

MAIMR Advanced Institute for Materials Research Magazine

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[Feature article]

Supercritical water: a dream fluid

The frontier where organic matter
and inorganic material meet

[AIMR in the world]

Thomas P. Russell

From Polymers to Working
with Math

Toward a Sustainable Society

[Special Interview]

What are the roles that universities and AIMR should play in order to solve the various issues confronting society?

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- Firstly Professor Russell, could you please tell us about your current research?

Professor Russell: I am currently researching organic photovoltaics, particularly polymer-based organic photovoltaics. I believe organic photovoltaics are part of the solution to the energy problem that mankind is facing. Our group has successfully acquired organic polymer-based devices with an exceptional power conversion efficiencies (PCEs) of >11%, which is the highest that has been reported to date.

- What specific area of organic photovoltaics are you focusing on?

Professor Russell: Our focus has been to optimize what's called the active layer, where light is absorbed and converted into electricity. This active layer is a mixture of carbon materials, namely fullerene C₆₀, and photoactive polymers. Key to the functioning of these devices is a bicontinuous morphology of the components with domains tens of nanometers in size, comparable to the diffusion of an exciton, a bound electron-hole pair. So, in addressing this issue, my co-researchers at the AIMR - Associate Professor Dr. Nakajima and Dr. Wang - used high resolution atomic force microscopy (AFM) to successfully look at the morphology at the surface which is in contact with the cathode and discovered the presence of crystals right at the surface, a key element in understanding the performance of these devices..

We have also been able to develop interlayer materials, that enhance conversion efficiencies by several percent. Our research has enabled us to create devices capable of PCEs > 11%, which is exceptional. Six years ago, standard devices were regarded as working well with PCEs of 5%. Attempts to commercialize flexible devices with these materials failed. With more than a doubling of PCEs in such a short period, with the promise of further enhancement, commercialization is viable with extensive potential applications.

- You've also been involved in research using nanoparticles; can you please tell us more about that?

Professor Russell: As you have pointed out, another important research field for me is the study of nanoparticle surfactants. Normally, a water droplet that is mixed in with oil forms a spherical shape, to minimize the contact area between these two fluids that do not mix together. If you deform the drop with, for example, an electric field, the spherical drop changes to an ellipsoid and, if the field is removed, the drop returns to its spherical shape. If, though, we introduce nanoparticle surfactants to the drop, after we deform the drop into an ellipsoid and remove the field, the drop retains its ellipsoidal shape and does not relax to a sphere.

- So why does the droplet maintain this deformed shape?

Professor Russell: When the water droplet deforms into an ellipsoid, the volume does not change but the surface area increases and more nanoparticle surfactants locate on the

surface of the droplet. So when the electrical field is switched off, the ellipsoidal droplet tries to return to a spherical shape which decreases the surface area. But, there are now too many nanoparticle surfactant at the surface. This is just like a large crowd of people in a room with the walls closing in on them. They become jammed up against each other, and are unable to move. This phenomenon of people getting stuck in a narrowing room represents an exceedingly interesting state of matter, which is referred to as a jammed system. This jamming actually prevents the droplet from relaxing to a spherical shape, so it stays deformed. So, we have actually structured the fluid, an interesting concept to say the least. Here we have a material with all the properties of a liquid, but the structural stability of a solid!

So where can you use this kind of technique? Let's say one fluid was an insulating material, such as a dielectric fluid, and the other was a conductor. Using nanoparticle surfactants to deform fluids, we can make a liquid electronic circuit. Now that's futuristic, but you have far reaching ideas to push the system to its limits.

My other research includes the study of self-assembly processes for generating 2D and 3D nanostructures from copolymers. We are increasing the complexity of molecules and the resultant morphologies where topological issues are important. This reduces to a geometric problem films, which I'm working on with mathematicians, like Professor Stephen Hyde from Canberra in Australia, who is interacting with AIMR, and Director of the AIMR Professor Motoko Kotani. I'm also involved in joint research with Associate Professor Nakajima and other colleagues on structural changes in glassy materials.

U.S. Energy Policy

- Professor Russell, you are currently serving as Director of Research on Polymer-Based Materials for Harvesting Solar Energy (PHaSE) at the research institute set up by the U.S. Department of Energy (DOE), while also conducting your own research on photovoltaics. Could you please elaborate on U.S. energy policy, and share your thoughts on the situation surrounding energy from here on?

Professor Russell: The U.S. Government, especially the DOE, is investing a substantial amount of money to encourage fundamental science and materials science, with the aim of achieving a sustainable society in the future; and solar energy is an important within this. So that's why we are researching polymer-based materials for use as photovoltaics. Polymer-based materials are effective, as they can be used to make highly functional and flexible devices, and as I mentioned earlier, they can reach PCEs > 10%.

