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BEYOND the SIMULATION

Where is Computational Science Today?

Beyond the Simulation

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Computational science technology enables computer simulations to run by setting desirable conditions such as combinations of atoms and temperatures.

But even with the power of computational science, it was difficult to reproduce real-world phenomena. For example, a reproduction of even a small experimental chemical reaction requires computations taking into account the simultaneous movements of hundreds of millions of atoms occurring in hundreds of millions of steps.

And yet, computational science is rapidly becoming capable of simulating real-world phenomena owing to recent advancement in computer technology.
Using the computational science approach, we are aiming to estimate the structures of materials with new functions, and reproduce them in experiments.

In this issue, we look at the current status of computational science, which has been evolving from a tool to merely reproduce empirical experiments to a tool that suggests plans to develop new materials.

Taizo Sasaki
Director of
Computational Materials
Science Unit

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Chikashi Nishimura
Director of
Hydrogen Materials Unit

Special Talk

How Far Has Computational Science Come?

In all areas of science, computation is now one of the most important and advanced research means, along with theory and experiment. The area of materials science is no exception. Computational science is expected to go beyond its conventional function of "explaining the experimental results" and to play a greater role in "forecasting" revolutionary new materials. What is the current status of computational science in the area of materials science, and what will become of it in the future? Two figures representative of different spheres of science, computational and experimental, discuss these issues extensively.

Beginning of collaboration among theoretical, experimental and computational sciences

Nishimura: Computational science has established its presence as the third pillar of science. I am in experimental science, but from day to day, I am feeling the presence of computational science becoming greater. I am curious about how theoretical, experimental and computational sciences will unite together in the future, so I have been looking forward to talking with you today on the current status and future prospects of this topic. First, let us look back at the history of computational science. What was computational science like when you joined the National Research Institute for Metals (NRIM), NIMS's predecessor, in 1988?

Sasaki: At that time, computational science began to be introduced in some disciplines, such as fluid dynamics which is indispensable for the design of aircraft, but it was rarely introduced in the field of materials science. I started my research career in theoretical physics, and to me, computers were "calculators," a tool for calculating theories. As I remember, the first supercomputer was installed in our institute in 1995, and it was only after the beginning of the 2000s that computational science started to be really recognized as a third research method following theoretical and experimental sciences.

Nishimura: Theoretical scientists study properties of materials on an atomic scale. However, in the 1990s, high-spec electronic microscopes were too expensive and not widely available, so experimental scientists rarely observed or analyzed the results of their experiments on an atomic scale. This probably caused a rift between theoretical and experimental scientists. I think they began to engage in debates on an equal footing when nanotechnology started to attract public attention.

Sasaki: Accordingly, findings were obtained at the nano-scale through experiments, and at the same time, the K computer development project was launched and the performance of computers dramatically improved. Along with this, useful calculation techniques were established.

Nishimura: As a result, an environment has been set in place where theoretical, computational and experimental scientists can discuss the characteristics of materials all on an atomic scale. As collaboration among these three moves on to the next stage toward solving diverse social problems, such as environmental and energy-related problems, progress is expected to be made in the development of new materials and innovative technologies that will change our industrial structure and lifestyles.

Sasaki: Your field of specialty is study of materials related to hydrogen energy. This field directly leads to bringing about significant change in the industrial structure and ↙

Our mission is to be the light of the lighthouse.
Taizo Sasaki

lifestyles. As a scientist who actually deals with experiments with materials, how do you recognize the role of computational science?

Nishimura: In general, first of all, computational science can be understood as something that fills the gap between theory and experiment. Computational science provides theoretical evidence of the underlying mechanism of the properties of materials that have been identified from the experimental results, and then presents such evidence in a visual form. I personally feel that when I submit papers to scientific journals, I need to present experimental results with evidence from computational science more frequently than before. Next, computational science can be a tool for selecting useful experimental conditions from among an infinite number of possible assumptions. Another important role I expect computational science to play is to visualize, through computer simulation, the reactions and the formation process of materials under experiments, and present them plainly.

However, there is also a concern. In computational science, parameters can be decided freely, such as at a super-high temperature or under super-high pressure, but in experiments, unexpected phenomena might occur under any situation, so the actual experimental results do not always agree with the computational results. What do you think about this?

Sasaki: You are right. For example, the surface of a specimen used in an experiment is not perfectly even and smooth as it is assumed in computer simulation. In most cases, the real surface has irregularity, such as kinks or holes, and these features can have an influence on the properties of the target materials. Computational science begins by creating a numerical model based on a theory. What both experimental and computational sciences should take note of is to check whether the created numerical model properly covers the point that the experiment aims to confirm.

By setting a goal precisely and creating a model of a high degree of perfection through mutual feedback of results, experimental science and computational science will be able to further enhance their relationship. ↙

Development of new calculation techniques will be the key to practical application of innovative materials.

Nishimura: Among the areas of materials science, which area would you cite as where computational science currently demonstrates its advantage?

Sasaki: Depending on their functional features, materials can be largely divided into structural materials and functional materials. In this respect, computational science is really fit for functional materials. A big reason for this is that the dramatic improvement in the performance of supercomputers has made it possible to reproduce the behavior of each atom fairly faithfully through computer simulation. Conversely, computational science may not be good at handling structural materials because it is difficult to grasp phenomena at the nano-scale.

Nishimura: It seems so. But even in such area, computational science may have a potential in developing designs of new materials through the integration of simulation and data science and reducing the time required from discovery until practical use of innovative materials.

In order to ensure that computational science will play a more active role in areas of materials science, do you think that improvement of the performance of supercom ↙

Interdisciplinary development of computational science will bring about new ideas.
Chikashi Nishimura

puters will be the key?

Sasaki: No, I can't simply say so. Of course, it is better that a computer has greater performance. But, when dealing with materials that have an uneven or irregular structure, even a supercomputer would be unable to do a complete calculation by the conventional method of the first-principles calculation, because the volume of data would be massive. This situation will basically remain unchanged even when an advanced version of the K computer becomes available. Therefore, we have also been working on the development of a new calculation technique that we call Order N (see p.6). This has enabled, for the first time in the world, the first-principles calculation of a system having tens of thousands of atoms. As a result, it is now possible to do calculations regarding nanostructured materials having a complex grain boundary and biological materials such as proteins.

