AIMR Magazine

Advanced Institute for Materials Research

AIMR Magazine January 2014

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03
January 2014

[Feature articles]

Metallic Glass, A Dream Material

Associate Professor, Tohoku University Advanced Institute for Materials Research (AIMR)

Akihiko Hirata

[AIMR in the world]

Science Talk Live 2013

by WPI

"Conviction and Responsibility"

Motoko Kotani

Director of the Tohoku University Advanced Institute for Materials Research (AIMR)
Distinguished Professor, Graduate School of Science, Tohoku University

[New Staff]

Sophie D'ambrosio

Science Talk Live 2013

by WPI

Saturday, December 14, 2013 Venue Sendai International Center

PROGRAM

12:00 – 13:00
Registration (Booth session)

13:00 – 13:05
Explanation of objectives
(Motoko Kotani, Director of Tohoku University AIMR)

13:05 – 13:10
Opening remarks
(Susumu Satomi, President of Tohoku University)

13:10 – 13:15
Congratulatory message
(Yoshitaka Sakurada,
Senior Vice Minister of Education, Culture, Sports, Science and Technology)

13:15 – 15:05
Lecture by five researchers (including breaks)

15:05 – 15:30
Booth session: Core time

15:30 – 16:40
SPECIAL PLAN **English presentations by high school students**

16:40 – 17:00
Review of presentations by the researchers

17:00 – 18:00
Booth session: Core time

SPEAKERS

Kenichiro Itami
Director of the Institute of Transformative Bio-Molecules, Nagoya University

Born in the United States in 1971. Specializing in synthetic chemistry (technology for synthesizing molecules), he aims to develop new nanocarbon materials, life function molecules, and pharmaceutical and agrochemical products. In the past five years, he has been featured on television, radio, newspapers, and magazines over 90 times.

Alan Lindsay Greer
Principal Investigator of the Advanced Institute for Materials Research, Tohoku University / Professor of the University of Cambridge

Born in 1955 in the U.K. After graduating from the University of Cambridge, he moved on to become a researcher at Harvard University, and worked in various capacities before taking up his current position. He is renowned as a world authority in research on the microstructural formation of metallic materials, and has published more than 350 papers to date.

Akari Takayama
JSPS Postdoctoral Research Fellow, Tohoku University

Born in Fukushima Prefecture in 1985. Since her time as a doctoral candidate, Takayama has been involved in the development of a spin-resolved photoemission spectroscopy with the highest resolution in the world. She has received the JSPS IKUSHI Prize and the Tohoku University President's Award for her achievements in the observation of the Rashba effect on interfaces. Takayama was conferred her doctoral degree in March 2013.

Kei Hirose
Director of the Earth-Life Science Institute, Tokyo Institute of Technology

Born in 1968 in Fukushima Prefecture. Hirose is a world-class Japanese geoscientist, and a recipient of the Japan Academy Prize. He was commended around the world for making a major discovery in the history of earth science for the first time in 30 years, for his discovery of the lowermost mantle (post-perovskite), and was featured on the cover of the American journal *Science*.

Masashi Yanagisawa
Director of the International Institute for Integrative Sleep Medicine, University of Tsukuba

Born in 1960 in Tokyo. He completed his doctoral course at the graduate school of the University of Tsukuba. Yanagisawa is a regular member of the National Academy of Sciences (U.S.). During his time as a graduate student, he discovered the vascular control factor endothelin, and in 1998, discovered orexin, the neurotransmitter that controls sleeping and waking conditions. He plays an active role on the global stage with the aim of unlocking the mysteries behind sleep.

Booth session

The World Premier International Research Center Initiative (WPI) aims to establish "visible research bases" with superior research environments and extremely high research standards, in order to attract researchers from around the world who are working on the front lines of their fields. The program was launched in 2007 by the Ministry of Education, Culture, Sports, Science and Technology. This booth session brings together the nine WPI bases from all parts of Japan, and features cutting-edge research that is being carried out in a wide range of fields, spanning research on atoms and molecules, to research on life, earth, energy, and space.

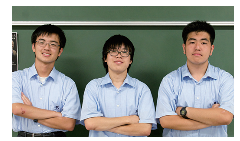
From the ability to see, to the ability to perceive.

The world-changing perspective of scientists

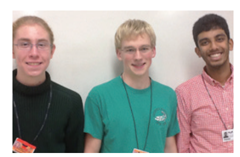
SPECIAL PLAN English presentations by high school students

「A Method to Change the Color of Metals by Oxidation」
・*Masahito Yamazaki* ・*Yusuke Sato* ・*Shotaro Yuzawa*
Sendai Daisan Senior High School (Miyagi, Japan)

「$KMnO_4$-$Na_2C_2O_4$ Redox Titration -The effect of Mn^{2+} as a catalyst-」
・*Takumi Machinaka* ・*Kenichirou Munakata* ・*Tomohiro Seino*
Sendai Dai-ichi Senior High School (Miyagi, Japan)



「Verification of Breed Difference through Anther Culture」
・*Kenji Itabashi* ・*Michitaka Yamasaki* ・*Daiki Takashima*
Furukawa Reimei Senior High School (Miyagi, Japan)



「Adaptive Control Using a Neural Net」
「Cooling of Linear Induction Launcher」
「Fast Single-Point Imaging Electron Paramagnetic Resonance Imaging to study fluctuating Tumor Physiology; k-space and Trajectory Design」
・*Matthew Early* ・*Michael Stevens* ・*Vishnu Rachakonda*
Eleanor Roosevelt High School (Maryland, US)

