Advanced Institute for Materials Research

Director
Motoko Kotani

A Unique Research Center Where Mathematics Drives Materials Science Innovation

AIMR was established to bring together scientists in materials science, physics, chemistry and engineering – research fields in which Tohoku University holds a world-leading position – who can contribute to society by creating revolutionary new materials. Since its establishment in 2007, AIMR has consistently produced interdisciplinary "fusion" research achievements across different fields, utilizing atomic and molecular control. In 2011, a new policy was adopted of introducing mathematics into all areas of materials science research, aimed at making fusion research more dynamic. Since then, promoting collaboration between mathematicians and researchers in the fields of materials science, physics, chemistry, and engineering, AIMR has become the world's first research center fully devoted to fusion research between mathematics and materials science.

Research Center's Information (FY 2015)

Center Director: Motoko Kotani (up to FY 2011: Yoshinori Yamamoto)
Principal Investigators (PI): 28 (including 13 overseas researchers and 2 female researchers)
Other Researchers: 140 (including 74 overseas researchers and 13 female researchers)
Research Support Staff: 75
Administrative Division:
  Administrative Director: Masaru Tsukada
  Administrative Staff: 30 (percentage of bilingual staff: 90%)
Satellites and Cooperative Organizations: University of Cambridge, UK;
  University of California, Santa Barbara, USA; University of Chicago, USA;
  Institute of Chemistry, Chinese Academy of Sciences, China;
  University College London, UK; Tsinghua University, China; and others
URL: http://www.wpi-aimr.tohoku.ac.jp

Major Research Achievements

1 Using mathematics to shed light on materials science

The structure of metallic glasses was elucidated after remaining a mystery for half a century. This revolutionary fusion research, by materials scientists working with mathematicians (in the field of geometry), is emblematic of AIMR innovation.

2 Research advancing porous materials

Nanoporous metal, with countless nano-sized holes, was applied to development of highly efficient catalysts. Using nanoporous metal as a mold, technology was developed for fabricating three-dimensional nanoporous graphene that preserves the electron mobility of two-dimensional graphene. AIMR continues to dramatically advance the field of nanoporous materials science

3 Elucidation of new principle relating to magnetic properties and spin

A principle was conceived whereby magnetic waves (spin waves) are used to transport thermal energy in the desired direction. Moreover, a spin- and angle-resolved photoemission spectroscopy system (spin-ARPES) was developed achieving the highest resolution ever, and is being used to clarify the mechanisms by which material properties emerge. AIMR is advancing at the forefront of the magnetism and spin science.

4 Applications of multifunction hybrid materials and complex hydrides

Using supercritical water as the reaction solvent, multifunction hybrid materials were created without the use of hazardous substances. Discovering the excellent ionic conductivities of "complex hydrides", researchers applied these new materials to solid-state electrolytes for next generation rechargeable batteries. Creating new materials, AIMR is also pointing the way to potential applications.

5 Design of MEMS and biosensing devices

In the field of MEMS (Micro Electro Mechanical Systems), visible only with a microscope, a micromirror was developed using metallic glasses. Researchers also developed a noninvasive high-resolution imaging method using NanoSECM and related systems, and applied it to monitoring of living cells.

6 Oxide electronics endowing common, abundant materials with novel functions

Superconducting was realized by field-effect doping of oxides, which are basically insulators that do not conduct electricity. Moreover, researchers observed the fractional quantum Hall effect in oxide materials for the first time. The results of AIMR research led to the birth of a transparent superconductor.

Research Paper's Information

Number of Research Papers:	2,609
Top 10% Papers:	17.6%
Top 1% Papers:	2.4%
Internationally Collaborative Research Papers:	43.3%

(Database: WoS between 2007-2015)

The background is graphene.
Two-dimensional graphene consists of a single layer of carbon atoms arranged in a honeycomb lattice pattern.

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Blazing new trails at the forefront of materials science

The moment people start using a substance, it comes to be called a "material." The science of studying materials is known as materials science. The field of materials science, which seeks to make substances serve humankind in useful ways, crosses over a wide range of natural sciences including physics, chemistry, engineering, and life sciences. AIMR was established in 2007, bringing together researchers from this broad range of areas to advance fusion research and blaze new trails at the forefront of materials science.

