NATIONAL INSTITUTE FOR MATERIALS SCIENCE

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Materials Research by Information Integration

Strategic Plan

Message from
the new President

Kazuhito Hashimoto

Since its foundation in 2001, National Institute for Materials Science (NIMS) had made various efforts toward strengthening its research capability and internationalization under the direction of its first President, Prof. Teruo Kishi, and second President, Prof. Sukekatsu Ushioda. Starting in 2016, NIMS will implement the fourth term of its seven-year plan. In addition to the existing goals of further strengthening its research capability and international competitiveness, NIMS is also accelerating to transfer its research achievements to the society, which I, as a third President of NIMS, consider a central goal.

Today, social expectations for science and technology are greater than ever, and the government considers the promotion of science and technology to be one of its paramount policies. As many people agree, Japan's industry is leading the world in the development of new materials and functional materials, and Japan's materials research that supports the industry is also world-class. Under such circumstances, expectations are high for NIMS to lead advanced materials research and play an active role in providing a foundation for strengthening the R&D competitiveness of Japan.

To meet these expectations, we intend to fundamentally enhance our "mediating function," aiming to accelerate the return of research accomplishments to society. Under the principle that "the true value of materials is in their use," we will continue to focus on building a close relationship with the industrial sector. Furthermore, I strongly encourage researchers at NIMS to be actively involved in the application of their research results to society in addition to their research engagement. This approach is also important in terms of providing researchers with an opportunity to gain new research insights. We will make continuous efforts to transfer our results to the industrial sector for use, and to become a hub to facilitate product R&D in academia and the industrial sector, so that NIMS can strengthen the research capability of the entire nation.

We will also continue to collaborate with organizations specialized in different fields. In particular, promotion of joint research with the information and communications technology (ICT) sector is an urgent issue, as is conformity with the Japanese government's fifth science and technology basic plan starting this year, which states to "strongly undertake a series of initiatives to realize the future vision of super-smart society (Society 5.0), which is an elaborate fusion of cyberspace and physical space (the real world)." NIMS founded the Center for Materials Research by Information Integration where initiatives have already been taken to fuse materials research with data science. As for future plans, through various activities, we intend to fuse materials research with ICT, thereby creating new research fields and industries.

Engaging in these endeavors, I hope that NIMS will further grow as an organization contributing to Japan and the international community. We would appreciate your support.

Sincerely,

Special Talk

Tripartite

MI^2 : A new trend in materials research

On July 1, 2015, the Materials Research by Information Integration (MI^2) Initiative (MI^{2}I) based at NIMS, was launched within the framework of JST's Support program for starting up innovation hub. The purpose of the initiative is to establish open innovation hubs to facilitate the R&D of new materials using a data science approach. Collaboration efforts are extending across different sectors, including industries, universities, and research institutes. Discussion was held on the circumstances behind the launch of MI^{2}I and plans for future activities by three panelists: director-general of the Institute of Statistical Mathematics, Tomoyuki Higuchi, representing all research institutes involved; JST program manager Satoshi Itoh; and Center for MI^2 (CMI^2) director Kiyoyuki Terakura.

* Throughout this article on the three-man talk, materials research using computational and data sciences are consistently referred to as "MI^2."

Tomoyuki Higuchi

Director-general, Institute of
Statistical Mathematics,
Research Organization of
Information and Systems

Kiyoyuki Terakura

Director, Center for Materials Research
by Information Integration
National Institute for
Materials Science (NIMS)

Satoshi Itoh

Program Manager,
Department of Innovation Platform
Japan Science and
Technology Agency (JST)

Accelerating materials research using the "fourth science"

Terakura: First, I would like to talk about how MI^{2}I has been started at NIMS. The key event that inspired MI^{2}I was the Materials Genome Initiative (MGI), which effectively started in the United States in 2012 after President Obama unveiled the plan in 2011. MGI is a national project endorsed by the U.S. government with a huge budget, aiming to promote materials informatics (MI). MI is a coined term likened to "BI" (bioinformatics), and its objective is to search and develop new materials in short time and at low cost using data science. Data science is considered to be the fourth paradigm for science, after experimental, theoretical and computational sciences. The U.S. took this initiative with strong motivation to restore the competitiveness of its manufacturing industry, which had fallen behind Japan and Germany, by taking full advantage of IT. Other countries, such as those in Europe, China, and South Korea, are also taking similar initiatives. Japan's first response to these movements took the form of a workshop hosted by the JST's Center for Research and Development Strategy in February 2013.