In the areas of materials science, the subjects of study cover a very wide range, and researchers wish to do as many calculations as possible under various conditions. So, not only supercomputers but also distributed computing systems consisting of multiple PCs connected together and small or medium-scale computers are assuming an important role.

Expectations for further advancement in computational science and a Nobel Prize-class discovery

Nishimura: These days, personal computers have seen remarkable improvement in performance and a lot of versatile software programs are available, so it is common that researchers who mainly engage in experiments do simple calculations using their PCs at hand.

Sasaki: Yes. This means that we, computational scientists, will have to do more than just doing calculations in the future. We have to be more creative.

At present, NIMS has a one-petaflop supercomputer. It operates at about 90% capacity, of which only about 20% is used by the members of the Computational Materials ↙ Science Unit, and the remaining portion is used by research units which are not in computational science, such as MANA and GREEN. When I joined the institute, among about 300 researchers, only four researchers including me dealt with computational science. I feel the trend of the times that led to today's rise of computational science.

Nishimura: GREEN aims to develop new materials for solving global environmental problems through the collaboration and integration of computational and experimental sciences. I feel that there should be more opportunities for such collaboration and integration. Interdisciplinary development of computational science will lead to the progress of computational science itself and bring about new ideas. Seven years ago, when I was present at the scene where GREEN was in the final stage to be selected as a MEXT-sponsored project, one of the judges, a great professor, said that he didn't think computation would be of any use. I still clearly remember this harsh comment. But the situation has greatly changed since then. Now I feel that the day the development of revolutionary materials will be achieved under the initiative of computational science is approaching.

What do you think will be demanded of computational science in the future?

Sasaki: My ultimate goal is to make proposals and give advice to materials researchers based on computational science. I would be happy if my proposal or advice would lead them to develop new materials that smash conventional ideas.

Nishimura: Theoretical scientists have predicted the existence of new materials based on their own theories, and then experimental scientists have proved it through their experiments. You mean, in the same way, computational scientists may predict the development of new materials based on their own computations.

Sasaki: I remember an interesting comment by a professor at Osaka University. "Theoretical scientists will discover a revolutionary theory and make a prediction, as if they serve as the light of a lighthouse to guide a ship which experimental scientists are aboard. But only a handful of theoretical scientists can be such a powerful light, and most of them act as nothing more than the dim light of lantern." I really agreed with him. As he said, the mission we have as computational scientists is to be the light of the lighthouse.

Nishimura: I hope that in the near future, computational science will pave the way toward a Nobel Prize-class discovery and the development of new materials that no one has ever imagined.

(by Kumi Yamada)

* The first-principles calculation is a calculation technique for elucidating laws of physics and estimating physical properties on the basis of quantum mechanics (first principles), which is the fundamental law for materials on an atomic or nano-scale.

Creating a dream device
through fusion of computational science and experimental science

Tsuyoshi Miyazaki, the leader of the First-Principles Simulation Group, studies the behavior of atoms and electrons in materials by performing the world's largest-scale calculations: he deals with 10,000-1,000,000 atoms. Meanwhile, Naoki Fukata, a leader of the Nanostructured Semiconducting Materials Group, is working to develop highly-functional devices using nanostructured silicon materials. Through collaboration, Miyazaki and Fukata are hoping to create a ground-breaking device.

To perform calculations that take into account a large number of atoms

"It was only five or ten years ago when computational scientists and experimental scientists were able to engage in constructive discussions about materials on the nanoscale," says Tsuyoshi Miyazaki of the First-Principles Simulation Group. This progress was made partly because Miyazaki's group developed an order-N first-principles calculation program called "CONQUEST."

First-principles calculations allow for computation of interatomic forces and the behavior of electrons based on quantum mechanics, the most fundamental principle in atomic physics. If you know the state of electrons in a material, you can reveal the properties of the material. However, this process requires very complex calculations, made worse as the computational complexity increases proportionally to the third power of the number of atoms in the material (N). For example, if N doubles, the computational complexity increases eight times. As such, the number of atoms that can be calculated is limited.

"The number of atoms that can be computed by first-principles calculations used to be only several hundred. Even a cube that has only 10 atoms on each side contains a total of 1,000 atoms. Standard computational methods cannot handle even such a tiny object. On the other hand, a material consisting of several hundred atoms is too small to handle in experimental science. So, experimental scientists had urged us to make progress in computational science, so that it could deal with much greater numbers of atoms. Of course, we ourselves were well aware of the issue, and therefore, we spent more than 15 years developing a first-principles calculations method capable of executing large-scale computations."

Then, Miyazaki and Professor David Bowler (affiliated with both the University College London, and the London Centre for Nanotechnology in the UK: he is also a NIMS-MANA member) succeeded in developing a new computational method called the order-N method. This is a ground-breaking method as it removes the cubic increase in computational complexity when N increases, replacing it with a linear increase. For instance, when the value of N doubles, the computational complexity also doubles based on the relationship that the computational complexity increases proportionally to N. In conventional first-principles calculations, a wave function needs to be calculated for every single electron. In contrast, in order-N first-principles calculations, the computational complexity is minimized by dividing the whole material into localized small units and calculating density matrices.

There are different types of order-N methods, and many groups worldwide are competing with each other in developing superior methods. CONQUEST has the advantages of conducting stable and accurate calculations and being efficiently compatible with a massively parallel computer. Because of these features, CONQUEST is capable of carrying out calculations involving more than 30,000 atoms routinely, and has been shown to handle as many as over 1 million atoms (Figure 1). This means that the computational power has been boosted by two orders of magnitude or more in CONQUEST compared to previously developed programs. "The first-principles molecular dynamics simulations involving 30,000 atoms are the world's largest scale, and our method has many features that other codes do not have," Miyazaki says.

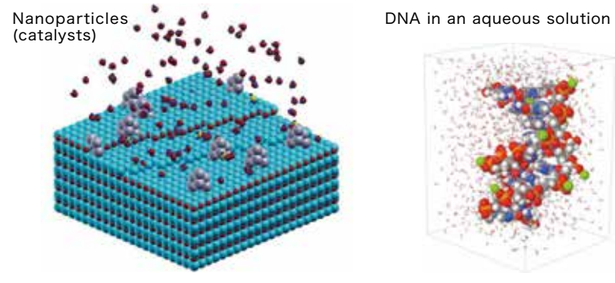


Fig. 1. Targets of the order-N first-principles calculation program CONQUEST.
CONQUEST is capable of computing interatomic forces and the behavior of electrons even in a large system consisting of more than 30,000 atoms.