In the first half of the decade since its founding, under the leadership of Director Yoshinori Yamamoto, a chemist, fusion research was carried out by people in the fields of materials science, physics, chemistry, engineering, and life sciences. Then in the second half, under current Director Motoko Kotani, a mathematician, fusion research was accelerated based on the policy of introducing mathematics into all areas of materials science research.

Today this policy has evolved further, moving in innovative directions with the aim of deriving common principles by describing various materials science phenomena and principles using mathematics, going on to mathematically predicting structures and other properties of previously unknown materials, and then actually creating these unknown materials.

Here we introduce some of the research results brought about by AIMR in each of the broad-ranging fields of materials science, starting with innovations achieved by introducing mathematics.

1 Using mathematics to shed light on materials science

Mingwei Chen (PI), Motoko Kotani (PI), Akihiko Hirata (Associate Professor)

A successful example of introducing mathematics into materials science is clarification of the structure of metallic glasses.

As is well known, the three states of matter are solid, liquid, and gas. Viewed at the nano scale, solids are made up of atoms packed tightly together in a regular pattern to form crystallized structures. In liquids, atoms are assembled close to each other but more disordered and free to move around. In a gaseous state, both the position and distance of atoms can change freely.

But are atoms arrayed regularly in all solids? Not necessarily. Glass, the material of windows and goblets, appears solid to the eye, but its atoms are not arranged regularly as crystals. They are disordered as in liquids.

Normally we tend to consider glass to be a "kind" of material. We think of the transparent material used for windows and drinking utensils as glass. In the world of science, however, the term "glass" is used rather as a material "state." The transparent material we call glass results from high-temperature melting of the main ingredients silicon and oxygen, followed by a cooling process, during which a "glass state" is reached in which the atoms have not had time to line up in an ordered array.

In the case of metal, when it is melted and then cooled, the atoms tend to become rapidly arranged in orderly arrays, forming crystallized structures. Under certain conditions, however, metal can become a solid without the atoms achieving an ordered arrangement. The resulting substance, while not transparent, is in glass state and is thus called metallic glass. Metallic glass is a new material exhibiting many times the strength of ordinary, crystallized metal. This is a material with many mysteries. The strength comes from the absence of crystal grain boundaries where fractures can occur, but the lack of order in the arrangement of atoms makes the structure difficult to characterize.

In 2013, a fusion research team of AIMR mathematicians and experimental scientists (materials scientists) succeeded in clarifying the structure of metallic glasses. First, experimental scientists identified a number of characteristic shapes (atom clusters) in which atoms are arranged in metallic glass, using electron diffraction. Then mathematicians analyzed the features of these atom clusters by means of a geometric method known as computational homology. While the existence of these atom clusters had been pointed out in the past, this was the first time anywhere that their structure was clearly determined. On the basis of these studies, researchers concluded that the arrangement of atoms in metallic glasses consists of clusters of icosahedra (polyhedra with 20 faces each) all distorted in the same way (Fig. 1).

How do metals, with their normal tendency to become crystallized structures, instead become glass with disordered atomic configurations? Hidden in what at first appear to be random atomic arrangements are distorted icosahedra, in large numbers and all similar to each other. However, regular icosahedra cannot completely fill up a three-dimensional space without forming gaps (they are not a space-filling polyhedron), making it theoretically impossible for them to form crystals. This leads to the conclusion that, because their atomic arrangement differs from that of crystal, they are hindered from crystalizing and remain in glass state.

In fact, the icosahedral structure of metallic glasses was theoretically predicted more than a half century ago; but direct confirmation could not be made despite