By the way, we name the initiative "Materials Research by Information Integration" Initiative (MI^{2}I) as its intention was more than just the use of "Informatics." In the term "MI," emphasis is given to the "I" part representing informatics. But we are rather aiming to conduct materials research using more tools than just informatics. Based on this idea, we decided to call it "MI^2" (materials research by information integration) rather than "MI." So I would like to use the term "MI^2" in this talk, consistently to mean materials research using not only data science but also experiment, theory, computational science.

Higuchi: I believe that data science refers to scientific methods for data analysis, such as statistics, machine learning, optimization, and data mining. The increasing interest in MI^2 among people in the materials field is attributed to the fact that data science is becoming practical as big data is now used in various fields. I first encountered MI^2 in May 2008. At that time, I was conducting research on "data assimilation," by combining observational data with simulation models. That is when I was called by Professor Terakura, who was then working at Japan Advanced Institute of Science and Technology (JAIST), to exchange opinions. There, I was introduced to MI^2 for the first time. I remember that, during our conversation, we really weren't on the same wavelength (laughing).

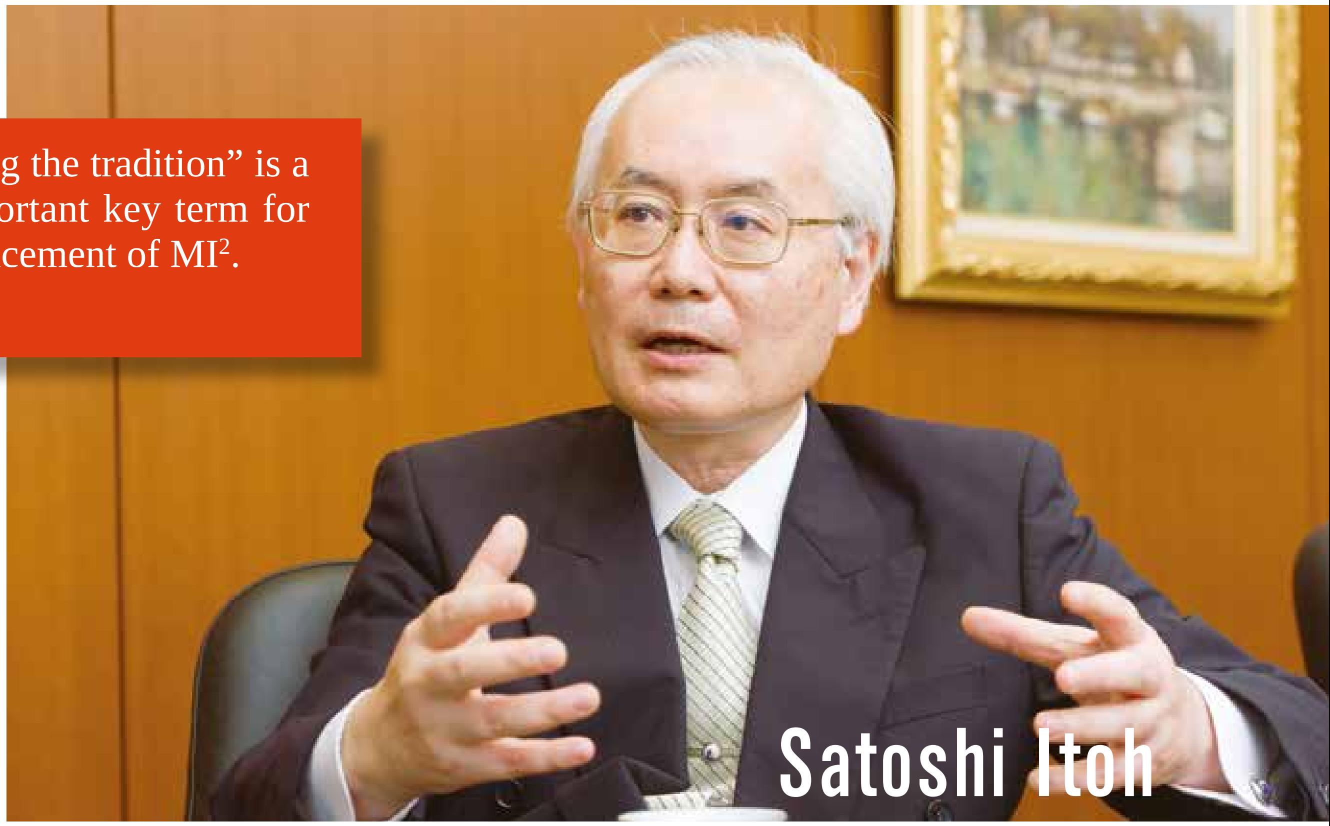
Terakura: I had an idea similar to MI^2 from around 2001. Then, I felt strongly that I could put the idea into practice when I moved to JAIST in 2007. After being exposed to leading-edge research on simulations, mathematical logic, and data mining, I had a hunch that material design may be accomplished by integrating these three methods.

