infrared region of the electromagnetic spectrum, are important devices with uses in optical communication and imaging instruments. They rely on the generation of negative and positive charges — electrons and holes — by optical excitation. Subsequently, the charges are separated and contribute to an electrical current. However, in graphene, a material well known for its exceptional electronic properties and the foundation of several established photonics components, the electrons and holes rapidly recombine.

As a result, the amount of photocurrent that can be generated from a watt of incident radiation — the photoresponse — is very low, and preparing a graphene-based photodetector has remained a challenge. Now, Haixin Chang, Hongkai Wu, Mingwei Chen and Yuichi Ikuhara from the AIMR at Tohoku University and co-workers have demonstrated the possibility of enhancing the infrared photoresponse of graphene oxide, a close relative of graphene, by controlling the structure and number of defects in the material¹.

Chang's team began by reducing few-layered graphene oxide through thermal annealing to improve its electronic properties. Then, they studied the structure and type of defects found in the original and reduced graphene oxide with transmission electron microscopy and X-ray photoelectron spectroscopy. While the original material contained large domains of highly ordered and disordered lattices (see image), thermal annealing decreased the size of both of these areas and also affected the nature of the oxygen-containing groups.

The researchers were able to directly link the structural modifications



Transmission electron microscopy image of graphene oxide, containing large regions of high disorder (yellow line) and order (blue line).

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introduced during thermal annealing to changes in the few-layered graphene oxide's photoresponse. Under infrared illumination, the team observed a photocurrent signal in the thermally annealed material that increased with the length of annealing — something they could not detect in the original.

Next, the team fabricated flexible infrared photodetectors from the reduced few-layered graphene oxide, finding the photoresponse of the devices to be over an order of magnitude higher than that of devices made from pristine graphene. The external quantum efficiency, a measure of the number of electrons and holes created by each photon under external bias, reached 97% — among the highest observed in graphene-based infrared photodetectors. Furthermore, the devices

were very stable, retaining their photoresponse after 1,000 bending tests.

According to Chang, these findings could provide new ways to control the optoelectronic properties of graphene-based and other two-dimensional systems. His team is currently working to improve the response time of the reduced graphene oxide, which is still quite slow. "We believe that there are further opportunities to improve the photoresponse by further optimizing defects and atomic structures," says Chang.

1. Chang, H., Sun, Z., Saito, M., Yuan, Q., Zhang, H., Li, J., Wang, Z., Fujita, T., Ding, F., Zheng, Z. *et al.* Regulating infrared photoresponses in reduced graphene oxide phototransistors by defect and atomic structure control. *ACS Nano* 7, 6310–6320 (2013).

Spintronics

Using nature's symmetries

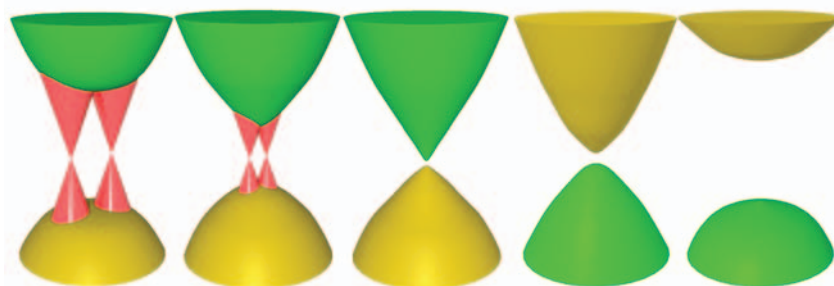
The different fundamental symmetries of tin telluride make it an ideal testing ground for the study of topological states

Symmetry is an important concept that must be taken into account to explain the properties of the Universe, as well as those of molecules and atomic crystals. Researchers from the AIMR at Tohoku University, together with collaborators from Osaka University, have now shown how the symmetry of crystals of tin telluride (SnTe) can be modified such that the material demonstrates various electronic effects^{1,2}.

Tin telluride is a conventional semiconductor with commercial applications in infrared photodetectors. A feature of the compound is that its crystals are mirror-symmetric, meaning that they do not change upon reflection. As a consequence, the electronic states at the surface of the crystal are protected against perturbations. Such crystals are classed as topological crystalline insulators and exhibit 'topological states' on their surface.

A practical advantage of these topological states, explains Seigo Souma, a member of the research team, is that the material's electrical conductivity is independent of size. "Normally, when we reduce the size of the conducting material, at some point electrons cannot move and the material becomes insulating. This is a real limitation when down-sizing electronic devices. However, materials with topological protection could overcome such limitations."

In tin telluride, topological states can be controlled by changing the atomic composition of the crystal. Souma and his colleagues replaced some of the tin with lead, discovering that when the lead content was 75% or higher, the topological states disappeared¹ (see image).



The surface of the topological crystalline insulator tin telluride (SnTe) has electronic states (pink) that differ from those in the interior (yellow: Sn or Pb; green: Te). When the lead (Pb) content of the crystal is increased (left to right), these surface states disappear as the character of the interior becomes inverted.

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As well as destroying these states, the researchers also found that they could alter them. When they replaced a low percentage of the tin with indium instead of lead, the samples became superconducting at low temperatures. Owing to the symmetries of the modified crystal, the resulting material, $\text{Sn}_{1-x}\text{In}_x\text{Te}$, is a rare form of a topological superconductor². Interestingly, topological superconductors are predicted to contain an unusual class of particle known as a Majorana fermion. As their own anti-particle, these fermions possess some unique properties and are very stable to external perturbations, making them appealing for use in electronic applications.

Souma notes that with the ability to control symmetries and topological states through atomic substitution, new possibilities arise — including further investigation into the existence of the

Majorana fermion. "One interesting future possibility is to create thin layers of tin telluride/lead telluride in a device. As topological states do not only exist at the surface, but can also arise at the interface between a topological and an ordinal material, one can encapsulate the topological state between these two layers."

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2. Sato, T., Tanaka, Y., Nakayama, K., Souma, S., Takahashi, T., Sasaki, S., Ren, Z., Taskin, A. A., Segawa, K. & Ando, Y. Fermiology of the strongly spin-orbit coupled superconductor $\text{Sn}_{1-x}\text{In}_x\text{Te}$: Implications for topological superconductivity. *Physical Review Letters* **110**, 206804 (2013).

