

M AIMR Magazine

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for Materials
Research

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Public Relations & Outreach Office,
Advanced Institute for Materials Research, Tohoku University
2-1-1 Katahira, Aoba-ku, Sendai
980-8577 Japan
Phone: +81-22-217-6146 Mail: outreach@wpi-aimr.tohoku.ac.jp
<http://www.wpi-aimr.tohoku.ac.jp/>
<https://www.facebook.com/TohokuUniversity.AIMR>



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Frontlines of Interdisciplinary Research

Paul S. Weiss

Principal Investigator, Advanced Institute for Materials Research (AIMR), Tohoku University,
and Fred Kavli Chair professor at the University of California, Los Angeles (UCLA)

Stanley J. Osher

Professor at the University of California, Los Angeles (UCLA), and Director of Special Projects
at the Institute for Pure and Applied Mathematics (IPAM)



Frontlines of Interdisciplinary Research

Two of the centers that promote interdisciplinary research at the University of California, Los Angeles (UCLA) are the California NanoSystems Institute (CNSI) and the Institute for Pure & Applied Mathematics (IPAM). For this issue, we chatted with Professor Paul Weiss, Principal Investigator at AIMR and former director of CNSI, and his research partner Professor Stanley Osher, Director of Special Projects at IPAM, about the potential in fusing mathematics and materials science.

Interview: Susumu Ikeda, Yasufumi Nakamichi
Text and photos: Yasufumi Nakamichi

CALIFORNIA NANOSYSTEMS INSTITUTE

Paul S. Weiss

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“I have no interest in pursuing research without mathematics”

- First of all, I would like to ask you both about your research activities. What are the research projects that you currently involved in?

Dr. Weiss: When I first started my independent research career, I was interested in nanoscience through the use of a scanning tunneling microscope (STM). One of the wonderful things about STM is that it allows us to study both electronic structure and chemical properties simultaneously, at the level of single atoms and molecules. We have improved imaging methods and the microscope itself, and developed methods to control molecules to make them even easier to observe. As a result of these efforts, we have succeeded in building microscopes that are able to observe even molecular function in molecular switches and motors.

Through this process, we learned something important. By using a microscope like the STM, we typically oversample the system observing a small number of functional molecules held in place by a field of many matrix molecules. For example, we typically have 50 functional molecules or assemblies in a field of 10,000 matrix molecules. We do not really need to measure the matrix molecules every time, but only need to focus on measuring the functional molecules that are our subject of research. This is where we began to cooperate with Professor Osher and Professor Andrea Bertozzi. We began using the concepts of sparsity^{*1} and compressive sensing^{*2}, to target information, rather than collecting multimodal images equally at every pixel.

^{*1} **Sparsity:**
The state in which information is distributed erratically. Efforts are made to create an overall picture based on inadequate information.

^{*2} **Compressive sensing**
Efforts are made to create an overall picture using only a few measurements. For example, in order to elucidate the three-dimensional structure of an object, conventionally, several hundred measurements had to be taken from various angles. In comparison, by harnessing methods such as statistical mechanics, algorithms are being developed to facilitate the understanding of a structure using just a few measurements.

Dr. Stan Osher: Sparsity is a mathematical concept of great importance when it comes to considering image processing and signal processing. In cooperation with materials scientists, I use sparsity to obtain new basic functions in order to solve problems relating to imaging.

Compressive sensing is a mathematical algorithm that is able to generate a large quantity of data using just a few measurements. It is now drawing much attention in the field. Through the Internet and computers, it is now much easier than before to incorporate such mathematical ideas into research that deals with practical problems. I also believe that scientists now accept mathematics more than they used to.

Dr. Weiss: Compressive sensing also plays an extremely important role in our research. Most images are now shown in JPEG or equivalent compressed formats. In short, they are being compressed in some way. Videos are similarly compressed into MPEG or equivalent formats. That is why we started asking, “Would it not be better to record our experiment data already in a compressed, information-rich form?” This is how our research started. Compressive sensing and sparsity are exactly the answer to our question.

Experiments using scanning probes, including STM, allow us to program the position of the probe tips that we use to measure the data.

Because it's possible to narrow down with real-time data recording and accumulation which algorithm is more effective, this provided us with a wonderful opportunity to test the importance of compressive sensing. Then, in an attempt to apply this method to all types and scale of imaging devices, such as electron microscopy, optical microscopy, astronomy, entertainment, smart phones, brain imaging, and medical imaging, we selected two mathematical algorithms that could be applied straightforwardly, and at the same time studied new methods of data analysis. Our collaborations on the mathematics enable us to carry out real-time analyses, and ultimately to discover new methods for recording data.

- That is very interesting. Have you noticed any changes in the research group as a result of the outcomes you have achieved through such collaboration with mathematics?

Dr. Weiss: There have been significant changes. In my laboratory, there are now students who do not want to work on a problem unless they are collaborating with mathematicians. I think that this is revolutionary. We plan to disseminate our results to everyone, so once it starts to get on track, it should have an impact across many groups and fields apart from ourselves.

At the same time, we are developing different mathematical approaches in parallel, although I would not say that they compete with each other. Eventually, the approaches that work best for a particular problem are selected, but we can also see the results of the approaches that were not selected. Students are conducting research in parallel for identical problems or related problems, and this process enables us to develop multiple approaches simultaneously. We do not bet on just one horse. We bet on all the horses, and see which is the fastest after they start running.

Dr. Osher: That leaves the very interesting mathematical question of why the selected method had been a successful one. By understanding the special factors that lie behind the background of that success, we are then able to improve the algorithms. I think that science is undergoing a rapid transformation in many places through such collaborations between mathematics and different fields of specialization, and I feel this especially because it is happening here in UCLA. Perhaps I'm biased because I'm a UCLA researcher.

“There's sort of a perfect storm here.”

- I believe the California NanoSystems Institute (CNSI) plays a central role in UCLA for its efforts to combine such different fields of research.