Itoh: Since I worked at a company for many years, I am aware that the industrial sector has been using MI^2 since very early times for product development. Especially, chemical and medical companies implemented it very early. For the development of agrochemicals and drugs, hazard assessment is essential. However, since it is difficult to test promising compounds by going through all kinds of biological experiments, those companies strived to improve the efficiency of R&D using technology similar to MI^2.

Manufacturers rely heavily on the experience and intuition of talented researchers and technicians for R&D activities, and I think this practice delayed the implementation of MI^2 into manufacturer's systems. However, they have realized that they cannot maintain competitive superiority if they keep practicing conventional methods, due to the issues of successor shortage and intensifying global competition in recent years. I think electronic manufacturers came to this realization before anyone else.

Conversely, materials manufacturers seemed to practice conventional methods to the last. That is because it takes more time for them from the R&D phase to commercialization, compared to manufacturers in other fields. It is challenging for materials manufacturers to discover totally new materials or new functions in existing materials in the first place. Furthermore, considering that they also need to put mass production technology in place, it takes them 30 to 40 years from the discovery to commercialization. However, motivated in part by the movements in the U.S. and China, Japanese materials manufacturers have finally become serious about incorporating MI^2 into their systems for quicker product development.

> Purposes of implementing MI^2 are to discover new materials and to make the R&D process intelligent.
>
> Tomoyuki Higuchi



> "Changing the tradition" is a very important key term for the advancement of MI^2.
>
> Satoshi Itoh

The role of MI^2 is like a treasure map

Higuchi: The purposes of implementing MI^2 are two-fold: to discover new materials and to make the R&D process intelligent. I think that materials manufacturers are interested in MI^2 mainly because they have been concerned about losing ground in global competition unless they go through the PDCA (plan–do–check–act) cycle more quickly. However, MI^2's capability varies greatly in terms of achieving these two purposes—MI^2 tends to be more useful in making the R&D process intelligent, and discovering new materials using MI^2 would be very challenging.

Terakura: My understanding is that the role of MI^2 in materials research is to solve inverse problems. Conventional materials R&D had been taking the approach of identifying the characteristics and functions of given materials, in other words, researchers were solving direct problems. In contrast, inverse problem solving addresses the question, "Which materials have desirable characteristics and functions?" MI^2 is the first means to efficiently solve inverse problems.

Recently, a company researcher asked if we would be able to make MI^2 perform like a treasure map. This metaphor is a good representation of the inverse problem solving approach. We are hoping that MI^2 will become capable of specifying target material groups from which we can search for optimum materials with desirable characteristics and functions.

Higuchi: On the other hand, MI^2 also has some issues of concern. Particularly in the materials field, experimental, theoretical, and computational science researchers had a strong tendency to work independently. So, to promote MI^2, it is vital to create a new framework that facilitates the integration of these different types of research and to have strong leadership.

Terakura: I totally agree with you. The aim of MI^{2}I is to create a platform for achieving those things.

Higuchi: It is especially important for experimental researchers to have deep understanding. There is a lot of world-class laboratory equipment at NIMS and valuable experiments are conducted daily. Until now, most unused research data had been discarded. However, from now on, it is important to save all data including those collected from failed experiments in order to boost MI^2. But if you store all data, like video data taken by surveillance cameras, on servers or in a database, data management would be very difficult, and it may be impossible to find the data you are looking for when you need it. For this reason, it would be essential to incorporate “edge-heavy computing,” which enables data compression and saving in the form corresponding to use purpose, into MI^2.