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Co-Host

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Institute for Integrated Cell-Material Sciences (iCeMS)
Immunology Frontier Research Center (IFReC)
International Center for Materials Nanoarchitectonics (MANA)
International Institute for Carbon-Neutral Energy Research (I^2CNER)
International Institute for Integrative Sleep Medicine (IIIS)
Earth-Life Science Institute (ELSI)
Institute of Transformative Bio-Molecules (ITbM)

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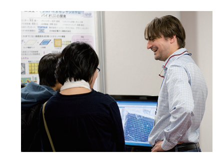

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“Conviction and Responsibility”

Taking up the challenge of innovative materials science while eyeing mathematics

**With the innovative vision of fusing mathematics and materials science,
Director Motoko Kotani has led AIMR for two years.
In the past year, her initiative has borne fruit,
demonstrated by the prestigious awards that AIMR researchers have been scooping up.
Director Kotani speaks about her passion for AIMR and for mathematics.**

Motoko Kotani

Director of the Tohoku University Advanced Institute for Materials Research (AIMR)
Distinguished Professor, Graduate School of Science, Tohoku University

text by Shouichi Kato / photographs by Masayoshi Harabuchi

Motoko Kotani

"Of course, I am delighted that the introduction of mathematics has yielded results far exceeding my expectations. But I am particularly happy about the fact that young researchers are finding joy in their research work."

This was how Professor Motoko Kotani, appointed as Director of AIMR in April 2012, assessed these past two years. It has been five years since AIMR was established, and confronted with the challenge of furthering fusion research, the institution is steering toward the new direction of introducing mathematics into the field of materials science. Professor Kotani was welcomed on board as the Director to push this initiative forward.

"Before accepting this role as the Director of AIMR, I did, of course, have some reservations. As a professor of mathematics in the Graduate School of Science, I had a vision of propelling my research in a certain direction, and would not face any problems as long as I stayed where I was. At the time, I thought seriously once again about 'the power of mathematics.' In history, mathematics has always played the role of joining with other fields and providing new perspectives contributing to breakthroughs in science and technology. Mathematics is tied closely to the field of materials science, and there was no doubt that this was the necessary and correct direction to head in. Although I had no confidence in my own abilities, I held a strong conviction in the power of mathematics, and felt that I should take on this appointment if the opportunity to move toward the correct direction was present here."

The significance behind the encounter between materials science and mathematics

Professor Kotani commented, "I held the conviction that incorporating mathematics would bring about new developments in materials science. On the other hand, AIMR itself was a project with a deadline, so rather than waiting slowly for results, I felt that we had to have a strong awareness of time and produce results."

"In my experience as a researcher so far, I have learned that if we attempt to bring something to fruition too quickly, we may wind up with insignificant conclusions. Normally, it is important to be patient and wait for results. However, in the case of AIMR, which has an existing track record over a span of five years, we were aiming to take new leaps forward based on these achievements. We were not starting from scratch. At that point, my thoughts were about harnessing the strengths of AIMR, and about the types of fusion research that would be able to make full use of the specialized knowledge that the new mathematics researchers have brought us. For one year, mathematicians and materials scientists tore down the walls that stood between their respective academic fields, and took their time to discuss these issues. We also held one-on-one discussions. As a result of these efforts, we came up with three target projects."

In order to achieve the vision of bringing about new developments in the field of materials science through the incorporation of mathematical methods, AIMR established three target projects. These were "Non-equilibrium Materials based on Mathematical Dynamic Systems," "Topological Functional Materials," and "Multi-scale Hierarchical Materials based on Discrete Geometric Analysis." In traditional materials science research, convention had been to observe new phenomena by conducting experiments and to obtain a logical explanation based on analysis. On the other hand, the target projects were, more than anything else, attempts to convert this trend into a bidirectional one.

"Even with the new approach of introducing mathematical methods into the field, as a research institute for materials science nothing has changed in our goal to discover the most cutting-edge functional materials. Rather, we could say that ours is one attempt to strengthen this goal. If we were only able to do what we have always done, then there would be no need to create a new 'encounter' between the fields of materials science and mathematics. By incorporating mathematics, we are aiming leap into discontinuity in order to bring about new, unprecedented developments in the field of materials science; or in other words, to achieve a breakthrough or a paradigm shift. While this is of great importance to the field of materials science, it also represents a new challenge and a motivational source from the perspective of mathematics. If we do not uncover problems like these, which pose interest to both perspectives, it would be difficult to achieve a breakthrough. Fortunately, and bringing a reprieve to us, we succeeded in identifying several such intriguing problems in under a year. I believe this is the result of unity among the AIMR members, who have put much earnest effort into tackling and discussing the problems."

The unique attempt to introduce mathematics into the field of materials science is supported by the Interface Unit, comprised of young theoretical physicists and theoretical chemists from around the world. The members do not belong to a specific research laboratory, but participate in multiple projects that interest them. In this sense, they serve as the bridges that link the mathematicians and the materials scientists.

"We have brought together researchers from around the world with an interest in the themes that we have established for our target projects. This group of researchers makes up the Interface Unit. It is natural for young researchers to consider problems freely and act independently, and I believe this how to attain the best results. Prior to that, the style taken at AIMR had been similar to a conventional research laboratory, with young researchers conducting research under a PI (principal investigator, who takes charge of the research). At AIMR, we recommend all researchers to come up with ideas freely, and to pursue their own interests. In addition to members from the Mathematics Unit and the Interface Unit, young researchers in experimental fields have also told us that they feel motivated, being able to conduct research in such a new and unique environment. Although we are only able to provide these researchers with this open environment for a limited period of time, I think that it is still a meaningful initiative."