Dr. Weiss, could you tell us some of the features of CNSI, which you had headed until June?

Dr. Weiss: One of the greatest features of CNSI is that researchers from many different fields of specialization engage in research here, with a focus on nanotechnology researchers. There are 135 faculty at CNSI from 30 different departments along with 1000 graduate students and post-docs. Science, engineering, and medicine each make up about a third of the faculty and students, with others from law, public policy, public health, art, film, and business. At CNSI, chemists and physicists learn the languages of the other fields and discuss common problems; materials scientists do the same. We include electrical engineers, bioengineers, clinicians, lawyers, and regulators. There are many such opportunities for communication. As a result, firstly, we have learnt that it is important to talk to people in different fields of specialization; and secondly, we have acquired the skills to do it. Consequently, we are able

to gain an understanding of the kinds of problems faced by specialists in other fields.

These researchers describe their refractory problems and say, “If this problem was solved, it would change our field.” Eventually, we had a growing number of participating faculty, students, post-docs, and staff who tackle such problems and have started to explore how they can contribute to solving them. By doing so, we have found ways to approach solutions for fields that have faced major roadblocks and have failed to achieve any advances in the past 10 years or more. This has also turned out to be really fun. It is what draws people to us. Everyone comes to CNSI to work on problems like that.



Dr. Osher: There's sort of a perfect storm here, because the math department is only about 100 feet from here, and the medical school is also very close. Most campuses are not like this. UCLA is very well situated, and the atmosphere is positive. People are not pretentious or stuffy. There are many people who are very nice and willing to work with one another, and egos do not get in the way. Students want to play active roles in this attractive environment, and we want to do more to make such environments prevalent.

Dr. Weiss: Exactly. The strength of such collaborations is that they allow us to recruit and to retain outstanding human resources. As I mentioned earlier, students, staff, and faculty have the opportunity to tackle problems outside of their fields of specialization.

Dr. Osher: There are also advantages in the aspect of employment. If students do more of this research and write more thesis papers, they will be able to get good jobs. Since this is an attractive place for students, we are drawing students at much higher levels than before. The students in the math department here are outstanding, and I think they are even better than the students were when I was studying. I am glad that I am not a student now. I think the situation is the same in Dr. Weiss' field.

Dr. Weiss: Yes, you are right. Thanks to this situation, we can do things that nobody else can, and that lets us open up new worlds.





“Harnessing WPI as a long-term grant”

-What issues does CNSI, which offers researchers a very attractive environment, face?

Dr. Weiss: We have very limited resources to develop new technologies and devices. To begin with, CNSI was meant to be a shared-use facility. In terms of the amount of funds used to develop new technologies, it is at a disadvantage compared to a government laboratory.

At CNSI, we have state-of-the-art electron microscopy, optical microscopy, and scanning probes, in addition to nanofabrication equipment. We can also conduct high-throughput screening at the scale of a major pharmaceutical company. We listen to what the users have to say to figure the problems of the future and tools and methods to address them. In other words, even when someone says, “I want to do this measurement,” and we can only answer, “No one can do that,” it eventually becomes clear that there is value in developing technology for it. There are many such examples. In that sense, we are fortunate in terms of the content and targets of research.

On the other hand, actual instrument development is very slow. There are multiple examples in my laboratory where it took 10 or 20 years to get an experiment to work. This does not fit very well with funding cycles in the United States, so what you have to do is patch together different sources in order to carry out such experiments. One of the advantages that AIMR has is funding that covers a long period of time, for 10 or even 15 years. This allows researchers to think about long-term problems. It is a tremendous luxury to be able to do so. There are special

research institutes like this in all parts of the world, such as the Max Planck Institutes in Germany. There are some extremely important institutions that offer long-term funding in England, as well. Hence, I think it is important for AIMR to take advantage of these long-term opportunities to develop and to apply new tools that are difficult to develop under other conditions.

- AIMR takes advantage of the long-term funding period to tackle the challenge, at the institutional level, of achieving collaborations between mathematics and materials science. What do you think is necessary in order to expand this initiative around the world?

Dr. Osher: Find a problem that is important, and solve it. That is the most important thing to do, and the world will then take AIMR’s challenge seriously. Do you not think so?

Dr. Weiss: Yes, indeed.

Dr. Osher: That is the best way to do it. There are many talented people in Japan. However, based on my understanding through interaction with Japanese mathematicians, the connection between the mathematics departments and industry seems to be weak. This surprises me. Japan does not have a tradition of disseminating mathematics out to the engineering, materials science, or medical communities.

Dr. Weiss: Is that also related to the type of mathematics?

Dr. Osher: Yes, because pure math is typically popular in Japan. I am speaking based on my experience, and I am sure that it is gradually changing. It is different in countries like Singapore, China, and Taiwan. There are more collaborations in these countries than in Japan. Hence,

while I think that it is good that there is much talent in Japan, it is also necessary to make some changes in mindset. I believe that Japan can do it, and should definitely put it into practice.



- Thank you for the interesting talk that you shared with us today. AIMR would like to provide mathematicians who want to collaborate with experimental scientists with opportunities to validate mathematical models through experiments. Going forward, we hope that such collaborations will be realized between AIMR and both CNSI and IPAM.

Dr. Osher: Well, I think that is a really good idea, and I also hope that my colleagues and applied mathematicians in other research institutes will play an active role in the real world. I believe that is actually the strongest desire of applied mathematicians. I hope it works out. We are excited about the possible collaboration with all of you.



Paul S. Weiss

Born in 1959, After obtaining his doctoral degree at University of California, Berkeley, he moved on to become assistant professor, associate professor, professor, and then distinguished professor at the Pennsylvania State University. Since 2009, he has held the Fred Kavli Chair in NanoSystems Sciences and has been a distinguished professor at UCLA. He also serves concurrently as Principal Investigator at the Advanced Institute for Materials Research (AIMR), Tohoku University. He was the director of the California NanoSystems Institute from 2009 to June 2014. He is the founding and current editor-in-chief of ACS Nano.