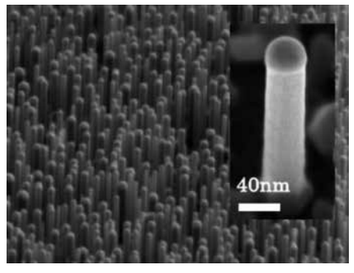


Fig. 2. Scanning electron micrograph of Silicon nanowires, and a magnified nanowire.
A nanowire is an elongated structure with a diameter of about 10-50 nm.

Perfect timing for collaboration between computational and experimental sciences

Miyazaki always had in mind that, "It is vital for us to develop a practical computational method that is applicable to actual materials, instead of merely developing a theoretical computational method for the sake of publication." Accordingly, he started searching for a target material to be simulated using CONQUEST. "A material consisting of 30,000 atoms is about 10 nm in size. Nanosized materials sometimes exhibit unique functions, which regular-sized materials do not possess. So I looked for nanostructures with interesting functions in literature worldwide. I was excited to find a paper on a very interesting material: silicon (Si)/germanium (Ge) core-shell nanowires. And to my surprise, the author of the paper was a NIMS researcher. I immediately contacted and met with him."

The author was Naoki Fukata in the Nanostructured Semiconducting Materials Group. "I first thought that Dr. Miyazaki contacted me because he was looking for a research partner within NIMS. But I was told just today that he contacted me because he was intrigued by my research while conducting an extensive worldwide literature review. That is an honor to me," says Fukata smiling. "Before I gained acquaintance with Dr. Miyazaki, I was also considering teaming up with a computational scientist in pursuit of conducting joint research. The problem was that computational scientists and experimental scientists dealt with different sizes of materials at that time. So, we gave up on the idea of working together in the end. When Dr. Miyazaki contacted me, however, computational science had made a significant advance, and computational scientists were able to handle simulations of larger materials. At the same time, experimental science had also made progress, and experimental scientists were able to handle the fabrication and characterisation of smaller materials. These simultaneous advancements in these two disciplines allowed us to deal with materials in the same size range. The timing of our collaboration was just perfect."

Tsuyoshi Miyazaki
Group Leader, First-Principles Simulation Group, Computational Materials Science Unit

Naoki Fukata
Group Leader, Nanostructured Semiconducting Materials Group, Inorganic Nanostructures Unit, International Center for Materials Nanoarchitectonics (MANA)

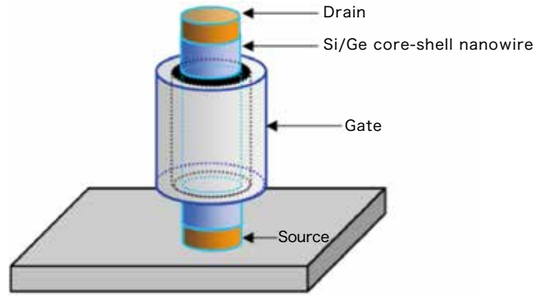


Fig. 3. Diagram of a next-generation vertical transistor using Si/Ge core-shell nanowires.
A transistor consists of a gate, source and drain. When a voltage is applied to the gate, electric current runs through a channel between the source and drain. Using nanowires in the source, drain and channel that are aligned vertically, it is feasible to create a transistor that is highly integrated, high-speed, highly controllable, low in power consumption and highly controllable.

What is a Si/Ge core-shell nanowire?

What is the Si/Ge core-shell nanowire which intrigued Miyazaki? Fukata explains, "A nanowire is an elongated structure with a diameter of about 10 nm. It is perceived as a promising next-generation transistor (Figure 2)." A transistor is a semiconductor device used to amplify electronic signals and serves as an electric circuit switch in electronic devices. Integration and functional improvement of transistors had been achieved by making them smaller. However, further miniaturization is very difficult. An alternative approach to miniaturization that has been proposed recently is the creation of vertical three-dimensional transistors. "In big cities, buildings are becoming taller and taller as the availability of building sites is dwindling. Similarly, we are attempting to develop a highly integrated transistor by arranging vertically-oriented nanowires side by side," says Fukata. He has high expectations for nanowires that have a special structure called a core-shell where a Ge nanowire is enclosed by an Si outer layer (Figure 3).

To realize the practical use of nanowires as transistors, it is critical to control charge carriers (i.e., electrons and holes) that flow in nanowires. One way of controlling charge carriers is to dope with impurities. However, in nanowires, this method has an issue that scattering by ionized dopant impurities may reduce the mobility of charge carriers. "This won't be an issue if Si/Ge core-shell nanowires are used," says Fukata. If the Si shell is doped with boron atoms (B), holes in the shell migrate to the Ge core, allowing charge carriers to flow only in the core (Figure 4). In this procedure, the doped area and the area in

which charge carriers are mobile are completely separated, and this arrangement prevents reduction of charge carrier mobility.

Computational science gives guidance and experimental science embodies a new device

"We succeeded for the first time in the world in measuring the state and behavior of impurities in nanowires using spectroscopic techniques. Furthermore, we observed holes migrating from the doped Si shell to the Ge core like water seeping out. In the future, we are hoping to observe phenomena taking place at the interface between Si and Ge. Unfortunately, spectroscopic techniques do not allow us to observe such phenomena due to their small scale. We need the aid of computational science to achieve this objective. The way of conducting research based solely on empirical experiments is a thing of the past."

Using CONQUEST, Miyazaki calculated atomic and electronic states at Si/Ge interfaces in Si/Ge core-shell nanowires (Figure 5). While they are not ready to tell us their findings in detail yet, the results are astonishing, to say the least. Fukata says, "I was shocked, like sparks ran through me, by the fact that the results of the computations were totally different from my expectations in terms of electronic state. The great thing about computational science is that it is able to show us the kind of the world we are unable to see in empirical experiments. It's just amazing."

While Si/Ge core-shell nanowires are perceived as a promising next-generation transistor, designing and producing truly practical products require the understanding of many aspects such as the movement characteristics of charge carriers and heat, stable structure and the control method.