The "Tea Time" sessions held every Friday is a space that provides students and young researchers with the opportunity to freely engage in discussions with world-class researchers. Here, researchers are not bound by any restrictions and are able to interact freely, and can also exercise their respective capabilities fully. This atmosphere is present in AIMR today.

"It is a matter of course for researchers to have a space where they can interact freely with one another. If they do not establish their own areas of expertise, insatiably absorb external stimulation, and create their own unique fields, they would lose the motivation to be a researcher."

Harnessing the conviction and responsibility toward mathematics as a driving force

Professor Kotani revealed that she loved to read, to think about things, and to explain her thoughts and ideas to others ever since she was a junior high school student. She had thought spending her lifelong career to do so, but had not known about what a researcher was back then. "Even so," she said, "my favorite subject was mathematics, so I may have wanted to become a mathematics researcher then."

Professor Kotani explained the appeal of mathematics for her. "To me, if we were to probe into the very fundamental essence of the universe that we live in, the result would be mathematics. I think that we can find mathematics in nature, in all the contexts of various phenomena in the natural world. Things that appear to be complicated or disorderly can look simple and uniform from the perspective of mathematics. The thrill in mathematics research lies in the euphoria I feel when I can see that. Furthermore, mathematics is a school of knowledge that allows us to set and pursue values and problems as we please, instead of having them dictated according to the demands of the outside world. Mathematics is the act of thinking about the correct 'settings,' and in that sense, it is very free and interesting."

Professor Kotani stands at the forefront of AIMR, and takes the lead in the unique initiative to fuse mathematics and materials science. Many members of AIMR have commented that she is a "cool" leader, but Professor Kotani told us that in junior high and high school, she had not been the type who exerted leadership skills.

"I read a lot because I was not good at dealing with people, and preferred to be alone. That has not changed today. Rather than leading a large group and communicating with everyone, I prefer to spend my time alone, quietly immersed in my own world. If you are unable to not talk to anyone for about a month and still be fine, then you cannot be a mathematician. Nevertheless, when you are placed in a position of leadership, you have to shoulder responsibility for many people. You must put in the greatest effort you are capable of. I have said that I hold strong conviction in the power of mathematics, but if I do not shoulder this responsibility, the trust that others have invested into the power of mathematics will also crumble. I do not know if I am capable of bearing this responsibility, but my strong conviction and sense of responsibility toward mathematics is likely the driving force that pushes me on."

Aiming to achieve a real breakthrough

Since her appointment as Director, Professor Kotani has established the Interface Unit, set up AIMR Joint Centers in three overseas locations, established a summer school for graduate students, founded an AIMR Fund with the aim of strengthening the institution's finances, and implemented other innovative initiatives founded on a clear vision. How does she perceive the future of AIMR?

"We have been through the Great East Japan Earthquake, and part of these two years were also spent in rebuilding efforts. We are now putting the finishing touches to these, and now aim to achieve a real breakthrough. We have identified our direction, and there are various approaches that we can take. It is important for each individual researcher to carry out research freely based on their own ideas, share their results, and move toward a positive direction as a group. We are gradually developing an atmosphere that recognizes mathematics as something that is close to us in our lives, and where it is natural to apply mathematics to research. I hope that we can strengthen that, so that this research institute can continue to exist as a leading research institute in the world, even after the projects come to an end. As a mathematician, I hope that the field of materials science can provide stimulation in various ways for the further development of discrete geometry analysis, which is my field of expertise."

Motoko Kotani

Professor Motoko Kotani was born in Osaka in 1960. She graduated from the Graduate School of Mathematical Sciences at the University of Tokyo in 1983. In 1990, she completed the doctoral program in the Graduate School of Science and Engineering, Tokyo Metropolitan University. In 1999, she joined Tohoku University as an Associate Professor, and was appointed Professor in 2004. She first served the Tohoku University Advanced Institute for Materials Research (AIMR) as Deputy Director, and was appointed to her current post as Director in April 2012. Professor Kotani received the Saruhashi Award in 2005, presented to female scientists working on the frontlines of scientific research.

EVENT REPORT

Welcome to Nano Tours!

"Atoms are movable!"
These were the comments from a participant, who had seen, under a special microscope, the words "AIMR" spelled out with atoms. This occurred at an AIMR open house in October this year, held in conjunction with the Katahira Festival 2013, which was organized jointly by the research institutes of Tohoku University.
The theme of this open house was "Nano Tours." A special tour route was set up in levels 1 and 2 of the AIMR Main Building. Following this route, participants would be able to see displays of beautiful photographs of atoms and molecules taken under a microscope, observe actual atoms under an electron microscope, and experience a "nano-world" that they are rarely exposed to. In addition, booths for experiments using rubber, magnetic fluid, and computers were also set up, where participants could learn about the amazing properties of materials while having fun.
At the "Castle of Mathematics" set up in the second half of the tour, participants were treated to a demonstration of a triple pendulum. The unpredictable movements drew out expressions of surprise on the faces of the participants.
The "Mini Talk Live" session held during this open house was also a first attempt in which 10 researchers held lectures about their respective fields of research. To prevent participants from thinking that they would not understand what the researchers were talking about, the young researchers who were in charge of the presentations made sure to provide elaborate and interesting slides, as well as live demonstrations, into the talks about their specialties. Dr. Qiu from the Saito Research Laboratory took up the theme of magnets. After giving a simple explanation about what magnets were, he displayed to the audience the sight of tomatoes moving as they repelled against magnets. Asking the audience to consider the reason behind the phenomenon, he obtained the correct answer from an elementary school student—that the water in the tomato had repelled the magnet. This in turn gave Dr. Qiu a surprise of his own.
In addition to enjoying scientific experiments, Nano Tours gave participants the opportunity to experience the world of atomic and molecular research from various perspectives, such as listening to talks given by researchers and experiencing the actual site of research. Participants commented that they had gained more in-depth knowledge about atoms, and that it had been a good learning experience. The Katahira Festival is held every two years, and the next has been scheduled for 2015.