Stanley J. Osher

Born in 1942. After obtaining his doctoral degree from New York University, he became associate professor and professor at Stony Brook University, The State University of New York. Since 1977, he has served as professor at UCLA. He serves concurrently as the Director of Special Projects at the Institute for Pure and Applied Mathematics (IPAM). He received the Carl Friedrich Gauss Prize in 2014.

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Editor
Yasufumi Nakamichi
Design/Printing
Hatakeyama Design Office Co.,Ltd.
produced by
Public Relations & Outreach Office,
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Math Changes Everything

Christian Ratsch

Associate Director
Institute for Pure and Applied Mathematics (IPAM),
University of California, Los Angeles (UCLA)

In August 2012, AIMR concluded an interdepartmental agreement with the Institute for Pure and Applied Mathematics (IPAM) at the University of California, Los Angeles (UCLA). IPAM is drawing attention from around the world as a research institute that promotes collaboration between mathematics and other fields of specialization through long-term programs. Here, Dr. Christian Ratsch, Associate Director at IPAM, shares with us the secrets to facilitating smooth collaboration between different fields of specialization; and the potential of AIMR, which promotes mathematics-materials science collaboration under one roof.



- First, could you give us a brief explanation about the Institute for Pure and Applied Mathematics (IPAM) at the University of California, Los Angeles (UCLA)?

Dr. Christian Ratsch, Associate Director: IPAM is one of eight national research institutes for mathematics in the United States. We are funded by the National Science Foundation (NSF), and our mission is to connect mathematics with other sciences including physics, chemistry, engineering, social sciences, and humanities. Twice a year, IPAM conducts long programs that last for 14 weeks, and researchers from various fields of specialization visit IPAM during these programs. For example, last year we conducted a program based on the theme of "Materials for a Sustainable Energy Future."

- Which fields of specialization did the researchers who participated in this program come from?

Dr. Ratsch: We had participants from a wide range of research fields, such as mathematics, materials engineering, physics, chemistry, and computer science. All of the participants discussed the common theme—materials for sustainable energy. Specifically, the discussions covered topics such as solar cells, batteries, and fuel cells; to name a few. In this way, IPAM aims to bring together researchers from various fields of specialization, and thereby connect mathematics with different fields of research.

- Why does mathematics play a central role in connecting the various fields of research?

Dr. Ratsch: First of all, all fields of research require theories, equations, or models to solve problems, and mathematics is necessary in order to acquire the fundamental knowledge about these theories, equations, and models. Mathematicians have a good grasp and understanding about the structure of equations; hence, when considering methods for verifying and solving problems in other fields of research, it is possible to gain various forms of synergy by working

in cooperation with mathematicians. Additionally, we often hear about "big data" these days. When handling big data, algorithms are needed in order to organize, search, and structure the data in a smart and efficient way. This is where mathematics is very important. IPAM's new tagline is "Math Changes Everything," which describes the ideas I have just explained.

- In workshops attended by specialists from various fields of research, do discussions between the specialists run smoothly?

Dr. Ratsch: The answer is both "yes" and "no." Depending on the field of specialization, there can be a lot of terminology that is interpreted differently. Hence, in most cases the discussions are fraught with difficulty at the beginning. We encounter situations where people use a word at the start of a discussion, but the participants are unable to agree on the meaning and concept of even just that one word. That is why we have established long programs lasting as long as three months, and we strive to facilitate discussions among the participants through various activities.

- Could you provide some specific examples of these activities?

Dr. Ratsch: For example, during the first week of the long program, we always have a set of tutorials. In the case of the Materials for Sustainable Energy program that I had mentioned earlier, we had a physicist explain to the mathematicians the problems related to solar cells and batteries, from the perspective of physics. They also introduced the specialized terminology. Next, we had the mathematicians give a tutorial about the equations that can be used for energy transport, and explain what the equations are like and how to solve them.

Hence, the first week of these long programs are spent literally introducing the specialized communities to one another. At the end of the first week, at the very least they are able to speak using the same

terminology, and during the three-month long program, the participants themselves realize that they are now able to hold discussions comfortably with specialists in other fields of research. While the long program is very effective, it also takes time and patience. That is why we believe that an institute like IPAM is necessary in order to facilitate such programs.

- How do you evaluate each long program?

Dr. Ratsch: We are struggling with the answer to this question. It is very difficult to evaluate the programs in an objective way, but we try to do so through a few methods. For example, we follow up with people who attend the long program every year, and count the number of papers they have written based on the outcomes of the program. We also keep track of the amount of joint research that has been initiated as a result of participation in the program, as well as the number of joint research grants that have been received.

Also, while it is not possible to really quantify this, if you look at the quality of the participants in the workshops, you would see that they are always the most outstanding researchers in their fields. I think that all the researchers who participate in our programs truly enjoy being away from their home institution and being relieved from daily work matters for three months, and to be able to discuss common problems with researchers from different fields in the open environment that IPAM provides. Based on this current situation, the NSF and review panels assess that IPAM's initiatives are very beneficial and effective.

- Researchers from AIMR who have participated in IPAM's long program have commented that they spent a very fulfilling time in an environment removed from their daily lives. On the other hand, AIMR brings together materials scientists, and particularly, experimental scientists and mathematicians, together in an everyday setting, in an attempt to create an entirely new form of materials science.

Dr. Ratsch: I feel that AIMR's initiative is a very important and ambitious one. IPAM brings together mathematicians and researchers in the field of computational physics, and these researchers contact the experimental scientists after the program. On the other hand, AIMR seeks to be the bridge between researchers and experimental scientists.