Fukata made requests to Miyazaki saying, "I want to know what is occurring inside the core-shell nanowire. I also want to know what structures are necessary for the nanowire to perform specific functions. In the past, I had no choice but to repeatedly perform experiments while changing the experimental conditions to answer these questions. But this approach is time-consuming and expensive. If the computational science approach gives us guidance as to what type of structure is necessary, we will be able to conduct experiments with confidence in addition to greatly saving time and expenses."

In response to Fukata's requests, Miyazaki replies, "In computational science, we make calculations based on an idealized system. As such, predictions resulting from the calculations may not always accurately be reflected in the actual materials. In such cases, we correct the models and calculations based on empirical data. Or, we sometimes even need to develop a new computational technique. Incorporating feedback from computational science and experimental science in a back-and-forth manner, we improve the prediction accuracy of our models and calculations, thereby contributing to the successful development of a new transistor consisting of Si/Ge core-shell nanowires. During this process, we may also discover a nanostructure with a function unknown to science."

Discussion is essential for the fusion of computational and experimental sciences

What needs to happen for fusion between computational science and experimental science in a manner that will produce innovative results? Miyazaki and Fukata answered simultaneously, "That's discussion." Then Miyazaki continues, "The two disciplines use different languages and are partially incompatible. Even so, I enjoy explaining my calculations to my partner as much as possible. I also want to understand my partner's experiment in detail. It is vital for both of us to understand each other's work."

Fukata says, "I want to create materials and devices with new functions using silicon, which is the second most abundant substance in the earth's crust, and thus is inexpensive and easily available. For example, using silicon nanowires, I am aiming to develop new solar cells that are superior to conventional silicon solar cells in terms of conversion efficiency from solar energy to electric power. I would very much like to team up with Dr. Miyazaki for this project as well." In response to Fukata's passionate request, Miyazaki responds, "I believe that a solar cell's power generation efficiency can be improved through the optimization of the structure and arrangement of nanowires. I am sure that computational science will be able to make great contribution to that problem."

The fusion of computational and experimental sciences is becoming key to the advancement of science and technological development. It is expected that the fusion of the two disciplines will continue to evolve and lead to many ground-breaking achievements and discoveries.

(by Shino Suzuki, PhotonCreate)

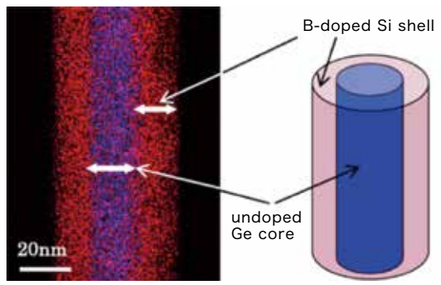


Fig. 4. Composition analysis of an Si/Ge core-shell nanowire and a schematic of the nanowire.
Si/Ge core-shell nanowire consists of a Ge core and an Si shell. Doping of an Si shell with boron atoms (B) causes holes to migrate from the shell to the core. Holes then flow in the core.

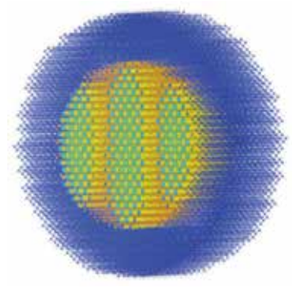


Fig. 5. Electronic state of a Si/Ge core-shell nanowire estimated by order-N first principles calculations.
A Si/Ge core-shell nanowire consists of a core, in which Ge atoms (orange) are arrayed, and an outer shell, in which Si atoms (blue) are arrayed. A wave function of electrons in an occupied state (i.e., electrons with restricted mobility) is depicted in yellow and its cross section in light blue. This indicates that holes carrying electric charge are stuck in the Ge core.

Making strong steel
using computational science

"Can you pound 5 mm to the left from there?"
"Right there?"
"There. Now can you increase the pressure level of the press machine?"
"I'm not sure. Alarm has been sounding continuously for some time."
"The current pressure level is not enough to produce deformation inside the steel. Could you raise the pressure to the maximum?"
"You are so demanding. Okay, I'll try."
This is a scene that took place in the operator room from which a 3,000-ton press machine was maneuvered at the Japan Steel Works (JSW) Muroran Plant.
To realize the dream of making super-strong steel, collaborative efforts were made between Tadanobu Inoue, leader of the Toughness Design Group at NIMS who is an expert on high-precision numerical simulations, and craftsmen with sophisticated steel processing skills.

3,000-ton press machine at the Japan Steel Works Muroran Plant

Doubling the strength of steel through ultrafine grained structures

In February 1998, Tadanobu Inoue joined the National Research Institute for Metals (NRIM), a predecessor of NIMS, where he participated in a project that started in fiscal 1997 called "structural materials for the 21st Century," or more commonly known as the "ultra-steel project." This 10-year project aimed at the development of ultra-steel materials that are twice as strong as conventional steel.

At that time, the mainstream approach to strengthening steel was to design an alloy by which such metals as molybdenum and chromium were added to steel. However, because they were rare elements and their stable acquisition might be difficult, the researchers wished to develop an alternative method to strengthen steel without using them. Consequently, they focused on the approach to create ultrafine grained structures.

Steel is an assembly of small grains, and it had been known that the smaller the grains are, the stronger the steel is. Crystal grains in conventional steel generally have diameters of about 10 μm. In the ultra-steel project, the researchers set the goal of achieving steel strength of 800 MPa, which is roughly equivalent to twice the strength of conventional steel, by reducing the diameter of the grains to one-tenth, of conventional grains, or to 1 μm

or less. Steel strength of 800 MPa means that permanent deformation of the steel does not occur unless a load of 800 N (about 82 kg) per 1 mm^2 is applied to it.

Process parameters required to create 1μm crystal grains identified

Inoue had expertise on theoretical science and computational science, and he was carrying out research mainly on dissimilar materials and composite materials. "This was my first time dealing with steel, and I hadn't even seen large structural materials being manufactured. Since I was new to this specific subject, I did a thorough literature review on miniaturization of grains of steel, and asked many questions to the project members from major steel manufacturers. After gathering information, I realized that there is no consistency among the different test results."