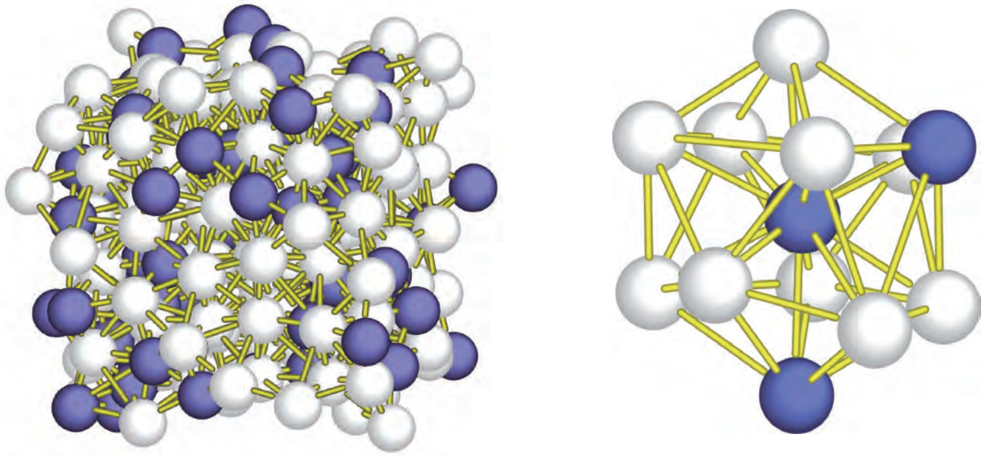

Fig. 1. Model of the atomic arrangement of metallic glass. The icosahedra structure hidden in what appears to be a disordered atomic structure of metallic glass (left) had long been predicted. This study revealed that the sequence of distorted clusters of icosahedra (right) prevent the glass state from crystallizing. The purple spheres in the figure are platinum (Pt) and the white spheres are zirconium (Zr).

attempts by numerous researchers. AIMR succeeded in verifying this hypothesis by combining the highest level of experimental techniques with leading-edge mathematics, settling discussions that had been waged for half a century. Optical fiber and other substances with glass structures are already widely used as practical materials. It is hoped that the knowledge gained from this elucidation of the structure of metallic glasses will lead to improvement of glass materials and development of new ones.

A. Hirata et al., Science 341, 376 (2013).

2 Research advancing porous materials

Mingwei Chen (PI), Yoshinori Yamamoto (PI), Naoki Asao (Professor), Takeshi Fujita (Associate Professor), Yoshikazu Ito (Associate Professor)

Materials with countless nano-sized holes are called nanoporous materials. AIMR scientists developed and applied technology for fabricating nanoporous metal (Fig. 2); moreover, using nanoporous metal as molds, they succeeded in developing new materials.

The process used for fabricating nanoporous metal is called dealloying. To make nanoporous gold, for example, first a gold-silver alloy is made, then the silver is dissolved in acid or the like, so that only gold remains. In the alloy state, gold and silver are mixed together at the nano level. The gold remaining after dissolving the silver is thus nanoporous, with very fine holes. The AIMR research team discovered that the nanoporous gold fabricated in this way acts as a catalyst to promote chemical reactions. Gold is an inactive substance resistant to corrosion, and was once thought not to function as a catalyst. Around 30 years ago, however, nanoparticulate gold was found to have catalytic activity. Thereafter, research on gold nanoparticle catalysts took off dramatically. The problem with gold nanoparticle catalysts is that their catalytic activity weakens as the nanoparticles agglomerate into larger particles. Solving this was a major research theme. The AIMR research team shifted their focus away from the gold nanoparticles that everyone had been studying, looking instead at nanoporous gold. Then they discovered that nanoporous gold had remarkable catalytic activity in the oxidization of organosilane compounds with water. In nanoporous gold, moreover, agglomeration does not occur as with nanoparticles. The high catalytic activity is retained and the catalyst can be re-used numerous times. Catalysts being essential to the chemical industry, nanoporous gold as a highly efficient catalyst is likely to contribute significantly to society.

AIMR is successfully using nanoporous metals like this to create completely new materials. Graphene is a substance consisting of a single layer of carbon atoms in a hexagonal honeycomb lattice structure. It became the object of public attention after the awarding of the 2010 Nobel Prize in Physics. Because of its very high electrical conductivity, graphene is expected as a