However, we are still heavily dependent on oil, coal and other fossil fuels, so photovoltaics are only a very small part of the energy supply picture. Reducing our reliance on these fossil fuels is not just figuring out a solution only for my country, the U.S., and your country, Japan; it has to be a global solution. It's essential that we can have access to energy sources that won't pollute the air or generate carbon dioxides and carbon monoxides, or sulfides and other such substances.

For example, I think we will see all vehicles becoming electrical vehicles (EV) in time; that's inevitable if we want to realize a sustainable society. And so we see the U.S. is steadily rolling out recharging stations for EVs. Finding oil alternatives will be one of the core issues we need to address from hereon.

- However, achieving this sustainable society requires many other things, such as making people consciously reduce their energy consumption, and developing new materials for enhancing energy efficiency.

Professor Russell: That's right. I believe developing new materials or redesigning existing materials for improvement is also fundamental in terms of enhancing efficiency. We also need to come up with some innovative and new ideas for how we can actually conserve or generate energy from different sources, whether it be thermoelectric, photovoltaic or hydroelectric. I think all of these things will become extremely important.

Preparing to foray into other fields

- So what initiatives are required for developing these new materials that can change society?

Professor Russell: In my opinion, the number one initiative that the AIMR has seen success in is the math-materials science collaboration. I think it's actually quite innovative, and if, through this collaboration, we can extract the key issues and find solutions for them, then I believe it has the potential to be groundbreaking. As for myself, I'm working with mathematicians at the AIMR on research in areas such as the self-assembly process. However, these types of initiatives take a long time to generate fruitful findings. Also, mathematicians and materials scientists need to find a mutual area of interest to work on.

So in that sense, I think tea time at the AIMR is a great chance for the people working there to interact with each other. When you give a presentation, if it's not in the area that some of the audience are working in, you lose their attention; some people may listen and see if they can make a contribution or suggestion; or others may listen and say "Gee, what about this? I might know how to do this. I bet if we worked together on it, we could produce some truly interesting results." Sometimes the research themes match, and sometimes they don't. We cannot predict the rate of success or failure, but I think having people gather in the same room and talking to each other is really important.

When I was working at IBM in San Jose, we used viewgraphs (OHP sheets) and gave a monthly seminar that we called a "tree-viewgraph seminar", a presentation to introduce a single idea using only three slides. We didn't have to present the fully worked out details of our idea; it was more just to show people what we were working on, where we saw noteworthy things happening, and where we could perhaps receive input and information from others. This seminar was held throughout the physical sciences group at IBM in San Jose, which was a fairly large number of people, and it was taken very seriously. If it

was done very formally, the presenters probably would've ended up announcing their final results. So from that perspective, it was also an excellent forum to present research results that weren't yet complete. Sometimes it's best to put ideas onto the table and get people discussing them.

- So first it's important to find topic to work on, and then look for an area of common interest.

Professor Russell: Exactly. In order to work in with a researcher of an area that you are not very familiar with, the topic you will tackle has to be a challenge for both sides; and you have to rely on the expertise of this person to complement yours, and vice-versa. You also need to really discuss your respective fields with each other. You must be ready to step outside of your own field, your comfort zone, and into that of your research partner; this is what matters the most.

- In closing, could you please tell us your expectations of the AIMR initiatives?

Professor Russell: As I've already mentioned, I believe in the significance of the math-materials science collaboration. It really is a key element in our work to develop new materials that can change society. And I'm confident that Tohoku University, in particular the AIMR, has the right environment for such collaborations to work effectively.



Thomas P. Russell

Born on November 18, 1952. He received a Ph.D. from the University of Massachusetts Amherst in 1979. After working as a Research Fellow at the University of Mainz in Germany for two years and as a research staff member at the IBM Almaden Research Center for sixteen years, he took up a post as a professor at the University of Massachusetts in 1996. Since 2007, he has also been working as a principal investigator at the Advanced Institute for Materials Research (AIMR).