In actuality, it is not so simple to create connections with experimental scientists. Other buildings are located at a distance from IPAM, so we would typically communicate by e-mail, and it would often take several days before we actually met up with one another. It is very rare to think, "I want to ask about this," and start an exchange of opinions five minutes later. In this aspect, I think that AIMR's system has an advantage. Going forward, I believe that will be one of the strengths of AIMR.

- To serve as a bridge between pure mathematicians and experimental scientists, we have also established "Interface Unit" that are composed of young theoretical physicists and chemists.

Dr. Ratsch: Yes, I think that it is extremely effective to have people who are able to understand the terminology on both sides. If the two parties are able to communicate patiently, they should be able to carry out discussions comfortably.

- Finally, could you tell us what your expectations are for AIMR?

Dr. Ratsch: IPAM signed an exchange agreement with AIMR, Tohoku University, in 2012. This is because AIMR is the first institute in the world that promotes mathematics-materials science collaboration at an institutional level. Through this initiative, we hope that AIMR will lead the world in mathematics-material science collaboration and achieve a breakthrough in both the mathematics and materials science fields.

Interview: Susumu Ikeda, Yasufumi Nakamichi
Text and photos: Yasufumi Nakamichi

Do sharks get tooth decay?

The secret to having strong teeth, revealed

through transmission electron

microscopy

Sharks have the healthiest teeth in the world

Do you know that sharks have the most powerful jaws on the planet? However, in order to determine whether sharks really have the strongest teeth in the world, we have to first understand the meaning of “the strongest.” If you think that the reason behind the strength of sharks’ teeth lies in their hardness, you wouldn’t be correct.

Shark teeth are indeed harder than iron, and are rated a 5 in hardness on the Mohs scale (on this scale, diamonds are positioned at the highest end of the scale with a hardness rating of 10), but this still does not mean that shark teeth are the hardest teeth. In fact, if we were to consider only hardness as a factor, the hardness of human teeth is almost the same as that of shark teeth. However, shark teeth have a significant advantage over the teeth of human beings. That is, sharks never suffer cavities. Not having cavities is of vital importance to the shark, because losing its teeth due to a cavity means death. In short, natural selection has provided the shark with ways to protect its teeth against cavities. We could say that nature is the best doctor of all.

Sharks have two ways to protect their teeth. Firstly, sharks have a mechanism in place for periodically replacing

their teeth. Usually, shark teeth are replaced once every two weeks. The secret to the second method lies in the material that shark teeth are made of. The internal part of shark teeth is made of soft dentin, which is enveloped by the hard and compact highly calcified tissue of enameloid. The enameloid, which forms the outermost part of the tooth, is composed of a compound that contains fluorine (fluoride). This fluoride is extremely important as it is effective in reducing cavities, and is believed to be the reason why shark teeth can stay healthy without succumbing to cavities. The effect that fluoride has on reducing cavities was a landmark discovery in the history of dentistry, and has been used as a way to prevent tooth decay up to the present day. That is why the toothpaste that we use often contains fluoride.

How does fluoride prevent cavities? Although various hypotheses have been put forth to date, such as the suppression of mineral dissolution, inhibition of acid formation by plaque bacteria, and remineralization promotion, the answer involves highly complicated processes, and we are still unable to provide a complete explanation for the mechanism of fluoride, even today. To gain greater insight into this mechanism, we have to conduct a detailed observation of the internal structure of enameloid.

Advanced Institute for Materials Research,
Tohoku University

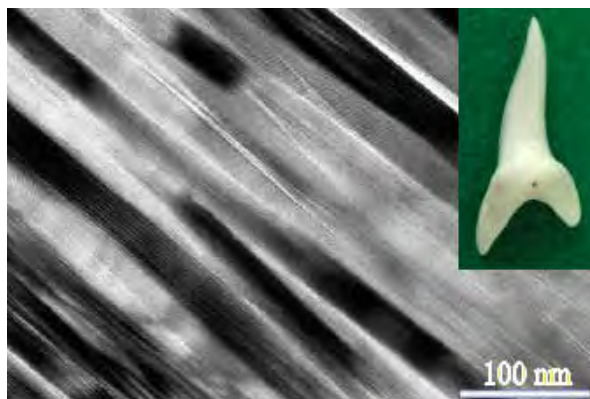
Yuichi Ikuhara
Zhongchang Wang

Difficulties in observing shark teeth using transmission electron microscopy

The minerals produced by living organisms, including the enameloid of shark teeth, as well as teeth, bones, and mollusc shells, are known as biominerals. Structural characterizations of biominerals reveal key information for advancing our understanding of many biological processes, ranging from bone growth and tooth development to the formation of kidney and salivary stones. For this reason, a great deal of research has been conducted over the past decades to investigate the microscopic structure of biominerals.

Shark tooth enameloid consists of a high density of fluorapatite crystals, and a low content of organic matrix (5~8 wt.%). The fluorapatite crystals are distributed over the surfaces of the shark teeth, and constitute well-arranged fibrous crystal bundles with a diameter of a few micrometers. When further investigation was conducted into the microstructural details of the interiors of these fibrous fluorapatite bundles, it was found that the enameloid consists of a bunch of single-crystalline fluorapatite in the form of small pillars (nanorods) (Figure 1). Each fluorapatite nanorod has an average diameter of 50 nm or less, grows in a bundle, and forms to reveal a fiber-like structure.

The observation of microscopic structures, such as in Figure 1, is carried out through the use of a transmission electron microscope (TEM). TEM is a microscope that obtains images by irradiating electron beams onto a sample and detecting the electrons that are transmitted through the sample, and enables the observation of the microscopic structure of various materials, including biominerals. However, the observation of biominerals through TEM poses a serious problem. This lies in the fact that biominerals are sensitive to electron beams, and are therefore easily damaged in the process. In order to analyze biominerals in even greater detail than the nanoscale structure obtained in Figure 1, it is necessary to observe the structure at the atomic level. While the supply of a high current is needed in order to improve resolution, raising the value of the electric current may damage the sample. Hence, there is a need to devise a better means of studying biominerals using TEM.