Materials that change the future of medical science

"The world's thinnest adhesive plaster is stuck here. Can you see it?"
When Assistant Professor Fujie (Faculty of Science and Engineering, Waseda University. Former AIMR research associate) pointed to the place on his arm where the plaster had been, everyone looked suspiciously where he pointed to. It looked as if nothing had been pasted there. This adhesive plaster is only as thick as a nanometer, or 1/100,000 the usual thickness. It is too thin to be seen when pasted onto the arm.
"We call this nano-plaster. It is made from material that does not harm the human body and which eventually breaks down and becomes absorbed by the body. Hence, it can be used to seal wounds without having to stitch up the injured area during surgery."
As Assistant Professor Fujie continued with his explanation using videos from an actual surgery, sounds of surprise and admiration arose from the audience seats.

AIMR and 9 WPI institutions held a joint booth at the scienceAGORA show held at Odaiba, Tokyo in November this year. During the show, each institution was introduced, a lecture titled "WPI Science Live!" was held, and experiment classes were conducted. Assistant Professor Fujie represented AIMR in delivering the abovementioned lecture, entitled "Nanotech materials pave the way for the future of medical science!" The nano-plaster was also put up on display at the AIMR booth, and a simple experiment about the surprising properties of rubber was conducted.
Visitors who had attended the event and witnessed the amazing properties of the materials in our environment, as well as the latest technologies, commented that they gained in-depth knowledge about the materials they had previously taken for granted, and hoped for further advancements in research to be applied to the site of medical treatment.

The amazing properties of rubber

"The world is moving"
This text was displayed in large fonts on a TV screen. Even when all objects appear to be stationary, the atoms are in fact moving. This is a key point to understanding the properties of rubber, which is the research that Associate Professor Nakajima is engaged in.
On 22 November 2013 (Friday), Associate Professor Ken Nakajima delivered a lecture at Renbokoji Elementary School in Sendai, titled "Let us experience the amazing properties of rubber." This lecture was held for students in the fifth grade.
Associate Professor Nakajima took out a rubber ball that was made in such a way that prevented it from bouncing at room temperature. However, he showed that it could bounce after it had been heated in hot water or cooled in liquid nitrogen. Associate Professor Nakajima's lecture, which explained the changing properties of rubber in different temperatures along with live demonstrations, roused the interest of many students. They seemed to have fun while gaining an understanding of the properties of rubber.
The final question posed to him was, "After rubber has melted and solidified again, will it return to its original state?" He replied that rubber does not typically melt, and if it did enter a melting state, it would lose its properties as rubber. His explanation was easy to understand. After listening to the talk by a researcher who is involved in cutting-edge research, the students were given much food for thought.

On the frontlines of research of the highly functional, high-performance dream material,

Metallic Glass

Associate Professor, Tohoku University Advanced Institute for Materials Research (AIMR)
Text: Akihiko Hirata

The atomic structure of metallic glass, which remained a mystery for five decades, has been revealed through the links between mathematics and materials science. The results of this research were published this year in July, in the American journal *Science*. Here, we will provide an explanation of metallic glass, from basic knowledge about the material, to the latest research about its atomic structure.

1 What is metallic glass?

Metallic glass research —from the beginning to the present

A certain material leapt into the limelight in 2012, when information was leaked that Apple Inc. might use it to produce the iPhone body. That material was called "metallic glass." When we hear the word "glass," the image that comes to mind would likely be that of a transparent material, such as the glass that we use for windows. However, metallic glass does not look anything like glass. Rather, it exudes a metallic gloss similar to typical metals (refer to the photograph shown on the previous page). While it is basically a type of metal, it has a structure that is similar to that of glass, giving it a greater strength and suppleness than normal metals. This property makes it an intriguing and wonderful material.

Figure 1: In the near future, will metallic glass be used for the iPhone as well?

Research on metallic glass started in the 1960s when a group in the United States discovered the formation of a glass using an alloy of gold and silicon produced through rapid quenching. This triggered an alloy hunt, when scientists began to combine various types of metals. Around 1990, a group from Tohoku University succeeded in producing an extremely stable metallic glass by combining more than three metals, resulting in the development of numerous types of metallic glass up to the present day. At the time, the production of metallic glass required rapid quenching technology that could reduce temperatures by more than 1000°C in 0.001 seconds. However, it is now possible to produce it using the same casting processes that are used to produce normal metals. This allows us to obtain much larger sizes (several mm to several cm) that could not be obtained in the early years of metallic glass production. This in turn has facilitated advancements in the development of various applications that harness the characteristics of metallic glass.

Difficulties in analyzing the atomic structure of metallic glass

The properties of metal are strongly influenced by how the atoms in the material are arranged. Generally, for metals, the atoms are arranged in regular, cyclic patterns, such as a face-centered cubic structure, or a body-centered cubic structure. When molten metal is cooled and solidified, it is normal and natural for the metal to form such regular, crystalline structures. However, across all samples of metallic glass, the atoms appear at first glance to be arranged haphazardly. It is this haphazard arrangement of atoms that holds the key to the superior properties that metallic glass has over typical metals.