Molecular magnets

Mathematical predictions

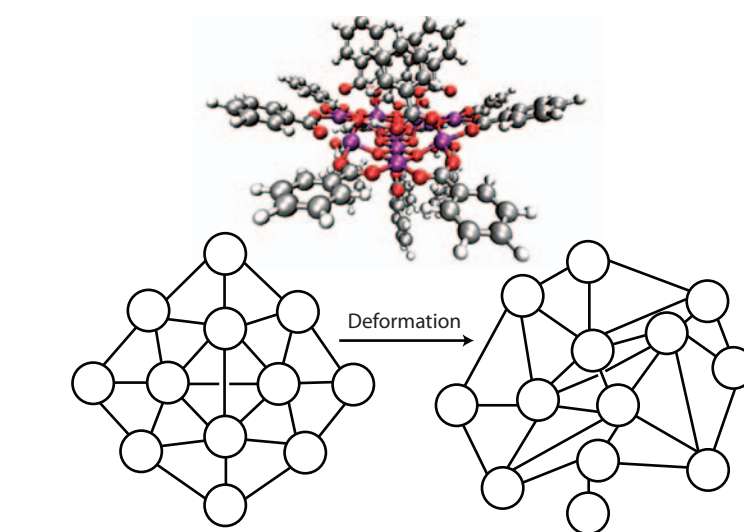
Mathematical analysis points to how robust nanomagnets can be made from surprisingly small metal–organic complexes

Molecular magnets can be handled like classical particles owing to their relatively large size, but they also exhibit quantum magnetic properties thanks to their unpaired electron spins. This unique behavior makes them attractive as high-density information storage materials and for spintronic-based computing. Currently, chemists struggle to attach molecular magnets to device surfaces, however, because these particles have a tendency to warp and lose their magnetic properties on adsorption.

To overcome this difficulty, an international team led by Daniel Packwood from the AIMR at Tohoku University has now developed innovative ‘mathematical chemistry’ techniques that can predict novel molecular magnets with deformation-resistant magnetic moments¹.

Most molecular magnets are made by linking transition metals, such as manganese and iron, into complex clusters through hydrocarbon or oxygen ‘bridges’ (see image). When the coupling interactions between the unpaired metal ion electrons within these metal–organic complexes are strong enough, the molecules acquire an appreciable magnetic moment. Packwood and colleagues hypothesized that the intimate relationship between structure and magnetic behavior in these systems could mean that certain geometric networks, currently unknown to chemists, exist with intrinsically stable spin properties.

To find these structures, the researchers devised an original model that examines how one physical property — the energy of the molecule’s ground spin state — changes with small, random shape deformations of a molecular magnet. “Creating a realistic model



A molecular magnet containing twelve manganese ions (top) is modeled with a new mathematical approach (bottom left) that randomly deforms the structure to predict spin arrangements that give highly stable magnetic moments (bottom right).

of a molecule is not so difficult,” says Packwood. “However, the key challenge is striking a good balance between physical realism and sufficient simplicity for mathematical treatment.”

The team’s analysis showed that two-dimensional molecules containing a sufficient number of spin centers can possess extraordinarily stable ‘weak topological invariant’ magnetic moments. “When mathematicians talk about topological invariants, they usually mean properties that don’t change under arbitrary stretching or squeezing deformations,” explains Packwood. “A weak topological invariant is similar; however, it can change under deformations that have a very low probability of occurring. This difference significantly broadens the applicability of the topological invariance concept to studying real systems.”

Surprisingly, the researchers’ calculations showed that only between 20 and 50 spin centers were needed for a two-dimensional molecule to achieve robust and stable magnetism. They also found that resistance to shape deformations improved when the number of ring-shaped networks in the model was kept to a minimum. As the structures predicted by this joint mathematics–materials science study are well within the size range of existing molecular magnets, Packwood and colleagues are confident that they represent practical targets for future chemical synthetic efforts.

1. Packwood, D. M., Reaves, K. T., Federici, F. L., Katzgraber, H. G. & Teizer, W. Two-dimensional molecular magnets with weak topological invariant magnetic moments: Mathematical prediction of targets for chemical synthesis. *Proceedings of the Royal Society A* **469**, 20130373 (2013).

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Batteries

The power of patterns

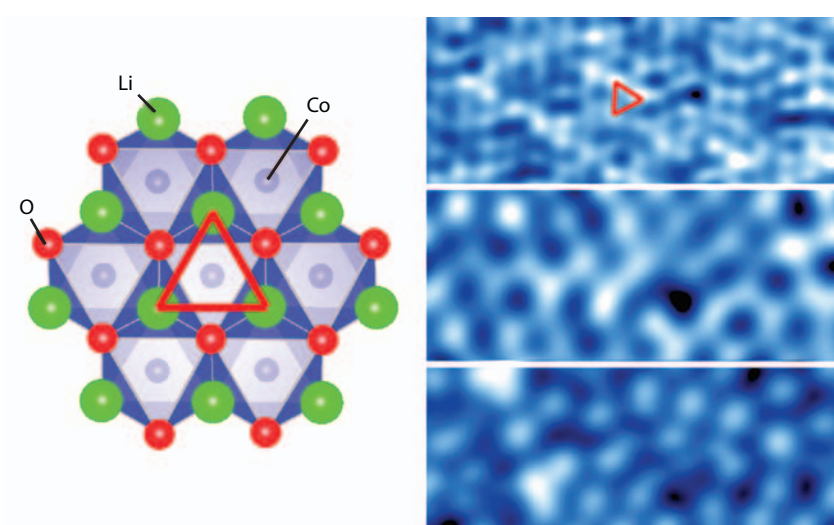
Atomic-scale images reveal that ordering patterns on lithium cathode surfaces can strongly influence battery performance

Lithium (Li) ions, which are small and light, are ideal for shuttling charge between cathodes and anodes in rechargeable batteries. But despite their widespread use, researchers still struggle to understand the atomic processes behind their movements at battery interfaces. Now, Katsuya Iwaya from the AIMR at Tohoku University and collaborators have captured unprecedented images of surface atoms on lithium cobalt oxide (LiCoO_2)¹, an energy-rich cathode material.

In its bulk crystalline state, LiCoO_2 has a structure consisting of alternating layers of lithium and cobalt oxide (CoO_2). This arrangement allows lithium and cobalt atoms to undergo interactions that determine the material's electronic activity. Understanding how these atoms arrange at cathode surfaces is difficult, however, because the behavior of lithium ions depends on the material's composition and can elude detection with traditional microscopes.

To resolve this problem, Iwaya and his team turned to the atom-resolved imaging capabilities of scanning tunneling microscopy (STM). Normally, STM requires atomically flat surfaces to produce useful data — a challenge when investigating LiCoO_2 surfaces due to their often polycrystalline and bumpy nature. The team devised a way to synthesize single crystals of LiCoO_2 with a controllable lithium content that they systematically changed. Peeling these crystals apart in ultrahigh vacuum conditions produced contaminant-free, smooth surface layers.

STM experiments revealed an abundance of atomic organization patterns on the cathode surface (see image). In



The surface of crystalline lithium cobalt oxide (LiCoO_2) contains a 'triangle' (red) of lithium atoms that forms part of a hexagonal array (left and top right). Scanning tunneling microscopy (right) also reveals other surface structures (ordered and disordered: middle and bottom right, respectively), which modify lithium-ion battery efficiency.

some areas, they saw hexagonal arrays of lithium atoms that scattered away when the researchers changed the voltage on the STM tip. Mostly though, they found cobalt oxide regions with either ordered or disordered structures. Depending on the degree of order in the cobalt oxide, the conductivity of the surface electronic states varied from insulating to metallic — a significant change from LiCoO_2 's bulk crystalline properties.