Beyond the nanoscale

Aberration-corrected transmission electron microscopes and scanning transmission electron microscopes (STEM) have been developed in

recent years, advancing to a level where it is possible to observe individual atoms in a material. STEM uses ultra-fine electron beams below 0.1nm to scan the surface of a sample, and annular detectors at the bottom part of the sample measure electrons that pass through the sample and are scattered. By presenting the intensity of these electrons as an image, a two-dimensional image is created. The image recorded at a high angle is called a high-angle annular dark field (HAADF) – STEM image. As the intensity of this image is proportional to approximately the square of the atomic number (Z), the image will be brighter the heavier the atom is.

However, biominerals are made of very light atoms. As such, the signals obtained through the irradiation of electron beams are extremely weak. In order to obtain strong signals, it is necessary to irradiate the material with strong electron beams. On the other hand, strong electron beams will damage the sample. This dilemma has made it difficult to study biominerals using this method.

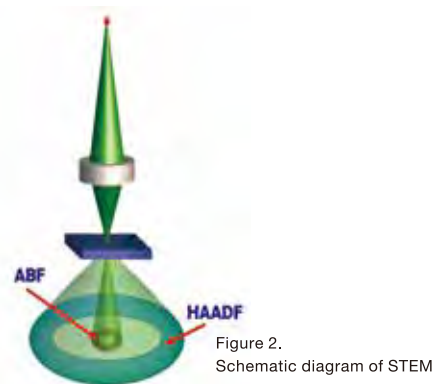


Figure 2. Schematic diagram of STEM

Unveiling the secret to strong teeth

We employed the annular bright field (ABF) method, which is effective in the study of a material containing light elements, to conduct our analysis. The ABF STEM method is a new method that enables the direct observation of atomic columns of all elements, from the lightest hydrogen elements to heavy ones. By combining this method with weak-beam technique, it is possible to obtain images for biominerals with a resolution at the atomic level. In order to protect biominerals from irradiation damage through electron beams, we conducted our study using the lowest probe current possible using the STEM, at 3 picoamperes.

Figure 3a shows a HAADF STEM image. This image represents one of the best atom-resolved images ever achieved in observing biominerals. Looking at this image, we can see that two types of calcium are present in the fluorapatite: one has a much stronger contrast (labeled Ca1), and the other a relatively weaker one (labeled Ca2). Since the strength of the contrast in the HAADF mode relies on atomic density, density in the atomic column is higher for Ca1 compared to Ca2. In short, one is stacked on top of the other.

To obtain images for atoms other than calcium, we show in Figure 3b the ABF STEM image collected at the same time as the HAADF image. In addition to conveying the identical structural information as the HAADF (Figure 3a), the ABF STEM image, in which dark spots represent atomic columns, can reveal all atomic columns in the fluorapatite. The fluorine atoms sit at the center of the hexagons formed by the Ca2 atoms. Near to the hexagons, three elongated dark

spots form an equilateral triangle, and two very close oxygen atoms are positioned at the top of each of these, arranged as if they were stuck together. The Ca1 atoms are found to sit at the center of triangles.

Theoretical calculations based on these observations reveal that there is a small extent of covalency between the fluorine atoms and their neighboring calcium atoms. Since covalent bonds are generally believed to be stronger than ionic ones, the identification of a small degree of covalency (even if it is very small) for Ca-F bonds suggests that strong Ca-F bonds are related to the mechanism for strengthening teeth.

These theoretical calculations clarify the strengthening function of fluorine in teeth from the aspects of atomic and electronic structures, and provide a clue to developing superior dentistry materials in the future.

This article is based on joint research with Yoshiro Takano, professor at the Tokyo Medical and Dental University.

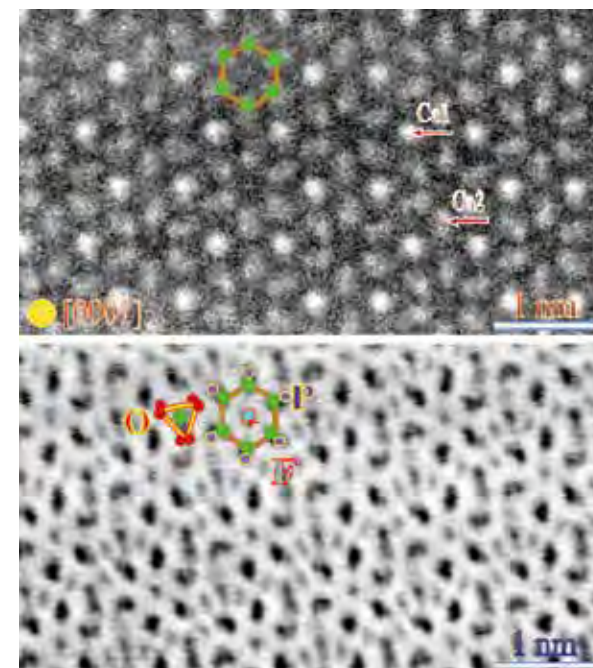


Figure 3. HAADF image (top) and ABF image of shark tooth enameloid

Yuichi Ikuhara
 Born in 1968 in Mie Prefecture. In 1988, he completed the doctoral course at the Interdisciplinary Graduate School of Engineering Sciences, Kyushu University (Doctor of Engineering). He has been a visiting assistant professor at Case Western Reserve University in the United States and principal researcher at the Japan Fine Ceramics Center (JFCC). In 1996, he was associate professor at the materials science department of the Graduate School of Engineering, University of Tokyo, and became full professor in 2003. Since 2007, he has also been serving concurrently as Principal Investigator at AIMR.

Zhongchang Wang
 Born in 1980 in Ma'An Shan, Anhui in China. In 2008, he obtained his doctoral degree (Doctor of Engineering) from the University of Tokyo. After working as research associate and assistant professor at AIMR of Tohoku University, he became associate professor at AIMR in 2013.