It had been confirmed based on many experiments and published papers that when a great force is applied to a steel material, strain energy builds up internally, which in turn facilitate grain miniaturization and strengthening of steel. Much literature has documented the relationship among the processing rate (i.e., % reduction in steel thickness), grain diameter, and the degree of increase in steel strength. What did Inoue mean by "there is no consistency among the different test results?"

"There are two methods of applying force to and processing steel: rolling, in which steel is extended while going through rotating rolls, and forging, in which steel is hammered or compressed using dies." Even if these two methods are implemented at the same processing rate, the strengths of forces applied to steel are different. As a result, the ways steel is strained are different between the two methods. Furthermore, change in processing speeds either add or removes heat, causing the temperature of the steel to vary. Therefore, it is important to quantitatively understand the relationship between various process parameters, including the processing rate, and the microstructure of steel. If this relationship is understood, you can specify appropriate conditions to fabricate 1μm crystal grains for the given processing method to be used and for the given size of steel to be processed."

To practice this approach, Inoue measured key process parameters such as temperature, strain rate, strain and cooling rate using a very small steel test piece, and recorded the relationship between these parameters and the resulting microstructure of steel. At that time, other research groups both in Japan and overseas proposed a technique called the severe plastic deformation process, and they later announced that they succeeded in creating 0.1μm grains and a steel material that is three times stronger than conventional steel by repeatedly compressing the steel."These high-profile studies attracted much attention. On the other hand, we continued collecting data in a steady manner based on the belief that quantification of the relationship between process parameters and the microstructure of steel is absolutely critical in soundly create stronger steel through the creation of ultrafine grains."

After five years in the project, Inoue's team finally quantified the process parameters necessary to create 1μm grains.

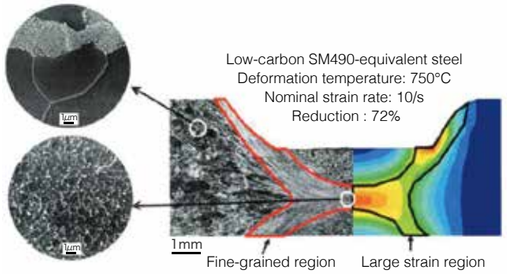


Fig. 1. Miniaturization of crystal grains illustrated in experiment and simulation.
Diagram on the right:Cross-section of a small steel test piece that was compressed (left) and strain distribution in steel estimated by simulation (right). Red areas indicate the highest level of strain.
Circular photos on the left:Diameters of grains in steel are about 10 μm (top) while diameters of ultrafine grains in steel that was greatly strained by compression are about 1 μm (bottom).

Success in the production of rod material and 18 mm thick steel plate

Since the beginning of the project, Inoue had noted another issue to be addressed. "So far, we used very small steel test pieces smaller than 1 cm in most experiments. However, we are aiming at developing structural materials that will be used for the construction of buildings, bridges, automobiles and ships. For this reason, we need to fill the large gap between the test pieces and end products in terms of size."

There was another research team engaging in the ultra-steel project, and the team was steadily dealing with the issue. Based on the knowledge gained from basic studies conducted by Inoue's team using very small steel test pieces, in 2000, the other team successfully produced steel rods that have an 18-mm-by-18-mm cross section, are about 20 m long, and consist of grains with diameters 1 μm or less that are uniformly distributed from the surface to the core of the material. Then, in 2001, the same team succeeded in the production of a steel plate that was 18 mm thick, 80 mm wide and about 2 m long, and weighed about 20 kg. The plate consisted of grains with diameters of 0.5 to 0.6 μm. Both the steel rods and plates were created using a rolling machine at an external facility after tests were conducted using a NIMS-owned rolling machine. While the rolling process is often performed at 800°C or higher so that the steel being processed becomes red hot, the NIMS team took a different approach of processing the steel at between 500 and 600°C. The use of lower temperatures facilitates buildup of strain energy and creation of ultrafine grains.

The next goal was to fabricate 25 mm thick steel plates. This is because 25 mm thickness is ideal while 18 mm thickness is too thin for practical use in civil engineering and construction. The NIMS team knew that 25 mm thickness cannot be achieved using the rolling process. To produce appropriately large steel plates with a sufficient thickness, it was necessary to develop a new production procedure. This is when Inoue's expertise in computational science came in handy at last.

Creating 35 mm thick steel plate in collaboration with steel craftsmen

Based on the process parameters obtained from the experiments using very small steel test pieces, Inoue numerically simulated the process of producing a large, 25 mm thick steel plate consisting of 1 μm ultrafine grains. Then, from the simulations, Inoue calculated three types of estimates: those concerning the microstructure of steel, the shape of the steel plate and the load on the steel processing machinery. "We tend to focus exclusively on the estimates concerning the microstructure of steel, but the shape of the steel plate is also important in terms of its relevance to the application of structural materials. So, it is critical to both enhance the properties of the material and shape the steel plate at the same time. In addition, the estimate of the load on the steel processing machinery is also important from the viewpoint that we must be careful not to break the valuable machine," explains Inoue.

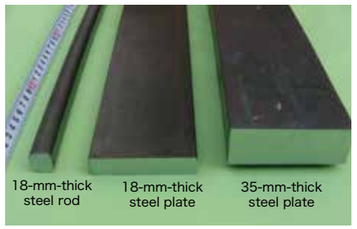


Fig. 2. Ultrafine-grained steel plates developed by NIMS
The 35-mm-thick steel plate was created using a 3,000-ton press machine at the Japan Steel Works Muroran Plant. The use of scrap steel in this production contributes to resource saving and reduction of environmental load.

The simulation itself is not the end goal of the project. Its outcomes need to be interpreted and applied to the production of steel plates using a new production procedure. To proceed with this plan, Inoue asked the JSW to allow them to use its 3,000-ton press machine at the JSW Muroran Plant. The request was granted.

Inoue immediately visited the plant taking the blueprint of the new production procedure he prepared based on the simulations. "The first trial was a complete failure. Due to my limited understanding of the specifications of the press machine, the precision of the simulation was very poor."

"I remember feeling encouraged when we obtained study results that were consistent with the concept: the internal microstructure and the external shape of a material are interconnected to each other as is evident from the fact that free forging produces uneven surfaces."