Changing the tradition is the key

Terakura: Valuable data is collected daily not only using laboratory equipment at NIMS, but also at other large facilities such as K supercomputer, post-K supercomputer, SPring-8, and J-PARC Center. However, most of the collected data is not used effectively. To improve the precision of artificial intelligence (AI), such as machine learning and deep learning, it is necessary to change the conventional practice and start saving unused data. But that is not easy to do.

Itoh: “Changing the tradition” is a very important key term for the advancement of MI^2. To realize this, it is vital to create a system by which data providers receive incentives. If active data providers are not benefited, or are even harmed, data collection will fail. People in the materials field are most reluctant to establish open data. In particular, since experimental data is the lifeline of competitiveness for materials manufacturers, it would be difficult to make data open in the immediate future. But looking toward the future, it is necessary to draw up long-term strategies, such as developing a business model by which a company’s profit increases as it provides more data, and changing the way researchers are evaluated in academia. The MI^{2}I has set up three applied research areas—battery materials, magnet and spintronics materials, and thermal management and thermoelectric materials—that are likely to have a widespread social impact. I hope that at least a few successful cases will emerge in this framework. I wish I had more ideas for promoting MI^2.

Higuchi: I suspect that the U.S. and other countries are putting forward the implementation of open data because they feel that their R&D enterprises have reached a plateau or deadlock situation. I speculate that they have come to the conclusion that different organizations must courageously share their data as only this approach allows them to break through this stagnant situation.

Itoh: In fact, until recently, many of Japan’s major companies believed in their capability to develop products independently. However, looking at the fact that national project applications by major companies are increasing these days, I assume that the industries are beginning to think that they cannot globally compete by solely relying on their own resources. Japan’s R&D budget is generally an order of magnitude lower than those of Europe and the U.S. I think Japan’s industries have to work together in solidarity.

Terakura: The Japanese government has to take the same approach to support MI^2. While the U.S. has allocated a huge budget for the federal government-led MGI, Japan has to implement MI^{2}I using a budget which amounts only to less than 10 percents of the MGI budget. We cannot resolve this issue by ourselves. We need to come up with ideas to address this issue.

Japan’s strength: database and collaborations in mathematics

Itoh: In Japan, JST and others have been building a materials database since around 1995. How do you think Japan should take advantage of its strengths, such as the database, in competition with other countries ?

Terakura: My view of the United States’ MGI is that they are trying to search for new materials through the approach of solving direct problems using simulations, as their materials data is not abundant enough. In contrast, Japan’s MI^{2}I is taking the strategy of solving inverse problems by using NIMS’s world’s dominant materials database MatNavi and AI from the beginning, through close collaboration among materials scientists, data scientists as well as mathmaticians. I consider this approach unique to the MI^{2}I to be Japan’s greatest strength. However, the U.S. has been conducting advanced AI research, and I am not sure how long we can sustain its superiority. What is your opinion in this regard, Dr. Higuchi?

The role of MI^2 in materials research is to solve inverse problems.

Kiyoyuki Terakura

Higuchi: I am not concerned about that. Much of what AI technology people are making a fuss about these days refers to deep learning, which requires a huge amount of data to estimate numerous parameters. So far, the MGI team has not acquired enough data to run deep learning programs. As such, I think the right strategy for us in implementing MI^{2}I is to keep strengthening MatNavi by continuing the collection of valuable experimental data while establishing collaborative relations with experimental researchers and computational science researchers, and by using edgeheavy computing.

Itoh: In the U.S., it is true that collaborative work in mathematics is going slow and almost no industries are involved in the project. I feel that we are certainly doing a better job in these regards through MI^{2}I. However, I expect that the human resources development will be a major issue for us in the future.

Terakura: I agree. I heard that in China, Shanghai University has already created a materials research course in which computational and data sciences are applied. Japan also needs to take a similar initiative as soon as possible. Amid the situation, Professional development Consortium for Computational Materials Scientists (PCoMS) was set up at Tohoku University after the plan was adopted by the government of Japan. We are planning to coordinate with PCoMS.