Signing of Agreement with the University of Chicago to Establish a Joint Research Center

On 16 April 2014, AIMR concluded a memorandum of agreement with the University of Chicago toward the establishment of a joint research center. The signing ceremony was held at the University of Chicago, and was attended by Professor Eric Isaacs, Provost of the University of Chicago, and AIMR Director, Professor Motoko Kotani. After the signing ceremony, accompanied by AIMR Principal Investigator Professor Hideo Ohno and Professor David Awschalom from the Institute for Molecular Engineering at the University of Chicago, both of whom had been involved in a joint research project from before, a discussion was held about operation of the Joint Research Center in future. It was also decided that a University of Chicago/AIMR Joint Workshop would be held at Sendai in September 2014. This workshop was held over two days on 18 and 19 September, during which participants discussed the possibilities of engaging in more joint research activities going forward.



Selection as Highly Cited Researchers

AIMR's Professor Mingwei Chen, Professor Takashi Takahashi, and Professor Ali Khademhosseini were selected as Thomson Reuters' Highly Cited Researchers 2014. Highly Cited Researchers are authors of papers that are cited worldwide in 21 fields, including the life sciences, medicine, physics, engineering, and social sciences. The top 1% of researchers with the most number of citations are identified and announced by Thomson Reuters. Professor Takahashi was selected for the field of physics, while Professor Chen and Professor Khademhosseini were selected for the field of materials science.

Professor Ikuhara Selected to be WAC Member

Professor Yuichi Ikuhara has been selected to be a member (Academician) of the World Academy of Ceramics (WAC). Once every two years, the World Academy of Ceramics selects world-renowned contributors to the advancement of the culture, science, technology, industry, and art of ceramics to become members of the Academy.

Professor Weiss Selected to be Member of the American Academy of Arts and Sciences

Professor Paul Weiss has been selected to be a member of the American Academy of Arts and Sciences. The appointment ceremony for the American Academy of Arts and Sciences will be held on 11 October 2014 at Cambridge, Mass. in the United States, where the headquarters of the Academy is located.



Japan-UK Young Scientist Workshop



discussing an agreement with the University of Chicago

Everyday life at AIMR

AIMR is a completely innovative international research institute that integrates mathematics and materials science. Researchers from around the world are gathered there, and conduct experiments, hold discussions, and generate many research results every day. These international research activities are supported by countless individuals, including the administrative and research support staff. Their activities, similar to those undertaken by the researchers, cover a global scope. For this issue, we will introduce several examples that characterize the international initiatives that the administrative and research support staff are responsible for.

Text and photos: Yasufumi Nakamichi

To establish a research support system that reaches international standards

At AIMR, the administrative staff is constantly engaged in the work of receiving, inviting, and dispatching foreign researchers. This covers duties such as receiving new researchers from overseas who are taking up their positions at AIMR, inviting lecturers when organizing international workshops, and dispatching researchers overseas through the Brain Circulation Program. In addition, when AIMR concludes a cooperative agreement with an overseas research institute, the administrative staff also makes detailed adjustments in coordination with the representative at the partner institution. This work has typically been carried out mainly by researchers. However, having the administrative staff make direct contact with researchers and administrative representatives overseas as well as various other coordination work helps to reduce the workload of researchers at AIMR. When carrying out such coordination work, various differences in regulations and conventions related to administrative procedures, such as execution of the budget, between AIMR and the overseas research institute can prove to be a barrier.

To resolve such issues, members of AIMR's administrative staff visit

overseas universities and research institutes directly to exchange views and opinions with the local staff. By comparing and recognizing the differences in the respective administrative systems, they seek to improve administration in order to facilitate the smooth completion of administrative procedures for receiving researchers and concluding agreements.



meeting at the University of Cambridge

In December 2012, Hiroataka Hirayama from the Accounting Section and Hiroshi Oikawa from the International Relations Unit visited the University of Cambridge, which is one of AIMR's satellite institutions. They also paid a visit to University College London, which is an AIMR International Partner Institution. During these visits, they held meetings with the local administrative representatives and conducted studies into their systems, including areas such as finance and funding. As a result of their studies, they learned that these universities have established rules that are equally or more stringent than the rules laid down by Tohoku University. For example, in principle, the actual cost for travel expenses are reimbursed, and receipts must be submitted for all expenses incurred including hotel accommodation costs. While it may seem that this is a common practice that is taken for granted, Hirayama said, "Compared to universities overseas, Japanese universities are often criticized for having strict rules and complicated procedures. However, this is not the case. We now understand that strict rules have also been put in place in the U.K., based on the need for accountability to those who are providing the funding." Hiromi Naganuma from the General Affairs Section, who visited Fraunhofer in Germany in January 2013, also returned with similar impressions. She commented, "At Fraunhofer Institute, expenditures that come

Special Lecture Conducted by Dr. Dan Shechtman

On 13 May (Tuesday), a lecture titled "Quasi-Periodic Materials—Paradigm Shift in Crystallography" was delivered by Dr. Daniel Shechtman at the Tohoku University Centennial Hall.

Dr. Shechtman discovered the quasi-crystal in 1982, and has received numerous awards for this achievement, including the 2011 Nobel Prize in Chemistry. This lecture, organized jointly with Tohoku University's Interdepartmental Doctoral Degree Program for Multi-Dimensional Materials Science Leaders, was attended by about 600 high school and university students who wished to listen to a lecture delivered by a Nobel Laureate.

Dr. Shechtman used diagrams and graphs to provide an easy-to-understand explanation about how the quasi-crystals he had discovered did not have a periodicity, unlike conventional crystals. He also explained that the transmission electron microscope (TEM) had played a significant role in this discovery. Furthermore, at the time of his discovery, the concept of quasi-crystals was not accepted in the field of crystallography, and he was put through an extremely difficult situation for some time. With this, he urged the audience to believe in their own capabilities at all times, and spoke about the importance of confronting and overcoming difficulties.