There were many other parameters that could improve the precision of the simulation such as the shape of the dies that pound the steel, the pressing speed, changes in applied pressure, the load on the manipulator that holds the steel plate, and the movement of the manipulator. However, a forging plant is a place where machines and equipment are operated by craftsmen who rely on their experience and intuition. "Outsiders were allowed to observe the press machine only from a distance. Due to this restriction, I was not able to gather necessary information, so I desperately asked the plant workers to allow me to observe the machine more closely. Then, to my surprise, the plant manager allowed me to observe the press machine from the operator room, which is normally inaccessible to visitors. Moreover, I received permission to videotape steel processing in action using a fixed camera. Diligently looking through the on-camera monitor, I made sure to record all necessary information in detail on the press machine, manipulator, and the operator controlling the system."

As soon as the experiment was completed, Inoue immediately flew back to Tsukuba (watching the recorded video over and over on the way). Then, Inoue ran simulations taking into account the information gathered during the experiment, additional specifications of the press machine provided by the plant workers, and the results yielded from running the press machine. The NIMS researchers tested the simulation-based production procedure by running it using a press machine. They repeated the test five times during the subsequent year. In 2004, for the first time in the world, they succeeded in producing a 35 mm thick and about 90 kg steel plate consisting of ultrafine grains with diameters of 1 μm or less that are uniformly distributed from the surface to the core. "The combination of high-precision numerical simulations and sophisticated processing technology capable of faithfully reproducing the simulation-generated blueprint contributed to this success," says Inoue.

The fundamental purpose of computational science is to make predictions

It is unusual for plant workers to permit outsiders to enter the operator room from which operators control a large forging press machine. Why did the JSW workers give the permission to Inoue? One of the plant managers told Inoue, "Steel production technology matured 20 years ago. No new technology has developed since then. Our current focus is to find a way to improve production efficiency and that's not exactly what I call ambitious. Under such circumstances, it is exciting to see someone attempting to develop a new production procedure. Everyone here is interested in such an attempt. Also, such an effort will revitalize the plant, and we perceive it as a very positive move for the JSW."

Until he became involved in the research on the creation of ultrafine grains, Inoue was not particularly interested in commercializing the new steel. But today he says, "As engineers, we are charged with a mission of making our research useful to society. Computational science could be a vital tool in serving such purpose," says Inoue. "That is because simulation technology may drastically speed up the steps from research planning to commercialization, thereby meeting the needs of society quickly."

Inoue concluded at the end, "The fundamental purpose of computational science is to make predictions. The discipline is not only a means to follow up empirical experiments, but also a means to facilitate the understanding of the results of basic research. Then we can propose, predict and verify new phenomena and experimental methods based on computations. That is the true integration between computational science and experimental science."

(by Shino Suzuki, PhotonCreate)

Tadanobu Inoue
Group Leader, Toughness Design Group, Structural Materials Unit, Research Center for Strategic Materials

Round-table talks

Viewpoints of a theorist and computation and experiment specialists

In the scientific research community, there are experiment specialists, who conduct experiments using lab instruments on a daily basis, theorists, who work with mathematical formulas, typically scribbling notes on paper, and computation specialists, who carry out calculations or simulations using a supercomputer. These specialists are in a delicate relationship—they rely on each other's expertise but at the same time, they tend to keep a certain distance. On June 22, 2015, four materials science researchers, including a theorist, a computation specialist and an experiment specialist, took part in a roundtable session at the University of Tsukuba to have a frank talk on such topics as their impressions of each other and their passions for their own studies. Here is how the discussion went.

Jun-ichi Inoue

Senior Researcher
Material Properties Theory Group
Computational Materials Science Unit
Advanced Key Technologies Division

Theorist. His expertise has been theoretical studies of solid-state physics on various materials. His research interest is to give simple picture to physical properties using such tools as quantum mechanics and statistical mechanics.

Tomoya Ono

Associate Professor
Center for Computational Sciences
University of Tsukuba

Computation specialist. For the purpose of developing high-performance electronic devices, he has been studying electronic structures of semiconductor materials using computer simulations.

Hiroshi Sakuma

Senior Researcher
Functional Geomaterials Group
Environmental Remediation Materials Unit
Environment and Energy Materials Division

Experiment specialist as well as computation specialist. Taking into account environmental and energy issues, he has been studying exploitable minerals using both experimental and computational approaches.

Takashi Aizawa

Chief Researcher
Electron Microscopy Group
Surface Physics and Structure Unit
Advanced Key Technologies Division

Experiment specialist. He has been studying physical properties of surfaces and interfaces of single crystals such as graphene, since he was a student of a surface science laboratory at a university.

Unexpectedly, these specialists get along well

Ono: At this session, we are planning to hear the frank opinions of a theorist, a computation specialist and an experiment specialist. I believe that many people can easily imagine what experiment specialists generally do. On the other hand, I imagine it is difficult for them to understand the difference between theorists and computation specialists. What is your opinion on that?

Inoue: To me, it seems that theorists tend to reduce a phenomenon to a simple description by extracting the essence of the phenomenon. On the other hand, computation specialists try to reproduce the phenomenon in more realistic way with a mathematical approach using a computer.

Sakuma: I agree with Dr. Inoue. In other words, computation specialists take specific scientific approach to a phenomenon and use a computer in trying to understand its physical properties. However, the computations cannot be performed without theoretical bases. So, theorists play a role of developing the necessary theoretical bases.

Aizawa: I see theorists as an experts dealing with something beyond my comprehension (laughing), whereas a computation specialist's job is to explain the incomprehensive matter in an understandable manner. I guess the two parties take different approaches in their research.

Inoue: I suppose another way of saying "different approaches," in more specific terms, is that theorists are interested in common features and universal properties, rather than differences, while computation specialists are more interested in differences and uniqueness than common features.

Sakuma: Like Dr. Inoue just said, I, as a computation specialist, get more excited when I find different properties between materials.

Ono: I don't have a feel for the difference in approaches taken by the two parties, owing to the fact that my mentor's academic background was the particle theory. Since all researchers in this field aim to identify a universal law, I believe both theorists and computation specialists feel excitement in a similar manner when they come up with a theory explaining a phenomenon.

Aizawa: How about your impression of experiment specialists?