Related to that, NIMS is also conducting a project in the field of materials integration under the Cross-ministerial Strategic Innovation Promotion Program (SIP), led by the Cabinet Office. Similarly to MI^{2}I, they are using simulations and data science for this project, whose primary purpose is to accelerate the development of structural materials. While there are some differences in purposes between this project and MI^{2}I, I hope for collaboration between the two in some aspects, such as the creation of development methods.

As an MI^2 hub center, MI^{2}I is aiming to speed up R&D activities through organic interactions among all researchers involved in materials research across different organizations. At the same time, we are planning to prepare a database, develop various kinds of software and foster human resources. Two or three decades ago, computational science was not considered to be dependable, but is now viewed as an essential third scientific method. Likewise, I am confident that MI^2 will also be considered as an indispensable tool in the near future. I hope that more people will show their understanding and support toward MI^{2}I.

(by Kumi Yamada)

Global Movement MI^{2}I

Global Trends in Materials Research Using Computational and Data Sciences

In 2011, the president of the United States declared the launch of the Materials Genome Initiative (MGI), and projects with a huge budget were kicked off in 2012. Thanks to this initiative, materials informatics (MI) has been quickly drawing worldwide attention. Since about 10 years ago, Japan also has been conducting studies on MI, and in 2015, the "Materials Research by Information Integration" Initiative (MI^{2}I), based at NIMS, was launched. Here, we report the current trends in related research conducted in some major countries.

Interviewees

Hiromoto Shimazu
Fellow, Center for Research and Development Strategy (CRDS), Japan Science and Technology Agency (JST)

Yibin Xu
Group Leader, Materials Database group, Materials Information Station, NIMS

Yukinori Koyama
Principal Researcher, Materials Informatics Platform, NIMS

Takuya Kadohira
Senior Engineer, Materials Informatics Platform, NIMS

The MGI in the U.S. inspired the inauguration of MI^{2}I projects

In Japan, MI^{2}I, based at NIMS, was started as a part of the Support program for starting up an innovation hub sponsored by the Japan Science and Technology Agency (JST). In addition, to promote MI, two research projects were launched: the Cross-ministerial Strategic Innovation Promotion Program (SIP), led by the Japanese government's Cabinet Office, and JST's Strategic Basic Research Programs (specifically PREST). The U.S. declaration of the MGI in 2011, for which a huge budget was invested by the U.S. government, inspired these Japanese projects.

The purpose of these projects is to realize quicker development of materials at lower cost by combining the use of data with conventional experimental and computational tools.

The U.S. government views the MGI as a part of the Advanced Manufacturing Partnership initiative. The purpose of this association is to restore U.S. manufacturing industries, which have fallen behind Japan and Germany, by making full use of data science in which the U.S. excels. The U.S. has taken this action out of a strong sense of crisis in terms of job security, assuming that the IT industry will not provide enough jobs to its people. The U.S. established the MGI to primarily promote materials research as materials production plays a particularly vital role in the manufacturing industry.

At present, such institutes as the National Science Foundation (NSF), the National Institute of Standards and Technology (NIST) and the Defense Advanced Research Projects Agency (DARPA) are promoting the MGI projects in coordination with federal departments and agencies under the direction of the Office of Science and Technology Policy (OSTP). The NSF forms and expands the MGI-related communities and fosters human resources; the NIST unifies research bases involved in MGI projects and develops various tools; and DARPA implements challenging research programs funded by the federal budget, assuming military applications. Also, the Department of Energy (DOE) is heavily involved in the projects. NIMS's Takuya Kadohira explains that "When the MGI was first proposed, it was declared that it had four focuses: clean energy, human welfare, national security, and next generation workforce. After three years, National Science and Technology Council determined the MGI strategic plan, in which nine types of materials including energy storage, lightweight and structural materials, also known as materials indispensable for sustainable societies, were focused on. Thus, it is obvious that the DOE is a major player in the MGI projects."

Integration of MGI-related projects by the U.S. government

Hiromoto Shimazu at the JST Center for Research and Development Strategy, who paid attention to the MGI from early on and made exertions to launch the related projects, explains that "There are three processes (communities)* that played a major role in the inauguration of the MGI. I presume that the U.S. government's idea was to achieve synergy and accelerate R&D by placing these three communities under the same umbrella."