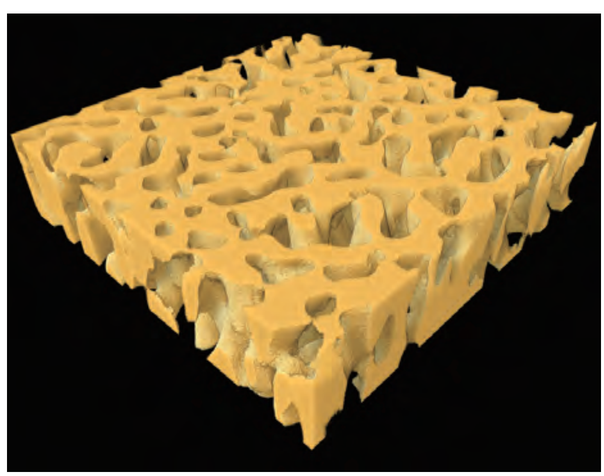

Fig. 2. Image of 3D nanoporous metal obtained by electron tomography using a transmission electron microscope

potential future replacement for silicon semiconductors and metal used in electronic devices today. Scientists have sought to create three-dimensional structures that maintain the high conductivity as demonstrated in two-dimensional graphene sheets, but none of the earlier attempts were successful. AIMR researchers, using the earlier-described nanoporous metal as a mold, developed a process for making a three-dimensional nanoporous graphene structure with high electron mobility. Graphene is grown by chemical vapor deposition on the surface of nanoporous nickel which is fabricated by a dealloying method. Then the nickel is dissolved leaving only graphene. Since this three-dimensional graphene preserves the properties of two-dimensional graphene, there are hopes for its application to electronic devices; but the discovery of its potential use as a catalyst for chemical reactions in hydrogen fuel cells has now suddenly become the focus of interest. Research is continuing toward enabling three-dimensional nanoporous graphene to contribute to hydrogen stations for fuel cell vehicles and to realization of the hydrogen society.

N. Asao et al., Angewandte Chemie International Edition 49, 10093 (2010).
Y. Ito et al., Angewandte Chemie International Edition 53, 4822 (2014).

3 Elucidation of new principle relating to magnetic properties and spin

Eiji Saitoh (PI), Takashi Takahashi (PI), Seigo Souma (Associate Professor)

AIMR has proven its excellence in the research area of magnetism and spin. One of the highlights is "spin caloritronics", which concerns interactions between spin and heat. By nature, heat flows from a hot place to a cold place and a control of the heat flow has been limited to a local heating and cooling. An AIMR joint research team has shown another way: a use of magnetic wave, a dynamics of spin, can control a heat flow in the desired direction. Applying this principle, it should be possible to develop heat flow control devices that transport thermal energy to places distant from the heat source, raising expectations for application to next-generation energy-saving devices.

Another remarkable achievement in this area is the development of a spin- and angle-resolved photoemission spectroscopy (spin-ARPES) system (Fig. 3) with the world's highest resolution. The system has been successfully applied to various novel materials for unraveling the mechanism and electronic states. To elucidate the mechanism of novel properties, it is essential to reveal the state of electrons, the fundamental basis of electronic properties. Photoemission spectroscopy is a powerful tool for this purpose. When materials are shone by light, electrons inside are emitted to outside from the surface (Einstein's photoelectric effect). By measuring the energy of photo-emitted electrons and comparing it with the energy of the light shone, one can estimate the binding energy of electrons in materials, namely the electronic state of materials. Of the three basic physical quantities of electron (energy, momentum, and spin), standard ARPES directly determines the first two quantities. To observe the last quantity (spin) which directly relates to the magnetic property of materials, AIMR researchers have developed a spin-ARPES system equipped with a mini Mott spin detector. The constructed spin-ARPES machine achieves the world's highest resolution. Using this spin-ARPES machine, they studied the electron