By comparing the STM results to quantum chemical simulations, the researchers deduced that the unusual surface properties of their cathodes arise from non-uniform concentrations of lithium ions. In turn, this produces distinct ordering patterns that significantly modify surface electronic states.

“These ordering patterns are closely related to diffusion of lithium within the crystal,” says Iwaya. “Understanding these processes in detail could lead to lithium-ion batteries with larger capacities and shorter charging times.”

Iwaya notes that these findings may also help to develop novel atomic-scale devices. “Because we can likely remove individual surface lithium ions with the STM tip, we can tune the surface electronic states at the nanoscale by controlling their ordering patterns — a potential route to very small electronic circuits.”

1. Iwaya, K., Ogawa, T., Minato, T., Miyoshi, K., Takeuchi, J., Kuwabara, A., Moriwake, H., Kim, Y. & Hitosugi, T. Impact of lithium-ion ordering on surface electronic states of Li_xCoO_2 . *Physical Review Letters* **111**, 126104 (2013).

Superhard materials

Shear resolution

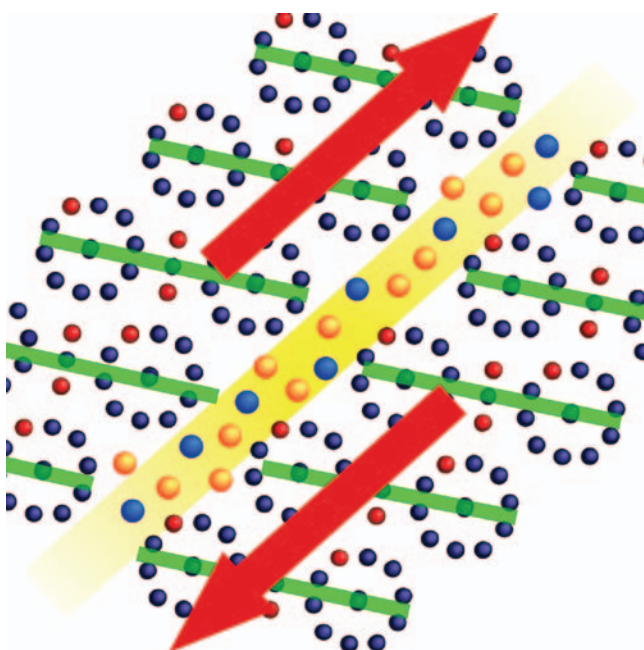
Microscopic analysis reveals the atomic structure of amorphous shear bands in boron carbide

Boron carbide (B_4C) is a superhard yet lightweight ceramic material. As a result of these characteristics, it is used as a protective component in bulletproof vests and tank armor and also has many other industrial applications. Despite its hardness, boron carbide's crystalline structure deforms under shear pressure, which creates amorphous regions that lead to the failure of the material. The precise mechanism behind this destructive amorphization, however, remains unclear.

Now, Mingwei Chen, Madhav Reddy and colleagues from the AIMR at Tohoku University have used Cs-corrected scanning transmission electron microscopy (STEM) to investigate the atomic-level deformation processes that take place during the formation of amorphous shear regions in boron carbide¹. “Understanding such processes is important for the design and development of new boron carbide-based materials with improved impact performance,” says Chen. “It is also important for understanding the basic failure processes of a covalent material.”

The crystalline structure of boron carbide comprises 12-atom icosahedra and 3-atom carbon–boron–carbon chains located within individual crystal planes. Under shear pressure, amorphous bands approximately 2 nanometers wide are created, which form within the plane containing the carbon–boron–carbon chains (see image).

Using a technique known as annular bright-field (ABF) imaging, which allows light elements to be observed at high spatial resolutions, Chen and his colleagues probed the finer details of the shear bands. The researchers were able to identify atomic-scale changes, which



When boron carbide (boron: red spheres; carbon: blue spheres) is subjected to shear pressure (red arrows), amorphous regions (yellow) form in the plane that contains the 3-atom carbon–boron–carbon chains.

led them to conclude that the shear bands were formed from disassembly of the icosahedra.

At the interface of the crystalline regions and the amorphous zone, the team observed deformed icosahedra. While some icosahedra were displaced from their original position by a considerable distance, others were hardly displaced at all, indicating that the conversion from a crystalline to an amorphous structure is progressive within the material. In the amorphous band, the icosahedra were irregularly shaped, randomly located and also lower in number than in the bulk of the material. The latter may either be due to the collapse of icosahedra during shear band formation or limitations of

the ABF-STEM imaging technique when observing tilted icosahedra.

“Our findings could help to fabricate boron carbide materials with improved mechanical properties by reinforcing atomic chains through chemical doping or changing the boron/carbon ratio,” says Chen. “We are now focusing on structural characterization and modification of the atomic chains in boron carbide by utilizing advanced Cs-corrected STEM and developing boron-rich boron carbide and heavily doped boron carbides.”

1. Madhav Reddy, K., Liu, P., Hirata, A., Fujita, T. & Chen, M. W. Atomic structure of amorphous shear bands in boron carbide. *Nature Communications* 4, 2483 (2013).

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IN THE SPOTLIGHT

The AIMR has grown rapidly since its inauguration in 2007, now with over 140 leading researchers from all over the world, including 31 internationally renowned principal investigators who are charged with pioneering new and innovative breakthroughs in materials science. The institute is also active in developing young, promising researchers with a focus on strong cross-disciplinary collaboration and creativity. *AIMResearch* spotlights these talented researchers of the present and future, detailing their daily research activities and scientific ambitions.



Comprehensive support for world-class research

In recognition of its researchers' efforts to successfully bridge the gap between mathematics and many different areas of materials science, the AIMR is committed to creating the most conducive environment for research and career building

Since its establishment in 2007, the Advanced Institute for Materials Research (AIMR), as one of the inaugural research institutes of the World Premier International Research Center Initiative (WPI), has consistently maintained a contribution to society through the creation of new and innovative materials. A highlight among the AIMR's many remarkable achievements is the creation of a pilot cross-disciplinary research program that brings together materials science and mathematics-related fields. This approach, dubbed 'fusion research', has the materials science community abuzz with its important discoveries.

Reflected in accomplishments so far, the success of the AIMR can be attributed

to its team of more than 130 researchers who cover the areas of materials science, physics, chemistry, engineering and mathematics. Going forward, the AIMR has pledged to inaugurate an even more attractive and robust support system for its researchers. "We have gained a lot of invaluable experience since the AIMR was established five years ago. We are now in an ideal position to build on our foundation and to offer the best support for all our researchers in recognition of their hard work," affirms Susumu Ikeda, deputy administrative director of the AIMR.