Ono: To me, experiment specialists are those who tirelessly carry out experiments, collect a huge amount of data, draw conclusions based on the data, and come up with a principle behind the phenomenon they studied. During this process, computation specialists play a role of data analysis for experiment specialists. That is my interpretation.

Sakuma: Supporting experiments is an important role of computation specialists, and as a computation specialist myself, I feel pleasure at experiment specialists finding my work useful. Also, I sometimes envy them when they discover new phenomena that had been unimaginable before through experiments. At the same time, I secretly perceive them as rivals due to the fact that I constantly pursue ways to predict new physical properties and phenomena based on computation results. In addition, there are some instances where researchers can make predictions only with computation approaches, and not with theoretical approaches, so it is vital for the three parties to complement each other.

Ono: I am also a computation specialist and would like to make amazing discoveries. For example, I hope to obtain computation results that totally deviate from the expectations of experimental specialists. Then, I want them to verify the results by conducting experiments. On the other hand, it would be difficult for a computational approach to faithfully reproduce experimental results due to the insufficient performance level of the current computers. As such, computation specialists simplify their computations as much as possible by excluding factors with minor influence from their computations. My vision of skillful computation specialists is those who are able to draw significant results under a given set of constraints.

Inoue: I think there are different types of experiment specialists. There are roughly two types: the first type includes those who perform measurements first, then try to draw some sort of conclusion based on the measurement results. And the other type takes a completely opposite approach: they first determine the expected conclusion, and then they carefully design the experiment in an attempt to obtain the kind of data that is consistent with the expectations. The first type appears to be a good match with computation specialists while the second type seems to get along well with theorists.

Aizawa: I think I am more likely to be the first

type. The most thrilling moments I have ever experienced as an experiment specialist are when I obtained totally unexpected experimental results. I feel great joy making a new discovery.

By the way, Dr. Sakuma said something earlier to the effect that computation specialists cannot perform computations without theoretical bases developed by theorists. What are your thoughts on that, Dr. Inoue?

Inoue: In this day and age when people are always asked to contribute to society, theorists seem to be least practical in real-world settings compared to the other two parties (laughing). The fact is that the theories that are of fundamental importance to computation specialists have been created by a few genius theorists. And most theorists, including myself, are just playing with the theories of the geniuses. In terms of being faithful to real materials, I think experiment and computation specialists are literally contributing more to society than theorists. That said, I always try to build theories useful to society, of course.

Ono: It is true that public expectations are often higher for computation specialists than for theorists in terms of contribution to society. However, I want the public to view science from a longer-term perspective as theorists' support is necessary for computation specialists to make contributions to society.

What promotes joint research among the three parties?

Aizawa: What kinds of matters do the three of you pay attention to when you work with other parties? In my case, I usually cannot draw any conclusion based solely on data collected from experiments. After all, you can't make any sense out of the data without analyzing them. So it is natural for me to work with computation specialists, otherwise, my research won't go anywhere. I choose a computation specialist whom I feel comfortable working with as a research partner.

In contrast, I only have a little interaction with theorists. Recently, new physical phenomena, such as topological insulation, have been discovered one after another, and it is required for us to develop new theories to explain these phenomena. When we try to reproduce these phenomena experimentally, we need a new theory for the analysis of experimental data. So this may be a good opportunity for me to start working with a theorist.

Inoue: I have an experience of working with an experiment specialist when he asked me to come up with a theory that explains his study results since the results appeared to be inconsistent (with existing theories). In this study, our attitude was: let's solve the puzzle together, and this type of project is often carried out collaboratively. In contrast, it is difficult for me to take part in the type of research in which the researchers believe that the study is already thorough and completed. This kind of study is typically presented at conservative seminars.

Ono: When I am involved in experiments conducted by a group of researchers, I take charge of computations at first. Then later, experiment specialists often ask me to work with them. This is usually how I get involved in joint research. In addition, I sometimes get involved in collaborative research during a drinking party or other social gathering. Basically, I always get involved in joint research on casual occasions (laughing).

Sakuma: Up until recently, many experiment specialists did not appear to trust computation specialists very much. In fact, when I showed simulation models of material surface structures to an experiment specialist, they angrily told me, "Don't talk to me as if you have seen the actual material." Today, it is easier for me to work with experiment specialists as mutual understanding between us has been deepening. Lastly, I would like to ask all of you about your future vision. I personally hope that the three parties will build a stronger relationship of trust, complement each other and collaboratively contribute to materials science.

Ono: I want to be the type of computation specialist capable of predicting material physics and designing materials using a computer.

Aizawa: My goal is to make amazing discoveries through experiments. Then I would like theorists and computation specialists to prove my findings on a theoretical basis and establish a new theory. It would also be my pleasure to conduct a specific experiment and develop a new material at the instruction of a computation specialist.

Inoue: I think the true worth of theorists is represented by their ability to identify interesting problems to work on. Today, websites for internet-based retailers are capable of making customer-specific recommendations. Similarly, I have a wild idea that in the near future, scientific journal websites will become able to make recommendations to authors about their next research projects when their manuscripts are accepted for publication. However, I want to be the type of theorist capable of identifying my own creative research projects that the journal websites can't recommend.

(by Kumi Yamada)

Science is even more amazing than you think (maybe...) 8

Computer simulations

In this day and age of modern technology, computers have become very familiar tools to many of us. We use or benefit from various types of computers such as mobile phones, PCs, household electronic products, car navigation systems and highly reliable weather forecasts on a daily basis.

However, the situation was much different 100 years ago; people then did not even dream that the computers would become reality. When they needed to calculate something, they used paper and pencil or an abacus as the most accessible calculation aids. Only few professionals in need of sophisticated calculations such as scientists and architects were able to perform complex calculations using such tools as slide rules.

At the beginning of the 20th century, new scientific and technological discoveries and developments were made in succession, which drastically transformed the ways in which people lived. People wondered how such scientific and technological development and popularization would further affect their lifestyles in the future. Then, some individuals around the world attempted to predict the future. Among them was a French novelist, Jules Verne, whose publication of a future-predicting novel attracted great attention at that time.

Similarly in Japan, one of the newspapers carried a special feature titled "Predictions for the 20th century" in its January 2 and 3 issues in 1901. There were 23 predictions in the feature regarding the kinds of inventions to be made and how they would change people's lives by the end of the 20th century.