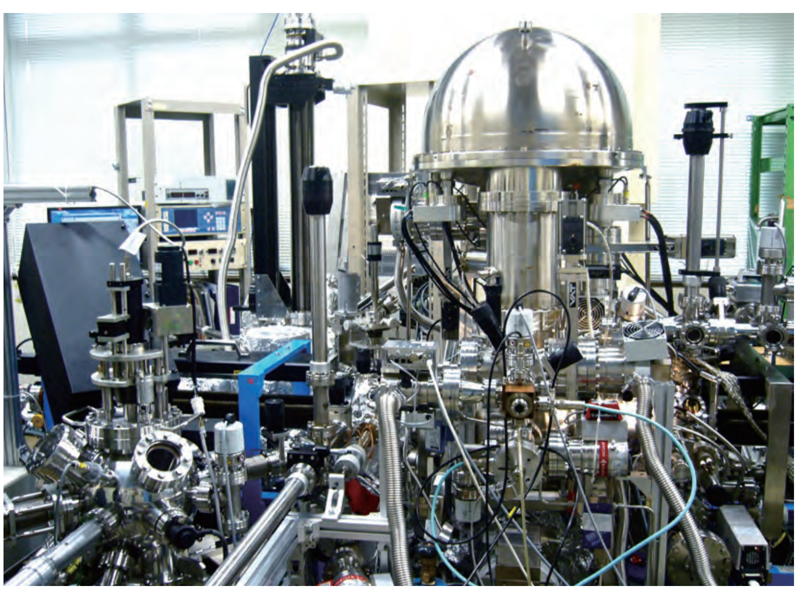

Fig. 3. Spin-ARPES system able to observe all three basic physical quantities of electrons (energy, momentum, and spin) in materials

states of various novel materials such as high-T_c superconductors and topological insulators.

By practical implementation of spin-based technology in personal computers and other electronic equipment, it is believed that energy savings of 80 percent can be achieved. The above studies, along with other spin-related studies pioneered by AIMR researchers in such areas as tunnel magnetoresistance effect and magnetic semiconductors, are major steps toward realizing the dream of energy-saving electronic equipment.

T. An et al., Nature Materials 12, 549 (2013).
Y. Tanaka et al., Nature Physics 8, 800 (2012).

4 Applications of multifunction hybrid materials and complex hydrides

Tadafumi Adschiri (PI), Shin-ichi Orimo (PI)

AIMR researchers are employing novel methods of materials science to create innovative materials with the potential for practical applications.

As one example, an AIMR research team discovered how to create multifunction hybrid materials without the use of hazardous substances, using supercritical water as a reaction solvent. At temperatures and pressure above the critical point, the state of materials turns into a supercritical phase that cannot be distinguished as either liquid or gas phase. Using water in supercritical state, the research team created CeO_2 nanocubes (cubic shape crystals of cerium oxide) of 10 nanometers or smaller (Fig. 4). The resulting CeO_2 nanocubes show higher catalytic activity at lower temperatures than normally seen in conventional catalysts. They are expected to be used for such applications as environmental cleaning and waste decomposition.

Another AIMR success was finding the excellent ionic conductivities of "complex hydrides" for next generation rechargeable batteries. Normally, liquid electrolytes are used in rechargeable (or secondary) batteries. The problem is that the liquid electrolytes become unsafe at high temperatures. Therefore, development of solid-state electrolytes has been socially desired. An AIMR research team discovered that, with the complex hydrides containing sodium, boron and hydrogen (stable salts substances such as $Na_2B_{10}H_{10}$), sodium ion conductivity at 100°C rises up to 100,000 times than that at room temperature. Research is continuing toward implementation of solid-state sodium rechargeable batteries using new complex hydrides with high ion conductivity even at room temperature.

J. Zhang et al., Nano Letters 11, 361 (2011).
T.J. Udovic et al., Advanced Materials 26, 7622 (2014).

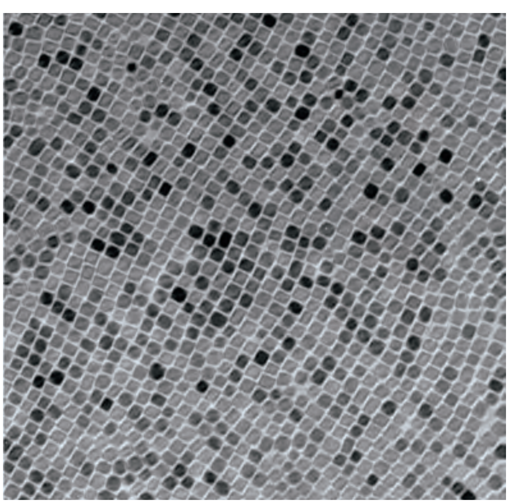

Fig. 4. Cluster of nanocubes fabricated by supercritical water thermal synthesis

5 Design of MEMS and biosensing devices

Masayoshi Esashi (PI), Thomas Gessner (PI), Tomokazu Matsue (PI), Yu-Ching Lin (Associate Professor)

AIMR has created highly innovative devices applying materials science knowledge. As examples, here we look at MEMS and biosensing devices.