The AIMR has identified several key areas of difficulty that a new team member or a visiting foreign researcher may face when they first embark on their research

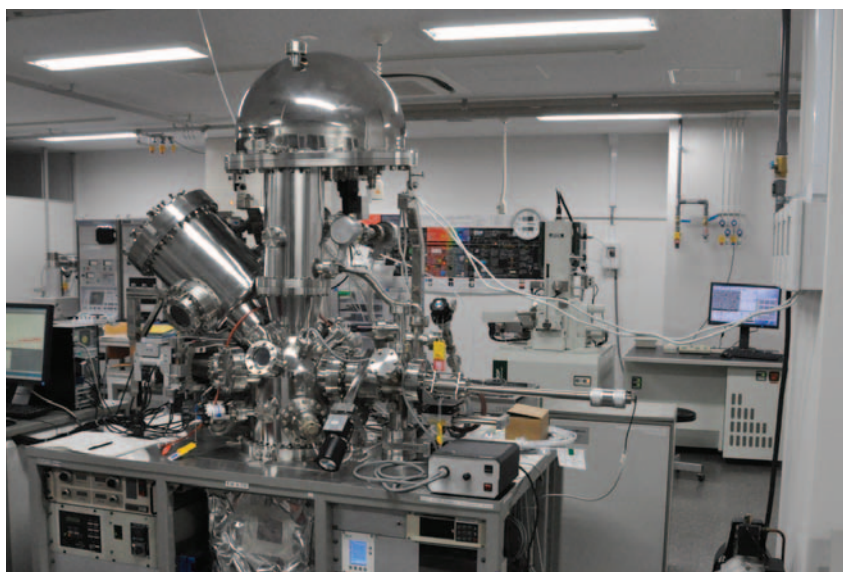
within the institute. In tailoring a comprehensive system to address those issues, suggestions from current staff members were analyzed together with studies of the organization and its facilities. The result of this extensive planning and implementation period was the opening of the Research Support Center, which consists of four divisions: the Common Equipment Unit, the Computation-Aid Unit, the Mathematics Collaboration Unit and the Researcher Support Office.

Access for everyone

In contrast to most overseas universities and research institutes, where access to common facilities and instruments is easy and guaranteed, experimental equipment usually belongs to an individual laboratory. New team members or visiting researchers may therefore find it difficult to gain access to equipment without formal collaborations. To address this issue, the Common Equipment Unit was set up to establish common facilities that offer essential apparatus such as electron microscopes, X-ray diffractometers and a photoemission spectrometer. Instruments located in associated institutions are also made available. "The Common Equipment Unit has since fulfilled many requests, from finding a specific piece of equipment, to designing appropriate experiments and providing training in English," says Ikeda.

Ensuring a smooth start

The innovative strategy of bringing together different areas of materials science with mathematics requires intensive theoretical studies and numerical calculations.



The Common Equipment Unit was set up to allow open access to essential apparatus, such as electron microscopes and a photoemission spectrometer, for all researchers at the AIMR.



At the Common Equipment Unit, staff members with fluency in both Japanese and English are available to assist with the design of experiments and provide training for AIMR researchers.

Correspondingly, the AIMR understands that an adequate and efficient infrastructure is crucial for supporting research of such magnitude. The Computation-Aid Unit is designed to offer a platform for the seamless inception of new projects. Operated by in-house theoreticians, the Computation-Aid Unit is particularly beneficial to newly appointed members of staff and visiting researchers. “Together, the Common Equipment Unit and Computation-Aid Unit provide support not only to the initial phase of a research project, but also extend continual support to ensure a successful outcome,” explains Ikeda.

Unifying materials science and mathematics

Traditionally, materials science research has been largely empirical and involved a great deal of trial and error. By contrast, mathematics concerns the setting of clearly-defined parameters, followed by the building and testing of theories. While the gap between the two fields has been bridged significantly over the last five years, ongoing effort is necessary to maintain the bond. The Mathematics Collaboration Unit was established to promote effective communication between AIMR materials scientists and mathematicians, and to encourage interactions with external mathematical communities. So far, the Mathematics Collaboration Unit has already made significant effort

toward connecting the AIMR with the Applied Mathematics Forum at Tohoku University; since the first joint seminar in June 2012, three more similar sessions have been organized to further strengthen the relationship.

Extending a helping hand

The AIMR appreciates that even the most gifted researchers may need assistance to advance their scientific career. Furthermore, AIMR staff members may also experience personal or family issues from time to time. In line with its commitment to ensuring staff well-being, the AIMR commissioned the Researcher Support Office — the fourth unit of the Research Support Center. “To equip young

scientists with competent writing skills, the Researcher Support Office facilitated an advanced scientific writing and publishing workshop conducted by Macmillan Science Communication,” says Ikeda. In addition, a mentoring system was initiated to enable younger researchers to connect with more established senior researchers and gain assistance with the important components of building a strong research career. Support is also available for administrative matters such as grant applications, working visa applications and renewals, and any other issues concerning daily life. “The AIMR knows it is important for foreign researchers to settle into their life in Sendai. We strive to provide all necessary support and assistance to make that transition a smooth one. A Researcher Support Office can be found in every building,” assures Ikeda.

Moving toward world-class status

With the new Research Support Center in place, present and future members of staff at the AIMR will undoubtedly find themselves in an environment that has a remarkable level of comprehensive support for the realization of their full potential and goals. Embarking on the next stage of its development, the AIMR is therefore set to continue attracting exceptionally talented individuals from all over the world, putting it on track to become a world-class research institution that offers both an excellent forum for research and an ideal working environment. ■



The Mathematics Collaboration Unit organizes joint seminars at which materials scientists and mathematicians can interact to benefit from each other's expertise.

Materials and math makes green

The AIMR International Symposium 2013 — convened by the AIMR in Sendai, Japan on 19–21 February 2013 — showcased cutting-edge research from leading international materials scientists and demonstrated how the power of mathematics is being harnessed to drive green innovation

Since its launch in 2007, the AIMR has built an enviable reputation for innovative fusion research in materials science, bringing together top international researchers in disciplines such as bulk metallic glasses, materials physics, soft materials and devices and systems. In 2012, a fifth research grouping — Mathematics Unit — was added, beginning a new chapter in the institute's scientific development.

Held since 2008, the annual workshop — renamed as the AIMR International Symposium — provides a forum for AIMR researchers, including those based overseas, and other internationally renowned materials scientists to discuss the latest developments in the field. The sixth symposium was held at the Sendai International Center from 19–21 February 2013 under the banner theme of “Challenge for green materials innovation through the fusion of materials science and mathematics,” and drew more than 240 participants from 14 countries.