The main processes under the MGI umbrella are called the "materials project" and "CHiMaD." The former has been carried out by a community led by Massachusetts Institute of Technology. The community mostly conducts prediction and search of functional materials. It has made major accomplishments in search of materials for lithium-ion batteries, which resulted in increased public awareness about the MGI. The latter project has been carried out by another community led by Northwestern University, which mainly conducts prediction and search of structural materials. This community contributed to the development of Ultra-High-Strength-Alloy to be used for airplane landing gears.

While the approach of the former community is to predict the physical properties of materials at atomic and nano levels, the approach of the latter community is to identify the physical properties of materials by integrating experiments and multiscale simulations.

Placing these communities under the same umbrella allows them to more clearly understand each other's materials research projects, and allows them to engage in active interactions between projects. It is expected that these arrangements will produce synergistic effects, allowing the fusion of multilevel studies at atomic, nano and macro levels and the broadening of application fields.

Similar projects were also launched in Europe, China and South Korea

In response to the MGI projects carried out in the U.S., similar projects have been initiated successively in Europe (by the EU and Switzerland).

The "materials modeling" project that launched in Europe aims to build an open platform available for the industries to conduct one-stop materials R&D. In particular, taking advantage of Europe's strength in computational science, the project's target was set to develop simulation technology capable of integrating multiscale studies ranging from nano to macro levels, and to promote industrial use of the technology. Furthermore, an additional goal of the project is to conduct prediction and search of functional materials using first-principles calculations. The main end products of the research are energy and ICT materials and drugs. An excellent system called "AiiDA" which performs automated calculations of electronic state in materials, was also developed by a Swiss research institute and others.

Yukinori Koyama at NIMS explains that "In Europe, the group taking computational science approach and the other group taking data science approach, work collaboratively to complement each other's results."

In Asia, China and South Korea have taken a major step. China in particular was inspired by the MGI in the U.S. and founded its own "China MGI," aiming to gain power in materials research.

What is notable about China is that several projects have been launched at a municipal level, not a national level, in cities such as Shanghai and Beijing. For example, materials genome research facilities were established at Shanghai University in April 2015 through financial support from the Shanghai municipal government and at the University of Science and Technology Beijing in May 2015. Furthermore, a private facility for international materials genome research was founded in Ningbo in September 2015. China intends to grow these local-level projects into national-level projects by accumulating results at each local facility.

China is also strengthening coordination with the U.S. "Given that Chinese students currently account for a large proportion of university students in the U.S., the relationship between the U.S. and China is rapidly deepening. Taking advantage of this situation, Chinese institutions such as Shanghai University have been inviting American professors to give lectures on materials research using computational and data sciences," explains NIMS's Yibin Xu. In fact, the facility in Ningbo was established by a Chinese researcher who studied in the U.S.

Assuming that the importance of materials research using computational and data sciences will increase, the matter of most serious concern is that there may not be enough workers in this field in the future. China is already looking into addressing this issue, assuming the situation in a decade or two, and making focused effort in creating more research facilities and fostering human resources.

Japan should more actively collaborate with Asian countries.

At present, while the U.S. is slightly leading other countries in this field, all relevant countries are nearly in the same position as they just took a first step. To prevent Japan from falling behind other countries, we should promote government-led projects like the U.S. does and begin fostering human resources at an early time like China does.

(by Kumi Yamada)

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* Three processes that played a major role in the initiation of the MGI

1. Process to identify materials with desirable performance and functions by creating data mainly using first-principles calculations.
Fuse the following three elements: a big data processing environment, various analysis tools based on data science, and a database based on experimental and computational sciences.

2. Process to conduct integrated computational materials engineering
Integrate primarily structural materials of different scales ranging from the crystal structure level (first-principles calculations) to the microstructure level while taking into account relationships of the materials with the process and its microstructure.

3. Process to conduct combinatorial synthesis and measurements.
Create materials using a high-throughput approach and measure them.

MI Report-1

Producing Outstanding Results Using MI

What can we actually do with Materials Informatics (MI)?
Kyoto University Prof. Isao Tanaka has produced a number of excellent research outcomes using MI, including the discovery of many materials with very low thermal conductivity, in a very effective fashion. We asked Prof. Tanaka about some of his successful studies using MI.