Interestingly, some of them came true rather accurately. For example, they predicted, "The development of radiotelegraphy and telephones will enable free communications across the world," "Invention of a new air conditioning machine will enable controlling the temperature of a room within a comfortable range," "Electricity will become a primary energy source," and "The advancement of railroad technology will enable people to travel between Tokyo and Kobe in two and a half hours."

However, mysteriously enough, none of these predictions forecasted the invention of computers. In fact, there was no mention of the invention of rapid-calculating machines that would lead to the development of information society.

Our predecessors 100 years ago did not imagine the advent of computers. However, in reality, the world's first computer came out in 1946 and computer technology has evolved very rapidly. Today, computers are indispensable not only as the heart of information society but also as the frontline tools in science and technology.

In particular, computer simulations are vital means of visualizing atomic behavior in chemical compounds and molecules, studying the structure of the universe, and measuring the resilience of buildings.

For instance, the universe had been thought to be made of matter, that is made up of atoms and molecules and energy. However, it has been discovered in recent years that most parts of the universe appear to be made of dark matter and dark energy, that are unknown to humans. Our understanding of the structure of the universe is making steady progress through computer simulation studies. Also, in the field of weather forecasting, the accuracy and precision of forecasting methods have dramatically improved with the evolution of computer simulations since when meteorologist Lewis Richardson attempted weather forecasting using manual calculations around 1920, and when mathematician John von Neumann succeeded in the first computer-based forecasting in 1950.

Computational science based primarily on computer simulations is probably the most advanced scientific procedure humans invented in the 20th century.

Written by Akio Etori
Title lettering and illustration by Shinsuke Yoshitake

Akio Etori: Born in 1934. Science journalist. After graduating from College of Arts and Sciences, the University of Tokyo, he produced mainly science programs as a television producer and director at Nihon Educational Television (current TV Asahi) and TV Tokyo, after which he became the editor in chief of the science magazine Nikkei Science. Successively he held posts including director of Nikkei Science Inc., executive director of Mita Press Inc., visiting professor of the Research Center for Advanced Science and Technology, the University of Tokyo, and director of the Japan Science Foundation.

NIMS NEWS

1 NIMS researchers awarded the 2015 Gottfried Wagener Prize

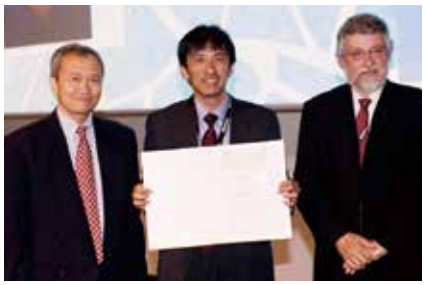
(June 30) NIMS researcher Hossein Sepehri-Amin and Yoshitaka Tateyama won the German Innovation Award "Gottfried Wagener Prize 2015". This award provides support for young researchers in Japan and encourages collaboration between German and Japanese industry and academia. The award was established in 2008 by technology-innovation-focused German companies and the Japan-based German Chamber of Commerce and Industry. To be eligible for the award, researchers must be under 45 years of age and be affiliated with a Japanese university or research institute. The research has to fall within one of the categories of Mobility, Materials, Life Sciences, or Energy & Industry, and must be an applied study that provides innovative and creative solutions.

Sepehri-Amin and his team member Takahiro Akiya, postdoctoral research associate, jointly received the award in the Materials category for the research titled "Development of Dy-Free high performance Nd-Fe-B permanent magnets by engineering of grain boundary phase." Meanwhile, Tateyama, leader of the Nano-System Computational Science Group, and his team member Keitaro Sodeyama (project researcher, Kyoto University) jointly won the award in the Energy & Industry category for the study titled "Theoretical elucidation of reaction mechanism on electrolyte interface in lithium-ion battery with highly-efficient use of supercomputers."

* Affiliations and positions of award recipients are those at the time of reception.

Yoshitaka Tateyama (left) receiving the prize

Hossein Sepehri-Amin receiving the prize.



Masamitsu Hayashi (center) receiving the IUPAP Young Scientist Prize, Professor Xiaofeng Jin (left, Commission Chair) and Professor Burkard Hillebrands (right, Commission Secretary)

2 NIMS Researcher Awarded the IUPAP Young Scientist Prize in Magnetism

(July 7) Senior researcher of the Magnetic materials unit, Masamitsu Hayashi, was awarded the IUPAP Young Scientist Prize in Magnetism at the 20th International Conference on Magnetism (ICM) held at the Palau de Congressos de Catalunya in Barcelona, Spain. This award recognizes outstanding contributions to the areas of magnetism. Hayashi won the prize for "the pioneering work on domain wall dynamics in magnetic nanowires and contributions to the development of current controlled magnetism in magnetic heterostructures using spin orbit effects". His work has contributed to advancing the understanding of electrical control of the magnetization direction of nanoscale magnets, which is a crucial technology for next generation information storage and computation devices.

Hello from NIMS

Hello, my name is Alexandre Fiori, I am French, and I love good food!

I really enjoy living in Tsukuba Science City. The city has a singular implantation of high-technology research centers in an agricultural plain, scattered with rice fields, forests, and residential places. Tsukuba City is a safe place, not too far from Tokyo, and very quiet at night.

Seven years ago, I joined NIMS for an internship under the supervision of Dr. Tokuyuki Teraji, at the wide bandgap semiconductors group, headed by Dr. Yasuo Koide. Since that, I have kept a strong interest in the synthesis of diamond and Japan. I came again to NIMS in 2011, during my Ph.D. course (Neel Institute, CNRS Grenoble). I experienced the big earthquake on March 11, the shortage of commodities, and a fast repatriation to France. Finally, in 2012, I joined NIMS a third time as a JSPS research fellow, and now as an ICYS-MANA researcher.

My research topic concerns the boron doping of synthetic diamond, superlattice architectures, and the study of metal/diamond interfaces.

Alex FIORI (French)
Feb. 2015 - Present
ICYS-MANA researcher

Caption: Enjoying the transient beauty of flowers at NIMS Namiki site. (from left to right : Toshie Mizuno, Alex Fiori, Suzuko Okamoto, Kumi Kurihara, Asuka Sakamoto, Tomoko Kudo, Mayu Nanbu, Shoko Manako).

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