In contrast to previous years, the meeting attracted a significant number of attendees and four speakers from the field of mathematics, mirroring the recent focus on mathematics-driven materials science at the institute. AIMR director Motoko Kotani, herself a distinguished mathematician, welcomed the development but pointed out that it reflected a natural evolution of the profile of the center. “We included a session on mathematics and computational science and one mathematician in the opening session but that was all,” she said of the inaugural workshop. “[This year], as in previous years, we called for recommendations of speakers from our researchers, and chose the best

from the list. I myself was surprised to find so many talks with mathematical hints in the symposium program. This shows our mathematics-driven materials idea has captured the imagination of our members.”

The decision to place mathematics-driven materials science at the heart of the AIMR's research strategy was announced by Kotani at the 2012 workshop, and the initiative has gained form and momentum since then. “I explained our idea of math–materials science collaboration to accelerate interdisciplinary research at the conclusion of the workshop last year,” explained Kotani. “But at the time, although we were confident we made the right decision, our ideas for the collaboration were then still largely unformed. In the intervening period, through much discussion and consultation, we have established three target projects to give a concrete strategy to our idea, and worked intensively to pursue research in this direction for one year.” While acknowledging that it is still too early to claim that the AIMR's mathematics–materials science collaborations have met the challenges of “green materials innovation,” Kotani remarked upon the encouraging initial results due to be presented at the 2013 symposium.

This year's meeting was opened by Susumu Satomi, president of Tohoku University, who extended a formal welcome to the delegates and congratulated AIMR members on their development of world-class research programs. This achievement, and the research-first, practice-centered ethos of Tohoku University, has ensured that the AIMR continues to play a central role in the life of the university, he said. Further development of the institute would be strongly influenced



Tohoku University President Susumu Satomi formally welcomed delegates to the AIMR International Symposium 2013, which focused on the theme of “Challenge for green materials innovation through the fusion of materials science and mathematics”.

by the success of the newly established, mathematics-driven materials science framework. Pledging the continued support of the university, the president also praised the international character of the AIMR and paid tribute to the role played by the institute's 19 overseas partners, and 3 satellite institutions at the University of California, Santa Barbara in the US, the Chinese Academy of Sciences' Institute of Chemistry and the University of Cambridge, UK.

Welcoming delegates to the symposium, Toshio Kuroki, program director of the World Premier International Research Center Initiative (WPI), which oversees the operation of the AIMR, reiterated the importance of mathematics-driven materials science research to the institute's work. Introducing the mathematics–materials approach had given the AIMR a “new



Nobel laureate Ei-ichi Negishi, from Purdue University in the US, discussed his research into zirconium-catalyzed addition reactions.

culture and paradigm shift,” in addition to a distinctive focus that complements the already high levels of research achievement established since its inception in 2007, Kuroki said.

In her symposium address, Kotani restated the institute’s goal to integrate materials science with physics, chemistry and engineering to create new materials that can contribute to society. Although a worthy and important aim, achieving this has not proved easy, Kotani noted. Working through the original AIMR launch plan had led to the realization that it was necessary to take greater account of the mathematical view of the field, she said. Further consideration had identified three target projects: Non-equilibrium Materials

based on Mathematical Dynamical Systems, Topological Functional Materials, and Multi-scale Hierarchical Materials based on Discrete Geometrical Analysis, that now form the mainstay of research at the AIMR. Kotani also spoke of the importance of the AIMR as an incubator for international research talent and encouraged researchers from around the world to join the AIMR’s research programs.

Following the introductory addresses, the conference’s academic program began with a special opening lecture entitled “The Magical Power of Transition Metals: Past, Present and Future” by Ei-ichi Negishi from Purdue University in Indiana, US. Negishi, who shared the 2010 Nobel Prize in Chemistry for his work on transition metal-catalyzed cross-coupling reactions, gave a wide-ranging survey of his research into zirconium-catalyzed addition reactions and spoke of his belief in the importance of transitional-metal chemistry for future developments in materials science.

The session continued with a lecture from Hideo Ohno, a principal investigator at the AIMR who presented the latest developments in ferromagnetism in semiconductors. Ohno was the 2012 recipient of the IEEE David Sarnoff Award — seen by many in the field as a precursor to the award of the Nobel Prize in Physics — and is also director of the

Center for Spintronics Integrated Systems at Tohoku University. The opening session concluded with lectures from Masakazu Aono, director of the International Center for Materials Nanoarchitectonics (MANA) — one of the original nine WPI institutes — who provided an extensive assessment of recent topics in materials nanoarchitectonics, and Shun-ichi Amari of the RIKEN Brain Science Institute who drew parallels between the modern differential geometrical analysis of neural networks and nanomaterials.

Plenary sessions featured lectures in mathematics and computation, spintronics, and processes and function delivered by delegates from Switzerland, Japan, Poland, Germany, the UK and the US, representing the research and geographical diversity of the meeting. In total, 32 lectures divided into 10 plenary and parallel sessions were presented during the symposium, supplemented by a 2-day poster session featuring 90 contributions from both Japanese and international AIMR researchers.

The AIMR International Symposium 2013 concluded on 21 February with closing remarks from Masaru Tsukada, administrative director of the AIMR, in which he thanked the organizers, speakers and participants and extended an invitation to all present to join the next symposium in 2014. ■



The symposium attracted 240 delegates, including a significant number of attendees and four speakers from the field of mathematics.

Scaling the heights of materials science research

Akari Takayama is a 2013 recipient of the exclusive JSPS Ikushi Prize for research excellence, awarded for her PhD work as part of the AIMR Materials Physics Group

Established in 2009 with an endowment from Emperor Akihito to encourage and support young scientists, the Japan Society for the Promotion of Science (JSPS) *Ikushi* Prize has been awarded annually to 16 outstanding early-career researchers in the natural and social sciences since 2010. Akari Takayama, currently a JSPS research fellow in the Materials Physics Group at the Advanced Institute for Materials Research (AIMR), speaks to *AIMResearch* about her recent award, her research, life at the AIMR and her plans for the future.

AIMResearch: Congratulations on winning the JSPS Ikushi Prize in 2013. How did you learn that you had won the prize?

I found out about it at the end of December when I passed the initial examination meeting of my doctoral thesis. I was talking through my progress and results when my PhD supervisor [Takashi Takahashi, a principal investigator in the Materials Physics Group] gave me the news. The moment I heard I'd won the prize, I was very surprised. Initially, I couldn't believe it but when it sank in, I was so happy and honored.

We were actually having a belated lab Christmas party at the time. We ate the cake as a sort of unofficial celebration since the lab was sworn to secrecy — the prize results had to be kept under wraps until the official announcement in January. However, I did get to tell my parents.

AIMResearch: The Ikushi Prize is only presented to a small number of top young



Akari Takayama, a 2013 recipient of the JSPS *Ikushi* Prize for research excellence.

scientists in Japan every year. What effect has winning this award had on your career so far?