Science Day 2014

In conjunction with Science Day, held on 20 July (Sunday), AIMR held an open house for the research institute based on the theme "Inside a Cutting-Edge Laboratory."

After conducting simple experiments to demonstrate the wonders of mathematics and materials, participants were led to the common equipment room to experience the observation using scanning electron microscopes (SEM), which is used in research. They searched for the tiny text "NIPPON" hidden in a 500 yen coin and invisible to the naked eye, observed the expansion of the legs of a jewel beetle to nano scale, and learnt about the mechanism that produces radiant colors through an extremely delicate structure. The participants were surprised to see invisible structures hidden in the materials and living things that we see casually in our everyday lives.

AIMR Becomes International Exchange Hub for High School Students

AIMR has held many international exchange programs this year. It organized the fifth International Exchange Program for high school students on 28 June (Saturday). For three days from 5 August (Tuesday), it also organized laboratory works for 14 Japanese and British high school students at AIMR research laboratories, as part of the Japan-UK Young Scientist Workshop. During these sessions, participants were divided into two groups, with one group in the research laboratory of Associate Professor Ken Nakajima, and the other group in the common equipment room. Using atomic force microscope and scanning electron microscopes, the respective groups observed and took measurements of biomaterials and polymeric materials, and summarized their experiment results in a presentation session. One of the Japanese students, observing the skillful ways in which the British students conducted the experiments and experiencing difficulties in communicating in English, had initially felt confused. However, by the end of the workshop session, commented, "We came up with a presentation after holding a joint discussion, and I was able to gain valuable experience in both the aspects of research as well as English."

from public sources such as the government are managed as strictly as at Tohoku University. With regard to procedures for business trips, there are even some aspects that Fraunhofer manages more strictly compared to Tohoku University, such as the need to submit documents as proof of having completed the assignment. This visit has dispelled my worries that Japanese universities may have been enforcing inefficient administrative procedures on researchers."

Furthermore, Oikawa also commented that there were many things we could learn from research institutes overseas. "With regard to travel expenses for business trips, the University of Cambridge, for example, uses a system that allows the university to arrange for air tickets and sometimes even hotel accommodations directly through travel agencies online. Unlike the system at Tohoku University, where researchers pay in advance for their own business trip expenses, such a system does not impose a heavy financial burden on researchers. I definitely hope that we can incorporate a similar system at Tohoku University."

Based on this study, AIMR played a leading role in negotiating with the university for the revision of Tohoku University's rules in February 2014. As a result, the university can now purchase air tickets and issue these directly to researchers who are invited to the university.

The experience gained through these visits was also harnessed when renewing the agreement with the Joint Research Center of the University of Cambridge and concluding an agreement with the University of Chicago, both of which took place from 2013 to 2014. Previously, when concluding agreements with research institutes overseas, a significant point of concern has been whether or not appropriate documents that serve as proof of the execution of research funds can be procured. However, Hirayama explained, "Based on our studies, we have learned that rules that are similar to those at our university are established and enforced. This has allowed us to make the necessary adjustments smoothly." On top of that, he added, "Whether we are talking about Japan or overseas, the staff in charge of accounts are responsible for accounting for the execution of the budget in a transparent and efficient manner. This mindset is the same for them as it is for us. I feel that the opportunity to discuss directly with the administrative staff of overseas universities and other organizations, and exchange detailed opinions about these matters, will contribute significantly to our administrative work in the future."

Aiming to spread these initiatives across Tohoku University

Tohoku University aims to make the leap toward becoming a world-class university. Under the leadership of President Satomi, it has put in place university-wide initiatives to become a global hub for brain circulation. Deputy Administrative Director Shin-ichi Sato talks about the role of AIMR in fulfilling these initiatives. "In order to receive outstanding students and researchers from around the world, we have to strengthen our bilingual support system across the university. AIMR's administrative department, which stands at the frontlines of international administration, could be described as the ideal place for employees with an interest in international work, as well as for many other administrative officers, to gain relevant experience. By widely providing the knowledge and experience gained here, we hope to contribute to improving administration at Tohoku University. I feel that we are already producing results in this aspect." Specifically, efforts have already begun to spread AIMR's knowhow

across Tohoku University. For example, in November last year, a session targeted at members of Tohoku University was held to report on international administrative work. An opportunity for an exchange of opinions was also provided to AIMR staff as well as staff from other parts of the university as part of the project to receive administrative staff from research institutes overseas, which was launched this fiscal year. Oikawa from AIMR's International Relations Unit, who had proposed and led this project for receiving administrative staff from overseas, said, "Staff members from other departments in the university have also been sent on business trips overseas. Of course, the fact is that there are many limitations to business trips in the aspects of finances and time. When I considered how to provide opportunities for international exchange for more employees, I turned the idea on its head and made the proposal of receiving staff from research institutes overseas instead."

In the first round of the project, Michelle Scholtes, a staff of the Carnegie Institution for Science in the United States visited AIMR in June. Over the four days of her stay, the various representatives of the general affairs, accounts, property, and international relations divisions explained the work that they do at AIMR. The Center for International Exchange and Public Relations Office of Tohoku University also provided her with information about work related to the university as a whole.

Takehito Saito, from AIMR's Accounting Section, commented, "It was useful to learn about the differences in remittance procedures based on the culture of using checks, which is different from Japan. Her surprise at finding out that our system provides administrative support for drawing up reports on research funds also left a deep impression on me."



meeting with Ms. Scholtes

At the end of her stay, Scholtes gave a presentation that summarized her visit. "AIMR is a research institute that produces the highest levels of research results. I was impressed at the generous and strong support that the supporting staff provide to the researchers here." She also said that the trip had been a very fruitful one for her. In particular, she wished to introduce the safety management system that seeks to prevent accidents, as well as the centralized gas management system, at her own research institute. Oikawa reflected on this project of receiving overseas administrative staff. "By receiving one person, we were able to spread the effects to dozens of people. From the perspective of cost-efficiency, we now realize that this is an extremely effective method. Going forward, I would like to harness such opportunities to let our staff gain familiarity with working in English, feel more at ease in their work, and strengthen their ability to provide even greater support as a member of the staff that underpin the work of an international research institute."