MEMS (Micro Electro Mechanical Systems) are mechanical systems so small they can be seen only with a microscope. This is one of Tohoku University's strongest applied research fields. An AIMR fusion research team used metallic glass, which does not break even under large deformation, to support a silicon micromirror (Fig. 5). The micromirror can be mounted on an endoscope and used for beam scanning in optical coherence tomography (OCT) imaging of tissue. The encounter between materials scientists and device engineers gave birth to the novel result of MEMS using previously unimagined materials. As an example of a biosensing device, the voltage-switching mode scanning electrochemical microscope (VSM-SECM) developed by AIMR researchers is a special kind of microscope. Detection at cell surfaces of neurotransmitters, reactive oxygen species, and other short-lived chemicals that are released and consumed by cells had been a highly difficult challenge. AIMR researchers, using this special microscope, succeeded in acquiring high-resolution topographical and electrochemical images of living cells simultaneously by non-invasive (non-contact) imaging. Their next challenge will be to monitor the changes in neuron topography when neurotransmitters are released. These advances have wide-reaching implications for the future of medical care.

Y.-C. Lin, Y.-C. Tsai et al., Advanced Functional Materials 25, 5677 (2015).
Y. Takahashi et al., PNAS USA 109, 11540 (2012).

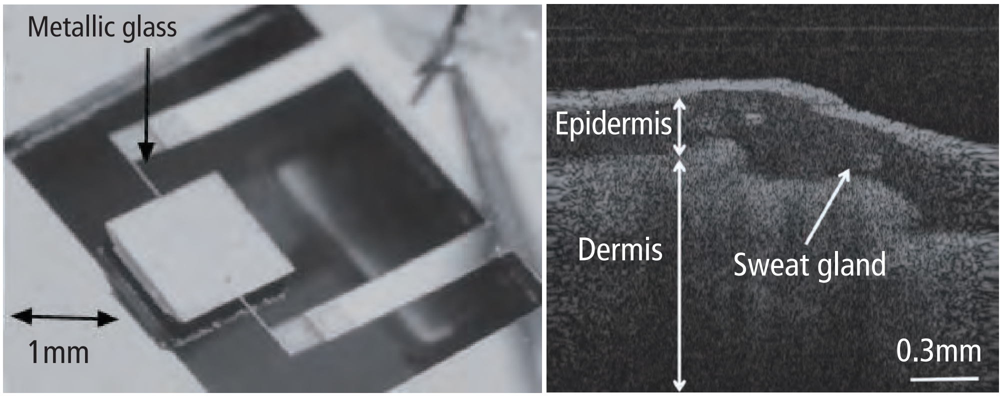

Fig. 5. Tomographic image of skin taken using a micromirror supported by metallic glass

6 Oxide electronics endowing common, abundant materials with novel functions

Masashi Kawasaki (PI), Taro Hitosugi (Junior PI)

Oxide electronics grew up rapidly as a research field soon after AIMR was established. Among the most important discoveries at AIMR, attracting the notice of researchers throughout the world, were superconductivity induced by field effect carrier doping and observation of the fractional quantum Hall effect in oxide materials.

When certain materials are cooled to very low temperatures, their electrical resistance rapidly drops to zero. This phenomenon is known as superconductivity. By making wires from superconductive materials, power transmission systems with very little energy loss can be realized, contributing greatly to solving the world's energy problem. The superconductors discovered up to now require cooling to reach the superconductivity state. As the search continues for materials that can achieve superconductivity at room temperature, besides the approach of looking for new materials, a breakthrough is being sought by coming up with a new way of inducing superconductivity. Here an AIMR research team has succeeded in establishing a brand new method, achieving superconductivity by field-effect doping of oxides.