I won the prize for my work as a PhD student, which I carried out under the direction of a supervisor. After receiving the award I feel a responsibility to step up, keep delivering even stronger results and make my mark as a researcher in my own right. However, the greatest immediate change was probably that my research became a lot better known. People now come up to tell me that they have read my papers and take an interest in my work, which of course makes me very happy. But more than the recognition, I value the opportunity this gives me to interact with other researchers, particularly those from adjacent fields. I learn a lot from them and am inspired to look at things

from a different angle and imagine different approaches.

AIMResearch: You achieved a tremendous amount during your PhD studies. What do you think has been the key to your success?

I think it helps that I'm a pretty observant person. In my view, it's really important in scientific research to have an eye for detail and to be able to notice subtle changes that are out of the ordinary. When developing equipment or optimizing an experiment, it is critical to be able to spot what makes one condition different from a previous arrangement and work out how this can be used to improve the experimental outcome. Similarly, when analyzing data, it's vital to be able to distinguish an unusual and potentially significant result from an artifact.

I'm also somewhat of a perfectionist: all the samples that I make in my research have to be meticulously prepared. If my materials aren't top quality, I won't use them. I'm proud of the quality of my samples — I don't want anyone to say my samples are a bit substandard.

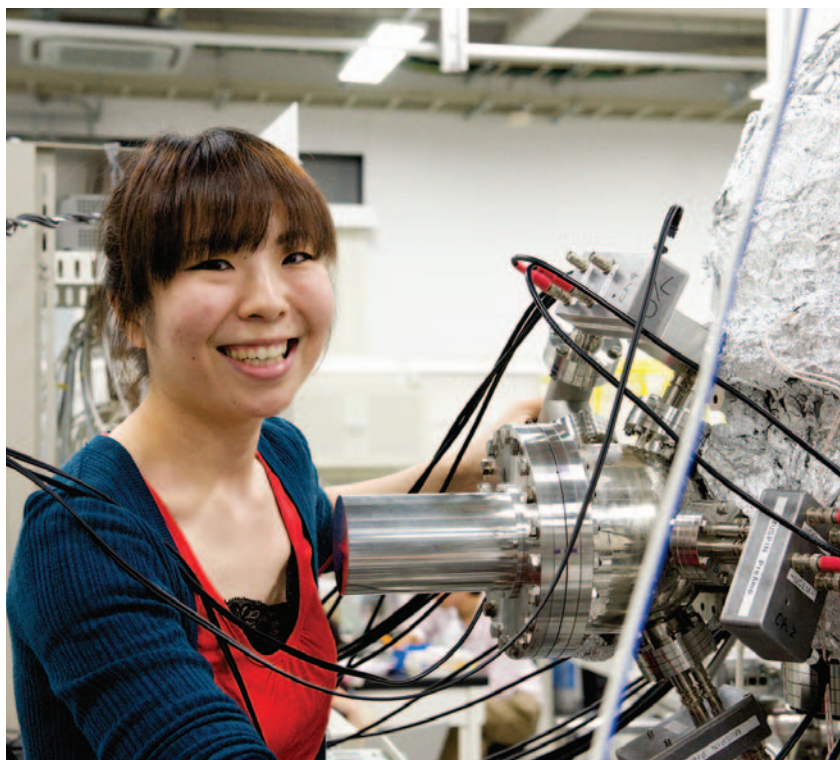
AIMResearch: Your PhD thesis discussed the effects of spin polarization in materials, which is extremely important for technologies such as 'spintronics'. What is spintronics, and how does your work contribute to the field?

Spintronics involves trying to control and manipulate the direction of the magnetic moment, called 'spin', that is one of the fundamental properties of electrons. One application for this technology is to use it to store electronic information as the basis for new types of computer memory, which would be many times smaller and more energy efficient than current devices. But in order to control these spins, we first have to be able to measure properties such as their size and the direction in which they are pointing. My work involves designing equipment and methods for measuring these properties very accurately, which can be quite challenging.

Thanks to the JSPS fellowship, I will be able to extend my PhD work to other materials systems and to study their spin-polarization phenomena. My research has discovered anomalous behaviors of spin, and the results suggest a new possibility of spintronics. To check the universality of this discovery, I am eager to investigate systems with different elements to the one I have been studying, but which theory suggests should display the same kinds of phenomena.

AIMResearch: What are the best things about working at the AIMR, and what attracted you to carry out your doctoral research here?

There are many reasons to study at the AIMR. You get to meet and work with a great number of extremely talented researchers from different, but related, fields and are therefore able to take



As a JSPS research fellow in the Materials Physics Group at the AIMR, Takayama is currently studying spin-polarization phenomena in materials as an extension of her PhD research.

advantage of their insight and ideas. For example, I often interact with colleagues from the recently incorporated Mathematics Unit at events such as the weekly Tea Time, and we have had many useful and interesting discussions. My interest in mathematics and my level of understanding has definitely improved as a result, and I am sure this will have a positive impact on my work in the future. Plus, AIMR researchers come from all over the world, which is enormously stimulating.

The facilities and the research support provided by the AIMR are truly excellent. Obviously, we have the necessary equipment within our lab to obtain high-quality data for experiments in our field, but with the kind of advanced, cross-disciplinary research that my group is performing, we often need to look at our systems from different experimental perspectives. Fortunately, at the AIMR I have access to all the other resources — both facilities and research collaborators — that I need, under one roof.

AIMResearch: You have already achieved a great deal in your career. What are your plans for the future?

I definitely want to stay in research, but I don't particularly feel the need to become a famous professor. The part of my research that I like best is designing and making new experimental equipment, then using it to explore new materials systems. The moment when I first obtain new data is really exciting. I'd like to keep working in an environment where I can pursue research and experience the thrill of discovery. I also want to try my hand at other experimental techniques. Up to now, I've specialized in photoemission spectroscopy, but I'd really like to learn new methods in order to evaluate the quality of samples more comprehensively. Wherever I am and whatever methods I use, I see myself always enjoying life as a researcher, though I think that it is hard to learn new techniques. For this reason, even small and incremental improvements please me when I am making samples or setting up machines. ■

RESEARCH SUPPORT FOCUS

Published online on 30 September 2013

No bridge too far

The Interface Unit, which bridges the gap between mathematics and materials science at the AIMR, is helping to transform the way the institute thinks about research in both fields

When the Advanced Institute for Materials Research (AIMR) embarked on its bold strategy of applying a mathematics-driven approach to materials science research under the directorship of Motoko Kotani, it faced a fundamental challenge: how to assist its mathematicians and experimental materials scientists — who respectively contend with abstract concepts and very concrete problems — to speak a common language.

To address this issue, the AIMR created the Interface Unit (IU), a group of eight young theoretical physicists and chemists charged to act as a bridge between the institute's mathematicians and researchers from three Target Projects — Non-equilibrium Materials, Topological Functional Materials and Multi-scale Hierarchical Materials — chosen as test beds for the mathematics-driven fusion research approach. In addition to carrying out independent original research, members of the IU work closely with their materials science colleagues to develop mathematical tools and models for theoretical aspects of the Target Projects, which subsequently guide the direction of experimental research. The radical approach is not only influencing the way that AIMR scientists tackle their work but also has the potential to break the mold of interdisciplinary research.