Furthermore, in metallic glass, the atoms are arranged in a way that appears like balls crammed into a box. If atoms are lined up in a regular arrangement like crystals, it would be easy to obtain this tight structure of closely packed atoms. However, it is more difficult than we realize to achieve such a structure while maintaining a haphazard arrangement. Besides crystalline structures, other known structures that are stable and tight include the icosahedral structure. Scientists have proposed models that suggest that the structure of metallic glass comprises numerous icosahedrons since the past, but they did not manage to come up with a solution for a major inconsistency—with only icosahedrons, it is not possible to fill a three-dimensional space completely without leaving any gaps.

In order to investigate how the atoms are actually packed together, researchers have conducted countless experiments to date, using mainly X-rays and neutron diffraction. Diffraction refers to a phenomenon whereby waves that encounter an object bend around the back of the obstacle to create a striped pattern. Using this phenomenon, the striped patterns or diffraction patterns that are formed when X-rays or neutron rays are applied to an object can be used to study the structure of the object. As normal metallic materials are crystals, their structures are cyclical, and their diffraction patterns show a clear repetition of similar patterns. Based on this, if we were to settle on the atomic arrangement that forms a metallic structure's basic unit, we would automatically be able to find out what the structure of the entire sample is like. However, the atomic structure is not cyclical for metallic glass, and the only observations gained from the diffraction pattern would be a small number of extremely blurred scattering. Hence, based on the sample, it would only be possible to find out the characteristics of the average structure. This has created great difficulties in conducting theoretical analyses on the structure of metallic glass.

2 Nearing the truth about metallic glass structure, using an electron probe and mathematics

Direct observation of the structure using an electron probe

Considering the existing situation, we decided to conduct a more direct observation of the structure of metallic glass, and attempted to carry out an experiment using an electron probe. An electron probe uses a fine electron beam as a needle (probe) to explore the properties of materials. As electrons have the property of waves, it is possible to study the structure of objects using diffraction patterns in the same way as in the use of X-rays and neutron rays. Furthermore, electron beams can be focused to scan much smaller areas than X-rays and neutron rays, making it possible to obtain diffraction patterns from extremely small areas. By narrowing the probe to below 4Å (Angstrom. 1Å = 0.1 nanometer), we succeeded in dramatically reducing the number of atoms contributing to the diffraction to several tens of atoms. If the probe is made too narrowly, we would then not be able to see the blurriness in the scattering. Hence, it was necessary to find the optimal degree of narrowness for the probe. In previous experiments using X-rays and neutron rays, researchers had studied the entire sample; that is, approximately 1023 atoms at the same time. This made our experiment drastically different. The result exceeded our expectations, and we felt that we would be able to apply this method to observing the structures of extremely small atomic organizations directly, and to discuss the results.

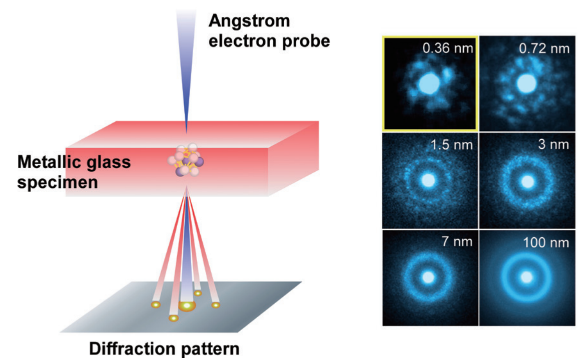


Figure 2: Schematic diagram of Angstrom-beam electron diffraction method (left) and the actual diffraction pattern of metallic glass

After some time, we decided to conduct an actual observation of the icosahedral structure that had earlier been proposed as the model for the structure of metallic glass. However, no matter how much we examined it, we could not see a neatly symmetrical icosahedral arrangement. At the time, we thought that perhaps our experimental technology had not been up to the job. Nevertheless, as we studied the data repeatedly for some months afterward, we realized that the pattern that we observed frequently was the result of a considerably distorted icosahedron. On top of that, we also found out that the structure combined both the characteristics of an icosahedron and a crystal (face-centered cubic structure). This made it possible to pack the atoms tightly into a three-dimensional space. In truth, the nature of the metallic glass structure made it impossible to see a regular icosahedron during the experiment.

Metallic glass research transformed by links with mathematics

Even if experimental technology advances even further in the future, making it possible to determine the complete atomic arrangement of materials, it does not mean that we would be able to grasp a complete understanding of the structure of glass. We have to find out the essence of the material from the data of the complex atomic arrangement, with, for instance the Voronoi polyhedral analysis method, which allows us to study fine differences in the local structure. However, as the structure of metallic glass is basically haphazard, we felt that it might be more appropriate to shut our eyes to these fine differences in the respective local structures and draw out the common characteristics instead, in order to uncover the underlying order of the atoms. Fortunately, in mathematics, the beginning of this century has brought about developments in the field of computational homology, which is an algebraic expression of the characteristics of how things are interconnected geometrically. Applications of this method in many fields has started, and with some manipulation, could also be applied to metallic glass. Since AIMR has a Mathematics Unit despite being a research institute for materials science, we can interact easily with mathematicians. From last year, we had held countless discussions with Assistant Professor Kaname Matsue and Professor Motoko Kotani, both of whom are mathematicians. When they analyzed the icosahedral structure in metallic glass using computational homology methods, they found a similar distortion across the entire sample. Together with the results of the observation conducted using the electron probe, these results were published in *Science** in July this year. In this way, we have gradually begun to see the different aspects of metallic glass, and look forward to future developments through the application of mathematics.