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 7
Tomography

Tomography is the generic term for using methods like sound waves or electromagnetic waves to explore the internal structures of objects that are not visible from the outside. One example of tomography is seismic tomography, which examines the internal structure of the Earth. This still might not give you a clear idea of what tomography entails. However, when we write “X-ray CT” (X-ray Computed Tomography), many people would probably remember what kind of equipment that is. Today, this equipment is installed in many medical institutions, and is used to diagnose diseases and injuries, as well as for health examinations. The representative form of radiography, utilizing X-rays, is roentgenography. This form of radiography takes its name from W.C. Röntgen, who discovered X-rays. In roentgenography (more commonly known as X-ray), X-rays are passed through one side of the body. The X-rays that emerge from the opposite side are captured by films or detectors and printed as photographs (images). Most of the X-rays are absorbed by parts made of elements with high atomic numbers, thereby reducing the intensity of the X-rays after they have passed through. As such, it is able to clearly distinguish bones in particular, which are mainly composed of calcium, as well as other parts of the body. However, passing the rays through the body in one direction means that, for example, if two bones are seen to be overlapping one another, it is difficult to tell just from the images which is in front and which is behind. To counter this problem, X-ray CT can acquire three-dimensional data. For cases like the aforementioned example, we can tell at a glance which bone is in front and which is behind.

The “C” in X-ray CT stands for “Computed.” This means that enormous numerical calculations must be carried out with a computer. Mathematics contributes significantly to tomography technology. If we were to carry out computations based on mathematical theories for the multiple transmission images (projection images) obtained by passing X-rays from various directions through a certain object, we could observe the internal structure of the object (three-dimensional distribution of X-ray absorption coefficient). The mathematical concepts applied here are the Radon transform and inverse Radon transform. The paper of this theoretical foundation was published by Austrian mathematician J. Radon in 1917. The American physicist A. M. Cormack, who was unaware of Radon’s achievements in the field, constructed his own theory equivalent to the Radon transform and inverse Radon transform, and published papers in 1963 and 1964 on calculating the three-dimensional structure of internal

parts of objects (called “3D image reconstruction”). Although the papers did not draw much attention at first, the British electronic engineer G.N. Hounsfield developed a practical X-ray CT device in 1971 based on Cormack’s theory. The following year, he announced the historical achievement of having successfully filmed images of the diseased parts of the human brain without carrying out a craniotomy procedure. With these achievements, Cormack and Hounsfield received the Nobel Prize in Physiology or Medicine in 1979. Although the MRI is a similar method used in the medical field, X-ray CT follows a largely different principle. Someday I will expound further upon it. MRI is also a form of tomography that makes use of computers, and therefore is considered to be a type of CT. However, CT is commonly used to refer to X-ray CT. Such tomography technology is also becoming indispensable in material science. It is useful as a non-destructive method to examine cracks and other details in materials; and the ability to view the three-dimensional structure of objects is a significant plus. For example, electrical conductivity and the behavior of fluids are dependent upon the three-dimensional connection state (network) of substances. However, even when connections exist three-dimensionally, they often appear to be disconnected when observed in two-dimensional cross-sections. Hence, it is crucial to be able to observe network structures in their three-dimensional forms. The development of equipment is also rapidly advancing. The resolution of CT scanners used in the medical field, which have been specially developed for filming the human body, is about 1 mm. This is not precise enough for materials research. High-resolution X-ray CT scanners that have been developed for industrial use and for use in fundamental research have resolution ranging from 1 to 10 micrometers. On top of that, the cutting-edge X-ray CT device developed at the large-scale synchrotron radiation facility, SPring-8, now has a resolution of about 0.2 micrometers (200 nanometers), and is being utilized in various materials research activities.

**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).

Song Toan PHAM

“I wanted to find out more about the world I live in, and I believed science could give me the answers I was seeking.” This is what motivated Dr. Pham to become a researcher.

Upon deciding to become a researcher, Dr. Pham felt that he wanted to make something new; so he started studying materials science. Among the various materials in this field, he was particularly drawn to organic material with its potentially high application in everyday life. “Apart from being flexible and extremely cost effective, with the use of spintronics, organic material is also able to transmit spin information over longer distances than inorganic material. As such, it is a fascinating material also for use in electronic devices.”

Dr. Pham is currently researching organic spintronics devices at Prof. Mizukami’s lab at AIMR. “Tohoku University is renowned in the spintronics field, and AIMR is well equipped with top level researchers and equipment. I greatly look forward to the opportunity to conduct research in such an excellent environment.”

Before coming to Sendai, Dr. Pham lived in Vietnam and Osaka. When asked if the cold winters here are particularly tough for him, he replied with a smile, “I like snow and skiing, so I’m really enjoying my life in Sendai.”

Song Toan PHAM

AIMR Research Associate
Born in 1986 in Hanoi, Vietnam, Graduated from Vietnam National University, Hanoi. After acquiring a Ph.D. at Osaka University, he started working at AIMR in 2015.

Text and photo: Yasufumi Nakamichi