Exploring new avenues

Miki Kobayashi, an assistant professor at the AIMR who specializes in non-linear dynamics, joined the IU in 2012. He admits to having had concerns at the outset about the viability of the mathematics-driven research strategy, which were ultimately unfounded. “Materials science is a well-defined field that has achieved



Members of the AIMR Interface Unit (IU). Clockwise from top left: Miki Kobayashi, Masamichi Miyama, Daniel Packwood and Koji Sato.

remarkable results without any special involvement from the mathematical community, so I wondered if these researchers actually needed our help at all,” says Kobayashi. “But I have been impressed by how receptive my experimental research colleagues are to using mathematics to explore new avenues in materials research,” he adds. Masamichi Miyama, a research associate in theoretical physics, also joined the IU in 2012 and echoes this sentiment. “When I started at the AIMR, I had my doubts about whether my background in statistical thermodynamics would be useful,” Miyama says. “But my experimentalist colleagues have welcomed our involvement, and I think we work really well together,” he adds.

An important tactic used by the IU to build connections between the AIMR's mathematics and materials research

groups has been to identify problems of interest to experimentalists that also have a mathematical ‘hook’. “It’s like a seed for creating discussion from both sides,” says Daniel Packwood, an assistant professor and theoretical chemist who originally hails from New Zealand. “Normally, experimentalists come to me with a problem then we discuss it further and I’ll go away and work on it — and that may lead to publishable research.” This exchange of ideas can work both ways, however, as the theoreticians often come up with mathematical concepts that may be of interest to the institute's experimentalists.

Research without boundaries

Free discussion and collaboration are encouraged at the AIMR and channels for interaction include weekly Tea Time sessions. In addition, there are regular

informal seminars aimed at stimulating open-ended discussion where participants are encouraged to ask questions, no matter how basic they may seem. “When I arrived at the AIMR, I was wary of approaching colleagues who were experts in areas I knew very little about,” comments Koji Sato, a spintronics researcher who joined the IU in early 2013. “At my previous institution, it would have been difficult for me to do this. But here, we are under pressure — in a positive way — to collaborate, so I made up my mind to not feel intimidated and to ask a lot of questions.”

Allowing members of the IU and experimental researchers to interact without boundaries has greatly improved communication within the AIMR, although there is still a need for a degree of ‘bilingualism’ on the part of IU members. “I do find myself needing to use different language depending on whether I am talking to a mathematician or an experimental researcher,” admits Packwood. A certain degree of individuality is inevitable — and even desirable — according to Kobayashi. “We’re not trying to amalgamate maths and materials science. Our job is to provide a bridge between the two.” Miyama agrees: “I would like mathematicians to retain their individual identity

but benefit from the different insight that working with materials scientists can bring.” Consequently, early concern about the viability of the mathematics-driven approach has largely been alleviated, and the institute is now harvesting the first fruits of this strategy — in the form of a number of international conference presentations made by researchers from the IU and papers jointly published with AIMR experimentalists in leading journals.

Breaking the mold of interdisciplinary research

The IU’s role in promoting efficient fusion research at the AIMR could also serve as a model for other universities and institutes — in Japan and around the world — who are seeking to boost their interdisciplinary research programs. “Given time, the AIMR could provide a template for creating truly functioning interdisciplinary research,” says Packwood. “We’re already producing innovative results that aren’t normally seen in the theoretical physics arena — but not yet in the mathematical arena because the results are so physical in character. Nonetheless, you can’t just mix people together and expect them to do interdisciplinary research. You need a catalyst.”

And while the IU provides exactly such a stimulus, it is also helping to create a new approach to research — one that is more predictive and theory-led than typical materials science, yet more descriptive than traditional mathematics. “It’s important to be able to discover new things and develop new methods, especially in a mature field like materials science,” notes Sato. “Hopefully our approach will help to unlock new potential, although it won’t be easy.”

Change is unlikely to come overnight and requires experimentalists and theoreticians alike to work outside their comfort zones, with the former accepting a more structured approach to carrying out experiments and the latter being willing to relinquish a degree of theoretical completeness. Although the potential rewards for the AIMR and any resulting interdisciplinary research are great, pushing forward with AIMR director Kotani’s vision for mathematics-driven research will take commitment, hard work and more than a little courage. “The experimentalists are changing the way they do research,” observes Packwood, “and as theoreticians, so must we. It’s exciting, but it’s challenging. We have to learn to think differently; maybe entirely new types of approximation are needed.” ■



The IU is bridging the gap between mathematics and materials science researchers at the AIMR.

ROUNDTABLE INTERVIEW

Published online on 20 December 2013

Reaping the rewards of a mathematics–materials approach

Founded in 2007 as one of the inaugural institutes of the World Premier International Research Center Initiative (WPI), the AIMR has now embarked on its second five-year term. In late 2011, the institute began an ambitious new mathematics-driven research strategy that is already delivering impressive results.

The mathematics-driven approach to materials science research at the AIMR is a distinguishing feature of the institute's research culture and sets it apart from the other institutes in the WPI program. Although still at an early stage, the strategy has already produced a number of exciting results. AIMResearch spoke to Mingwei Chen, a principal investigator in the Bulk Metallic Glasses Group, and Motoko Kotani, director of the AIMR and a principal investigator in the Mathematics Unit, about their collaborative work which was the subject of a recent *Science* paper.

AIMResearch: Your recent paper — entitled “Geometric Frustration of Icosahedron in Metallic Glasses” — is an excellent example of mathematics-driven materials science research. How would you summarize the paper's main findings?

Chen: Our work presents conclusive evidence showing that metal atoms pack into the glass state as geometrical fluctuations of 20-faced units called icosahedrons. This had previously been suggested, but we combined experimental results with extensive modeling and simulation to confirm that this motif could be used to make theoretical predictions of long-range disorder in metallic glass systems.

To understand structure–property correlation in metallic glasses, we need to work on the atomic scale because, unlike crystalline materials, glasses do not have a clearly defined microstructure, such as grain or defects. This is extremely challenging because glasses essentially consist of long-range disorder. Uncovering the



Mingwei Chen, a principal investigator in the Bulk Metallic Glasses Group.

atomic arrangement of glasses helps us to gain insight into fundamental processes such as the liquid to glass transition, the formation of shear transformation zones — the movement of atoms when force is applied — and the breaking of atomic bonds and failure of the glassy material. The work in our latest *Science* paper¹, which follows our 2011 paper in *Nature Materials*², establishes local structural features such as the geometrical and topological atomic arrangement and shows how these are distorted in the glass state.

AIMResearch: Your discovery was achieved by combining experiment, theory and mathematical modeling. What respective roles did these play in the research?