* A. Hirata *et. al.*, *Science* 341, 376-379 (2013)

3 Future outlook

The starting point in fields of study that deal mainly with the properties of crystals, such as metal physics and solid-state physics, lies in the study of crystal structures. Crystal structures are cyclical, and it is possible to establish various superb theories based on this characteristic. However, in the case of a non-regular structure such as metallic glass, this characteristic has not yet been determined, making it extremely difficult to establish any theories. As such, the revelation of non-cyclical structures is an urgent task. We hope to be able to continue with this research to further develop the basic science in this field, by combining past conventional methods with new ones, such as the electron probe experiment and computational homology described here. Furthermore, we are now considering the application of these methods to materials other than metallic glass that also have non-cyclical structures, such as phase-change recording materials and electrode materials for secondary batteries.

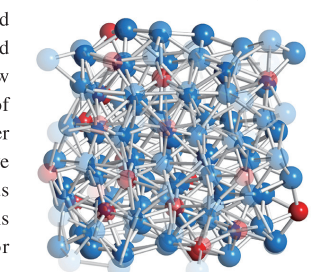


Figure 3: Model of the structure of metallic glass ($Zr_{80}Pr_{20}$)

The success of this research is the result of the efforts and cooperation from many researchers, including and not limited to Professor Mingwei Chen (AIMR), Professor Motoko Kotani (AIMR), Professor Alain Reza Yavari (AIMR, Grenoble Institute of Technology), Associate Professor Takeshi Fujita (AIMR), and Assistant Professor Kaname Matsue (Faculty of Science and now Institute of Statistical Mathematics). I would like to take this opportunity to express my gratitude to all who contributed to this research in various ways.

Akihiko Hirata

Akihiko Hirata was born in Tokyo in 1974. He completed his studies at Waseda University's Graduate School of Science and Engineering. He was previously an Assistant Professor at the Institute of Scientific and Industrial Research, Osaka University and Assistant Professor at AIMR, Tohoku University. Since 2012, he has been appointed Associate Professor at AIMR, Tohoku University. He holds a doctorate in engineering.

AIMR gave me insight into new possibilities in mathematics.

In this issue, we have featured the breakthrough research that revealed the structure of metallic glass by combining mathematics and materials science. Assistant Professor Kaname Matsue (currently affiliated with the Institute of Statistical Mathematics), who took charge of the mathematics part of the research, spoke about the journey that led to the fruition of the research, and his thoughts on tying-up with the field of materials science from a mathematician's perspective.

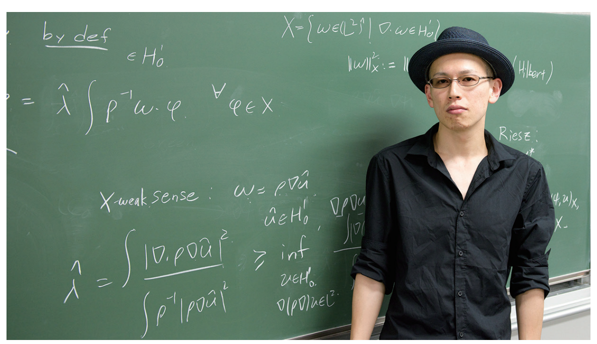
Assistant Professor, School of Statistical Thinking / Coop with Math Program, Institute of Statistical Mathematics **Kaname Matsue**

text & photographs by Yasufumi Nakamichi

"During my doctoral course in graduate school, I conducted research on topology in pure mathematics, with a focus on analysis using homology. After I received my doctorate, I felt a keen desire to continue engaging in pure mathematics research for the rest of my life. However, upon coming to Tohoku University and becoming involved in research with materials science researchers, I began to take a greater interest in applied mathematics; that is, how mathematical knowledge is applied to other fields of study."

So explained Dr. Matsue. In fact, after he took up his position at Tohoku University, he has taken up the structural analysis of metallic glass in joint research with a materials scientist, Associate Professor Hirata. In July this year, their paper was published in "*Science*." Thanks to this achievement, Matsue has been transferred to the Institute of Statistical Mathematics within just two years of his appointment, and has also been invited to participate in the Coop with Math Program. His life of research at Tohoku University seems to be going well. However, it was not smooth sailing right from the start.

"Soon after I came here, Professor Kotani, who was my team leader, asked me if I would like to talk to someone who was engaged in the research of glass. This glass researcher that he was talking about was, in fact, Associate Professor Hirata."



Hirata had consulted with Matsue about whether it was possible to use topology to analyze glass structures. Matsue told us that at that moment, he instinctively felt that his own area of specialty in homology analysis might come in handy. "However," he said, "at that point in time, I was completely unable to imagine how to proceed with this research. I only had a vague idea that something could possibly be done."

The two then began to discuss the possibility of conducting structural analysis on metallic glass using homology. In particular, they began to conduct intensive discussions after Hirata's research plan was selected as a Fusion Research Proposal by AIMR. Even so, during the initial stages of research they experienced great impatience, as they faced difficulty in holding any concrete discussions.

"It is often said that different fields of research do not communicate in the same language. This was when I truly understood what this meant. It is true that the language is different." Of course, although both the researchers could speak English and Japanese, the same word could mean completely different things to both of them. "For example," he explained, "The Japanese word 'iso' refers to topology for mathematicians, but means phase for physicists. In other words, it is also used to refer to wave properties."

When they encountered such differences in language, they would deepen their mutual understanding by explaining the terms to one another. As they went through this process repeatedly, Matsue gradually began to understand the meanings of terms used in physics. "Nevertheless, even if we understood the meaning of individual words, attempting to understand the research contents of the other party was of course saddled with even greater difficulty."

Matsue did not give up, and went around earnestly to inquire and talk to materials scientists. "In any case, nothing would begin if we do not make any moves ourselves. If you do not understand something, you have to ask someone. If not, nothing will advance forward."