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 5

Crystals and Minerals

At shopping centers, you may often come across shops selling minerals and rocks. A variety of beautiful crystals, minerals, rocks, and ores are laid out in these shops, and you would likely never tire of looking at them. We tend to be attracted to the mysterious figures of such naturally-formed objects.

Although crystals, minerals, rocks, and ores are listed casually above, what exactly are the differences between them? The relationship between minerals and rocks, and between rocks and ores is perhaps easier to understand. Objects with many mineral particles are known as rocks, and those rocks containing a particularly large quantity of material that can be harnessed as a resource or industrial raw material are known as ores. The differences between crystals and minerals are perhaps the most difficult to understand.

Crystals: Solid matter made up of atoms that are arranged in a regular pattern. This also includes artificially synthesized matter. As the atoms are arranged in a regular pattern, they create flat surfaces (crystal planes) that are characteristic of crystals. (Matter consisting of irregularly arranged atoms is described as an amorphous material. Glass is a representative example.)

Minerals: Minerals are naturally-formed materials that have a chemical composition with a fixed chemical formula. While minerals are generally also crystals, there are some examples of non-crystalline materials, such as natural mercury (liquid).

We focus on the arrangement of the atoms with regard to crystals, whereas we focus on natural or artificial formation when it comes to minerals. Many minerals are also crystals, but there are many crystals that are not minerals. The technology for materials synthesis is now developing, and various crystals can be made. However, man-made crystals whose chemical composition and crystal structure (how the atoms are arranged) do not correspond to naturally-formed materials are not called “minerals.”

Quartz is a mineral made up of silicon dioxide (SiO_2), consisting of silicon (Si) atoms and oxygen (O) atoms arranged in a regular pattern. When quartz is heated to 573°C at one atmospheric pressure (1 atm) the arrangement of the atoms changes and it becomes high quartz. If the

temperature is raised further, it will transform into different types of crystal, such as tridymite and cristobalite. This phenomenon whereby a crystal structure undergoes changes under certain conditions such as temperature and pressure is known as phase transition. The phenomenon whereby materials with the same chemical composition form various crystal structures depending on the condition is known as polymorphism and the products created through this process are known as polymorphs. Low quartz, high quartz, tridymite, and cristobalite, are all polymorphs of SiO_2 . Such phase transition occurs also through changes in pressure. In 1953, L. Coes, Jr. applied a high pressure of 35,000 atm and discovered a new polymorph of SiO_2 that was named “coesite.” However, the coesite artificially produced by Coes could not be labeled as a mineral at the time because this polymorph had not yet been discovered in nature. Thereafter, in 1960, coesite was discovered at the renowned Barringer meteor crater in Arizona, the United States. When the meteorite collided with the surface of the earth, it produced an extremely high pressure, and coesite was formed through the phase transition of quartz. Thus, coesite was included in the category of minerals through its discovery in nature. In fact, stishovite, which is produced at an even higher pressure than coesite, was also discovered at the Barringer meteor crater in 1962. This also led to the categorization of stishovite as a mineral.

In materials science, regardless of whether or not a material is found in nature, all substances that have functions are regarded as the subject of study and research, and the concept of “minerals” is not important. However, through careful observation of “natural minerals,” human beings have come up with the concept of “crystals” which are composed of regularly-arranged atoms, molecules, and unit cells, and which have become the foundation of materials science today. As such, one cannot deny that looking at minerals in a shopping center is somehow related to materials science.



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).

Koji Yoshida

“I get the impression that those who work in the corporate world analyze each and every piece of data that they obtain properly, and also put in place careful measures in terms of intellectual property.”

Dr. Yoshida laughs, as he explains that this does not mean that researchers at universities do not do things properly. He has just taken on his new post this August at the new research laboratory at AIMR, established in cooperation with Hitachi, Ltd. During his graduate studies, Dr. Yoshida consistently carried out research on a nano scale using scanning tunneling microscopes and atomic force microscopes. He is currently working with corporate researchers to develop all-solid-state batteries. According to Dr. Yoshida, while there are some cultural differences between researchers in universities and those working in corporations, motivation toward research remain unchanged. “I have liked chemistry since I was in high school, so I entered the faculty of engineering at Tohoku University because I wanted to do research that would be useful to society. Compared to what I felt during graduate school, I am now gradually beginning to get a sense that my research is moving closer to society.”

Even compared to Switzerland, where he underwent his doctoral course, he feels comfortable carrying out research at AIMR. “The atmosphere at AIMR is very similar to where I was at the University of Bern. Everyone is very friendly, and it is possible to hold candid discussions. I am grateful for this. I was also surprised that there were drinking parties with the Director held for young researchers!”

When asked what he wanted to do upon returning to Japan for the first time in years, he answered that he wanted to visit a hot spring. “There are good places nearby, such as the Toogatta hot springs. I would definitely like to visit these hot springs. If I have time, I would also like to start hiking again, which I often did when I was in Switzerland.”

Koji Yoshida

Research Associate, Hitachi, Ltd. Next Generation Innovative Battery Laboratory, AIMR Industrial-Academic Partnership Project

Born in 1983 in Kagawa Prefecture, Dr. Yoshida is 31 years old. After obtaining his master's degree at the School of Engineering, Tohoku University, he further continued his studies under Professor Thomas Wandlowski at the University of Bern, Switzerland. After obtaining his doctoral degree there, he returned to Japan and took up his current appointment in August 2014.

Text and photo: Yasufumi Nakamichi