Chen: As you might expect, technical aspects were extremely important in this work, and, in particular, the angstrom-beam electron diffraction method. This technique uses a modified transmission electron microscope to precisely focus a coherent electron beam of about 3 angstroms in diameter, without which we would never have been able to observe the local atomic arrangement of the sample. This is the first technique that allows us to image not only metallic glasses but also oxide glasses and other disordered systems in such detail.

Kotani: A major part of the work involved translating the experimental data into a picture of the overall structure of the

metallic glass. This issue was addressed by Akihiko Hirata (associate professor in the Bulk Metallic Glasses Group) and Kaname Matsue (assistant professor in the Kotani Laboratory) who used advanced topological methods to derive a global structure from local structural data using a modeling program provided by the Computational Homology Project (CHomP).

This web-based software provides non-mathematicians with a relatively pain-free way to analyze complicated datasets using topological techniques. As a result, many researchers at the AIMR have become interested in using topology to get essential data from complex figures and hierarchies for working on glassy and nanoporous materials.

AIMResearch: The scientific value of this research is very clear. What is its significance in terms of the mathematics-driven materials science agenda that has been adopted by the AIMR?

Kotani: When we proposed the new mathematics–materials-driven research approach, many thought it was an attractive idea but also very challenging. What that really means is that they thought the strategy was rather high risk. I always believed that the direction we chose was the correct

one but did not expect that we would get concrete results so quickly. While I think we are yet to make a real breakthrough, results like those in Professor Chen's paper give us confidence that our research program is moving in the right direction.

Chen: I agree that it is important to have been able to prove the concept of combining mathematics with materials science in such a short time. As an experimentalist, I can say that working collaboratively like this has not only given us a tool for research, but has also changed our conceptual viewpoint and opened my eyes to a new research philosophy. Taking a more fundamental approach, such as looking at the topological interpretation of the system, has helped to keep our minds on the bigger picture, as well as on the details.

AIMResearch: How do you expect the current collaboration to develop?

Chen: We believe that there is a common link between the behavior of all types of glassy materials and we are working to apply our methods to other systems such as polymer and oxide glasses, as well as chalcogenide glasses. Using theoretical models derived from experimental data, we can eventually begin to design materials with enhanced properties.

Kotani: Gaining a comprehensive understanding of glassy substances is one of the main areas of work at the AIMR. In the future, we will concentrate on establishing a universal framework for these systems. Glassy materials exist at a phase interface between particle dynamics, which obeys certain mathematical rules, and continuum dynamics, which can be described using tools such as Navier–Stokes equations. At the moment we do not have a master equation that describes these phenomena, so developing a mathematical theory that can handle these areas is a big challenge.

AIMResearch: How did the research environment at the AIMR help to make this discovery?

Chen: One important reason for the success of our study is the way in which the WPI program has fostered real fusion research that, in the case of the AIMR, puts mathematicians in the same building as experimentalists like me. This gives us the opportunity to discuss research directly, rather than having to travel to different campuses, and to establish working relationships with the right people, straight away.

Kotani: I am also very grateful to the WPI program for giving us the opportunity for this kind of interaction and support. It allows us to physically meet with the best people to discuss problems on a daily basis, which would not be possible under any other system. The same commitment to exchange has allowed us to set up the Interface Unit, which provides a bridge between young independent researchers in mathematics and experimentalists. The system has really stimulated our young academics and has provided a model that is being considered for roll out across Tohoku University. As is apparent, this is a very exciting time to be researching mathematics and materials science at the AIMR. ■



Motoko Kotani, director of the AIMR and a principal investigator in the Mathematics Unit.

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INTERNATIONAL WORKSHOP

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Strengthening scientific exchange and joint research

The AIMR represented Tohoku University and showcased some of its best science at joint workshops held with the University of Cambridge and University College London in November 2013

While the AIMR is well known for its world-leading research and international research partnerships, the history of international academic exchange in Japan is still relatively recent. The year 2013 marked the 150th anniversary of the first Japanese students — known as the Choshu Five — beginning their studies in England. In recognition of this milestone, UCL (University College London) — the university that hosted the students — organized a number of commemorative events, including several held in conjunction with Tohoku University. The AIMR's visit to the United Kingdom offered a further opportunity for academic exchange through a workshop on mathematics and materials science at the University of Cambridge.

Joint AIMR–University of Cambridge workshop on mathematics and materials science

On 20 November, 14 researchers from the University of Cambridge and 12 young researchers from the AIMR converged in Cambridge to attend the AIMR–Cambridge Workshop and Discussion on “Hierarchical materials for green energy.” The AIMR's connection with the University of Cambridge was formalized in 2012, when an agreement was signed to establish an AIMR Joint Center (AJC) where UK and AIMR scientists can perform joint research into metallic glasses, soft materials and mathematics.

Attendees at the workshop included Alan Lindsay Greer, an AIMR principal investigator and a professor at the University of Cambridge, and researchers Jiri Orava, Katherine Orchard and Demeter Kiss from



The AIMR–UCL Materials Workshop focused on recent developments in materials science.

the AJC in Cambridge. “The workshop provided a relaxed atmosphere in which the young and promising researchers could hold intense discussions on mathematics and materials science,” noted Masaru Tsukada, the administrative director of the AIMR.

Celebration of research with UCL

On 21 November, Tohoku University signed a Memorandum of Understanding with UCL to further promote scholarly collaboration and international exchange, building on several years of successful scientific cooperation under academic exchange agreements fostered between the AIMR, two other institutions at Tohoku University and UCL faculties. The signing ceremony was followed by a forum to commemorate 150 years of academic exchange between Japan and the United Kingdom, including speeches by eminent professors from Tohoku University and UCL. Representing

the AIMR, Director Motoko Kotani gave a commemorative address on the theme “An Introduction to the AIMR: Toward World Premier Status and Beyond.”

The following day, a well-attended AIMR–UCL Materials Workshop was held. Focusing on recent developments in materials science, the session featured 16 talks, including keynote lectures from AIMR principal investigators (PI). Alexander Shluger, a PI at the AIMR, expressed his expectations for future research development, in consideration of the many researchers — and potential collaborators — in attendance. “Each presentation stimulated in-depth discussions, and we expect further collaborations to develop as researchers find common agendas.”

Continued opportunities for exchange

The AIMR UK-based workshops proved stimulating and provided researchers located in Japan and the United Kingdom with an opportunity to share research ideas and findings. The workshops' success is expected to lead to further opportunities for personnel exchange and joint research projects, particularly in partnership with UCL. Additionally, the workshops highlighted the value of promoting multidisciplinary exchange through AJCs at the University of Cambridge and other AIMR satellite institutions.

“I am pleased that the AIMR's UK research activities are contributing to Tohoku University and providing an opportunity to strengthen its globalization efforts,” commented Director Kotani. “The AIMR and Tohoku University have now established themselves as top-class research institutes with a firm base in the United Kingdom.” ■