In research, progress is first made after countless rounds of discussion. Matsue realized that this was the same in other fields of research. He explained, "We tend to hesitate to speak to researchers in other fields. However, since we are engaged in research work, we should not put up defenses; rather, we should tackle problems earnestly with the intention of exploring all possibilities. This passion will eventually convey itself to others, and those who feel the same way will respond in kind. This is what I learned here." In particular, in AIMR, there is an Interface Unit that is comprised of young theoretical chemists and theoretical physicists. According to Matsue, this Unit played a useful role as the go-between for mathematicians and materials scientists. When he approached researchers in the Interface Unit with the question 'I would like to find out something about this topic; do you know anything?' they would introduce him to a researcher who was an expert in the field and speak to the researcher together with him, or sometimes participate in the discussion themselves.

Furthermore, Matsue also held his own study sessions on topology, and created opportunities to help materials scientists learn about the various methods used in mathematics. "As I continued to keep up these efforts, the materials scientists began to feel that it might be possible to conduct interesting research using mathematics. Similarly, as I continued to raise questions about materials science research, I began to grasp a clearer idea of the subject." Finally, half a year after they began discussing the research in earnest, the researchers discovered that an analytical method used in homology, known as CHomP, could be used to analyze the structure of metallic glass. This then led to the research results described above.

Matsue reflected on his experience of conducting joint research with the field of materials science in AIMR.

"We succeeded in producing one significant result. However, we are still unable to say that mathematics has been integrated into the field of materials science. Conversely, I also do not think the power of mathematics is limited to this. Even though I have moved to a different workplace, the fact remains that I will continue to collaborate with materials science researchers to conduct research. I plan to continue with my joint research with AIMR researchers. Someday, ideally, I hope that we will be able to use the power of mathematics to overcome the differences in materials and lead the way in theorems we can adapt to. On top of that, I hope that we can give feedback of the knowledge we have gained in materials science into the field of mathematics. For example, I would like to make an attempt to bring significance to abstract hypotheses."

Kaname Matsue
Assistant Professor,
School of Statistical Thinking /
Coop with Math Program,
Institute of Statistical Mathematics

Kaname Matsue, 30, was born in Hiroshima Prefecture in 1983. After obtaining his doctorate at the graduate school of Kyoto University, he joined Tohoku University's Mathematical Institute as an Assistant Professor (under the Kotani team, CREST), before moving on to his current appointment.

NEWS & INFORMATION

Dr. Akari Takayama receives the L'Oreal – UNESCO Japan Fellowship

A JSPS Postdoctoral Fellowship researcher (a member of the Takahashi Laboratory at AIMR, Tohoku University), has been awarded the Japan Fellowship 2013 of the 8th L'Oreal – UNESCO Award for Women in Science.

This award was established in November 2005 by Nihon L'Oreal K.K., in collaboration with the Japanese National Commission for UNESCO, with the aim of encouraging young female scientists in Japan to continue their research activities in domestic educational and research institutions. Dr. Takayama was highly commended and awarded for her contribution to the discovery of electronic spin behavior on semiconductor-metallic interfaces, known as the giant Rashba effect, through the world's highest-measurement resolution. This led to the revelation of the electronic spin state that forms the basis for the development of spintronic elements.

At the award ceremony, held at the official residence of the French Ambassador on 11 September, speeches were given by H.E. Mr. Christian Masset, the Ambassador of France to Japan; as well as Nihon L'Oreal President and Representative Director Klaus Fassbender; and Minister in charge of Support for Women's Empowerment and Child-Rearing, Masako Mori. Honorary Professor Akiko Kobayashi from the University of Tokyo, a member of the jury panel, introduced the research conducted by Dr. Takayama, which had been the reason for her selection as an award recipient. With that, Mr. Fassbender presented the award to Dr. Takayama. After the conclusion of the awards ceremony, Dr. Takayama spoke about her happiness for receiving the award. "It was only 100 years ago that Tohoku University was the first institution in Japan to open its doors to university education for women. This has led to my research activities today. There are still very few women researchers. As we celebrate 100 years since the first female students entered Tohoku University, I am honored to be a recipient of the L'Oreal – UNESCO Japan Fellowship, which commends women researchers. I would like to express my gratitude to my supervisor and all the members of the research laboratory, the members of the jury, and everyone at Tohoku University who has continued to support women researchers for the past 100 years, in the spirit of the university' s open-door policy."

Principal Investigator of AIMR, Professor Alexander Shluger receives the Daiwa Adrian Prize

Principal Investigator of AIMR, Professor Alexander Shluger (concurrently Professor at University College of London) has received the 2013 Daiwa Adrian Prize. This award is presented once every three years by the Daiwa Anglo-Japanese Foundation, to recognize scientific research activities conducted by collaborative research teams comprised of Japanese and British members. Principal Investigator Prof. Shluger received the award as commendation for his long years of collaborative research work conducted with researchers in Japan. The ceremony was held on 27 November at the Royal Society.

Column

A short detour

MATERIALS

This corner contains essays that cover topics relating to materials science research at AIMR, including fundamental facts, history, research trends around the world, and advanced research at AIMR.