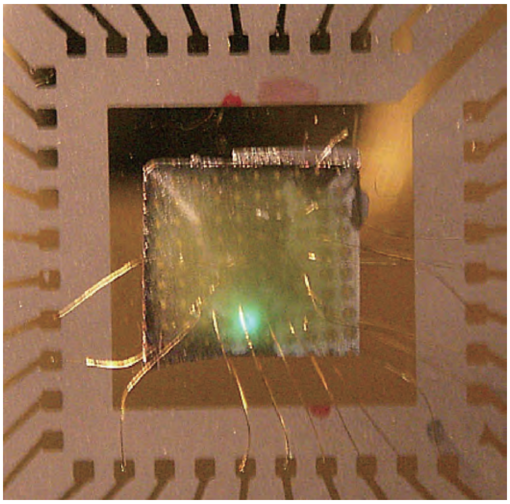

Fig. 6. Light from light-emitting diode made using zinc oxide material

Strontium titanate ($SrTiO_3$) is normally an insulator that does not conduct electricity. The team used field-effect doping to inject a large amount of electrons onto the surface of this oxide, inducing superconductivity. Previously, electron injection by doping with impurities had been tried, but the studies had been limited because very few oxides lend themselves to efficient impurity doping. Discovery of this new method suddenly broadened the search for superconductive materials, greatly impacting the world's materials scientists.

In addition to the above advances, AIMR researchers using zinc oxide confirmed the fractional quantum Hall effect in an oxide for the first time. This is a phenomenon in which electrical resistance take on values given by fractional times of a combination of fundamental constants of quantum mechanics. They also succeeded in developing high-luminance zinc oxide light-emitting diodes (Fig. 6). The key to both these achievements was the relentless effort of researchers to overcome the difficulties of controlling atoms on oxide thin films. A further accomplishment was creating transparent superconducting thin films of lithium titanates (spinel), exhibiting up to 70% transmittance of visible light. This was achieved by precise control of the atomic ratio. These research successes demonstrate the potential for creating highly functional electronics materials from oxides, which are abundant and found everywhere.

K. Ueno et al., Nature Materials 7, 855 (2008).
A. Tsukazaki et al., Nature Materials 9, 889 (2010).

The Path to Creation of Novel Scientific Fields

AIMR has produced a large and diverse array of remarkable research results, including those introduced above.

The number one reason that these accomplishments have been possible is that the center has attracted a large number of excellent world-class researchers. Tohoku University as the host institution has a long history of leading the world in materials science, and it is against the background of trust in this history that so many outstanding scientists have come to AIMR.

The second reason is the environment conducive to carrying out fusion research provided at AIMR, and many different innovative measures devoted to enabling its implementation. The center is equipped with the facilities and equipments for conducting world's top level research, and provides scientists appointed from outside Japan with extensive support for both research and living. It also holds various research events inside and outside the organization. The AIMR International Symposium is held annually, assembling scientists from more than 15 countries; many joint workshops are held with partner institutions from outside Japan; and interdisciplinary exchanges are encouraged in a wide range of materials science academic societies.

The third reason behind AIMR's success is the adoption of a clear policy and bold strategy of introducing mathematics into all areas of materials science research. Setting ambitious target projects that are highly compelling to researchers, research fusing mathematics and materials science has been carried out. Today research continues in AIMR on four target projects: Non-equilibrium Materials based on Mathematical Dynamical Systems, Topological Functional Materials, Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis, and The Core Technology for Nano Energy Devices.

That the policy measures relating to the above three reasons could be carried out successfully is in each case due largely to AIMR being a World Premier International Research Center. Along with these measures, AIMR has consistently devoted energy to supporting and developing the young scientists responsible for the next generation.

AIMR: Looking Ahead

Throughout its ten-year history, AIMR has continued to encourage and support young scientists willing to take up the challenge of interdisciplinary fusion research. In fact, young researchers from different disciplines, who would have few chances to become acquainted at an ordinary university or research institution, can frequently be seen talking to each other at Tea Time or debating at workshops, as they transcend the wall between disciplines. It is not hard to imagine that they will further advance the results that have emerged from such interchanges, and in the future will themselves create new fields of science. The fact that there are ambitious young scientists who grew up, transcended the walls between disciplines, and went out to the world, is the largest accomplishment of AIMR as a research center, and the core of the organization (Fig. 7).

Fig. 7. Director Kotani with young AIMR scientists.
They will go on producing research results by transcending the walls of nationality, gender, and academic fields

The goal of AIMR as an organization today is to create and give root to new materials science that enables prediction of new functions based on collaboration between mathematics and materials science. To bring about a completely new academic field and a brand new science, AIMR will continue to steadily produce research achievements. It will also nurture scientists who will create the future.

Osamu Shimizu (AIMR)