Difference between rotary dial phones and smart phones

── MI is rapidly attracting attention. How do you view this situation?

Tanaka: My impression is that while many researchers are aware of what MI is, they seem to be hesitant to introduce MI into their studies due to their unfamiliarity with it. For example, can you tell what has changed as rotary dial phones were replaced with smart phones? The basic functions of the phone per se have not changed much. But the amount of information one can gain from the phone has increased drastically. Rotary phones still work fine today if they are used only for making telephone calls. But for those who don't want to fall behind in certain businesses, a smart phone is a critical tool. Similarly, you can develop materials using conventional methods, but if everyone else starts using MI, you cannot compete. It is not difficult to understand the advantages of using MI. In traditional materials science, researchers rely on their own experience and ideas to carry out research. But by using MI, you have access to the power of information science, which will greatly expand the information available to you.

Extending the life of lithium-ion batteries by six times

── You have been engaging in materials development using MI since early days. Could you give us some specific examples of your accomplishments?

Tanaka: One example would be the development of a cathode material for lithium-ion batteries. Associated company members and I jointly conducted research to extend the lifetime of lithium-ion batteries used to store electricity generated by household solar panels. My research partners thought that capacity degradation of lithium-ion batteries is caused by repeated expansion and contraction of the cathode material—lithium iron phosphate ($LiFePO_4$)—resulting from exposure to the charge and discharge cycle. They also thought that they might be able to reduce the extent of volume change occurring in the cathode material by substituting some atoms in $LiFePO_4$ with other elements. However, there are limitless combinations and ratios to be selected for substitution. It is impossible to synthesize and test every possible combination in experiments. So, I decided to search for the right combination using MI.

── What kind of calculations did you perform?

Tanaka: I carried out so-called first principle calculations by which I computed the behavior of electrons based on quantum mechanics (first principle). These results allowed me to determine the structure of the material. Once the structure was known, I could calculate the volume. I first determined the structure of the material after some atoms in $LiFePO_4$ were substituted with other elements. Based on that structure, I then calculated the structure after the separation of Li. Comparing the two structures, I calculated the change in volume. I conducted these calculations for 2,000 different structures resulting from substituting different combinations of elements and their ratios. Through this process, I was able to identify materials that undergo a very small volume change.

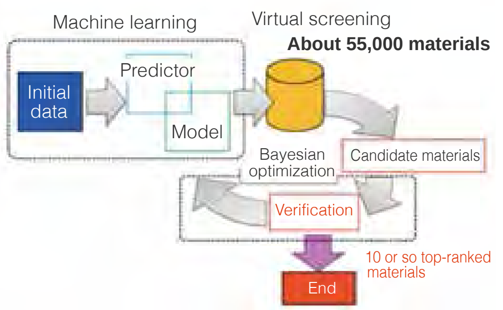
We synthesized a material with the optimum composition determined by the calculations and examined its charge-discharge characteristic and other features. I was very nervous while waiting for the results. When we found that the synthesized material has six times longer life than $LiFePO_4$, I felt relieved at last. The material was very difficult to synthesize. And the person in charge of the synthesis told me that he would not have tried to create that material without the computational evidence. This success is attributed to an advantage of using MI. Once a material difficult to synthesize is successfully produced, the synthesis usually becomes easier as it is repeated.

Discovery of various materials with low thermal conductivity

── In November 2015, you successfully identified various kinds of materials with low thermal conductivity using MI. Why did you focus on thermal conductivity?

Tanaka: Because very little calculation efforts had been made in that aspect. In fact, first principle calculations are used to determine the state of materials at absolute zero (−273.15°C). But since we don't handle materials at absolute zero, those calculations do not make sense. For this reason, we developed a computer program in which a user can specify the value for heat in first principle calculations. Since heat is conducted by lattice vibration, the program we developed called Phonopy (pronounced phono-pie) performs calculations of lattice dynamics based on first principle calculations and enabled systematic calculations of thermal conductivity for the first time in the world.