Part 3
Theory and Experiments

The world of science comprises theoretical research and experimental research. Theoretical researchers are sometimes called "riron-ya" (literally, house of theory), while researchers who are mainly engaged in experimental work are sometimes called "jikken-ya" (literally, house of experiments). In the independent research assignment for science that is often handed out for the summer for elementary and junior high school students, results are first obtained through experiments, followed by inquiry that aims to reveal the significance behind the experimental results. To do this, students attempt to mold their experiments by the principles they have learnt from books, or to guide the experiments toward an original principle that they have conceived of independently. This thought process of arriving at a principle can also be called theoretical research. In other words, in independent research, the same person is carrying out both theoretical and experimental research. However, the more complicated a problem becomes, the more difficult it is for the same person to theorize and experiment. This creates the necessity of dividing up the work. Science advances and develops when theorists and experimentalists share and discuss the results of their research work. Of course, the independent research assignment does not call for students to go as far as that. Arriving at a principle also includes the work of explaining the phenomenon and finding the mathematical formulae. Theoretical research uses mathematics, and describes phenomena using mathematical formulae. The ability to compose mathematical formulae is an advantage here. For example, if the weight (mass) of an apple is m, the weight of two apples would be $2m$. This "$2m$" is also a mathematical formula, but we understand instinctively that 2 apples would weigh twice as much. However, if we were to change this question, assigning the height of one apple as h, and asking how much more potential energy we can obtain from it than from the other apple, it would become difficult to use our instinct. Expressing these ideas using the simple formula mgh (where g is the gravitational acceleration) requires theoretical inquiry in order to find the formula. We are told that Newton saw the apple falling as a result of an attraction between the Earth and the apple, and deduced that there is also an attraction between the celestial bodies in a relationship that establishes the entire universe. Based on this law of universal gravitation discovered by Newton, we are able to come up with the formula mgh. Once we have obtained the formula mgh through theoretical research, we would be able to replace mgh with the weight of any object, or values on any planet (the value of g on other planets differ from that on Earth), and use that to compute potential energy without conducting any experiments. When described in this manner, it would seem that experiments are not necessary as long as you have theories. However, before we think about theories, it is necessary to first explore trends and regularity in the world of nature through experiments. In addition, after an experiment has been completed, you must repeat the experiment in order to verify the results. In 1964, Professor Peter Higgs theoretically predicted the existence of the Higgs boson. The Higgs boson was discovered in an experiment conducted using a large accelerator LHC at CERN in France between 2011 and 2013. Professor Higgs and Professor François Englert, who had worked on the same theory, were awarded the 2013 Nobel Prize in Physics for their work. This recent happening is still fresh in our memories. The actual discovery of something predicted using a theory is a beautiful and wonderful result of science. Through the collaborative work of theorists and experimentalists, research advances and moves forward toward the elucidation of truth. Materials are collective entities of a large number of atoms. The differences in their constituent elements and structures bring forth an infinite variety of properties. There is still no theory that can describe all these changes in property completely. However, through their collaboration, AIMR's mathematicians, theoretical physicists, theoretical chemists, and experimental materials scientists have recently discovered a simple principle lying beneath the structure of materials, which appears to be complicated at first glance. For example, one of the research results that Tohoku University has presented proudly to the world is technology that can convert metals—which tend to have a strong tendency toward crystalline structures (atoms are arranged in regular patterns)—into an amorphous state (glass), with disorderly atomic structures. On the other hand, through the application of geometry, AIMR researchers have discovered a rule underlying the mostly disorderly arrangement of atoms. While it will still take much time to complete the theories that can explain all the properties, the links between theory and experiments, or in AIMR's case, the collaborations between mathematicians, theoretical physicists, theoretical chemists, and experimental materials scientists brings us one step closer to the day when we will be able to gain a uniform understanding of the relationship between material structures and properties. At AIMR, theory and experiment work hand in hand, and further incorporate the perspective of mathematics. Through this method, we aim to uncover universal mechanisms that are applicable across various materials, and to build a predictive materials science that is supported by theory.

Susumu Ikeda

Born in Saitama in 1967. Ikeda graduated from Tohoku University's Faculty of Science in 1990. After working at a cement company, he received his Ph.D. degree from the Graduate School of Science, the University of Tokyo. He became an Assistant Professor at the Graduate School of Frontier Sciences at the same university, and then moved on to become an Assistant Professor at AIMR. In 2010, he was appointed Associate Professor, and in 2011, took on a second position as the Deputy Administrative Director (for Research).

NEW STAFF

Sophie D'ambrosio

Why did you want to become a physics researcher?

Although the question had come up casually, Sophie D'ambrosio paused for thought before answering. "This is a very difficult question. To answer this question, I would have to explain my past, my life, and everything else, and then go on to discuss this philosophical question—who am I?"

When I appeared a little bothered by the unexpected answer, she smiled and continued, "But yes, a very simple explanation would be to say, it is because I like physics."

She explains that the sense behind the explanation, "because I like it," is similar to that of an artist, and that there are fundamentally no differences between the lives of a researcher and an artist. "For example, creativity is required in both professions. Without creativity, we would simply be allowing ourselves to be swept along by the main currents, and we would be chasing after others. This might actually make our working lives easier. On the other hand, we would not exist in any special way or produce anything to change the world, in the way that Einstein discovered the theory of relativity, and the Rolling Stones created rock and roll."

Creativity that changes the world—Sophie D'ambrosio feels that AIMR is fiercely committed to the pursuit of creativity. She says, "The goal of bringing together mathematics, physics, chemistry, and materials science poses an extremely difficult challenge. However, if we succeed, it would then become possible to capture and think about all of these fields based on a multidisciplinary perspective. This would then bring about dramatic advancements in research. AIMR has shouldered the risks and provided the boost for researchers to take up this challenge, in order to achieve this major goal. This is why I am here now."

Sophie D'ambrosio
AIMR Research Associate

Sophie D'ambrosio, 27, was born in France in 1986. After obtaining her doctorate from Aix-Marseille Universite, she joined AIMR in July 2013 as a Research Associate.

text & photograph by Yasufumi Nakamichi