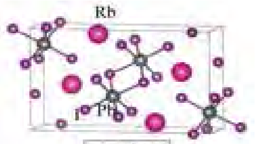
There is an inorganic material database, which covers about 55,000 registered materials. We attempted to search for materials with low thermal conductivity in the database using Phonopy. However, since calculations of thermal conductivity were very complex and time-consuming, it was impossible to conduct precise calculations on all of the registered materials. So, we first precisely calculated the thermal conductivity of about 100 materials, and based on these results, we built a simple thermal conductivity estimation model based on a machine learning method. Then, we applied that model to the 55,000 different materials and ranked them according to thermal conductivity. This sort of procedure, in which a simple model is used to select the most desirable materials rather than conducing precise calculations for each and every material, is called virtual screening. While virtual screening is commonly used in the development of pharmaceutical products, it has been seldom used in inorganic materials research.



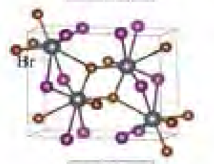
Steps in virtual screening

Conduct precise calculations on about 100 different materials and prepare initial data. Build a relatively simple estimation model based on a machine learning method and rank all materials in the library according to the outcome of running the model. Conduct precise calculations on top-ranked materials and verify the model. If the model is not accurate, correct it and repeat the virtual screening.

Ranking	Score	Compound	results of thermal conductivity calculations (W/m·K)
1	1.90	$PbRbI_3$	0.10
2	1.76	PbIBr	0.13
3	1.56	$PbRb_4Br_6$	0.08
4	1.56	PbICl	0.18
5	1.56	PbClBr	0.09
7	1.44	$PbI_2(R\,3m)$	0.29
8	1.43	$PbI_2(P\,6_3mc)$	0.29



$PbRbI_3$



PbIBr

Results of thermal conductivity virtual screening

We included 54,779 different inorganic compounds in our study. The ranking based on the model and the outcome of precise thermal conductivity calculations were somewhat inconsistent in terms of ascending order. However, the fact that all of the top-ranked materials had low thermal conductivity confirms that virtual screening was conducted soundly. The structures of the materials, which were confirmed to have low thermal conductivity based on precise calculations, are shown on the right.

* "Scores" represents estimated thermal conductivity obtained from the simple model.
Values of scores increase as the value of the predicted thermal conductivity decreases.

Isao Tanaka
Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University

Then, we determined the thermal conductivity of 10 or so top-ranked materials by carrying out precise calculations for each of them. Our plan was that if the calculation results are greatly inconsistent with the ranking, so that the simple model is not accurate, we would correct the model and run the virtual screening again. We would repeat this process until sufficient consistency is achieved between the calculation results and the model. In this study, we succeeded in identifying various materials with thermal conductivity of 0.10 W/mK, which is one order of magnitude smaller than the lowest conductivity of the conventional material. These results will greatly increase the choices of materials to be used as heat shields or for thermoelectric conversion.

Three purposes of MI

── There are high hopes for MI to facilitate the discovery of new materials

Tanaka: Application of MI is clearly useful for searching for new materials, but I am concerned that if we speak too much of that aspect only, it might trivialize the power of MI. In fact, I consider that MI has three purposes: discovery of new materials, discovery of materials' structures and discovery of laws related to materials. Once we identify the structures of materials, we can also reveal characteristics of the materials. Furthermore, if we recognize laws associated with the materials, we can design materials with desirable functions. Discovering these laws is of the greatest importance.

── Japan is said to be behind in the application of MI compared to some other countries.

Tanaka: Japan has been one of the world's leaders in terms of the productivity of the materials industries. Japan had been very successful in this area while practicing traditional methods. That might be a reason for the delayed introduction of MI. However, if other countries discover many new materials using MI and obtain basic patents for them, Japan's chances of competing internationally in this area would rapidly deteriorate. We cannot keep using rotary phones forever.

── What are your expectations for the "Materials Research by Information Integration" Initiative (MI^2I) at NIMS?

Tanaka: I hope that the center will fully demonstrate its hub function and disseminate MI-related information to materials industries. NIMS should provide a venue where industry people can learn MI methods so that they can apply them to materials development at their bases.

I also strongly hope that NIMS will provide training to prospective MI users. We need the type of people who are not only familiar with computational and information sciences but also have ample interest in materials science. Only those who are diligently studying certain materials can identify what types of characteristics need to be supplemented in those materials. Computational and information science specialists would not be able to make these kinds of critical decisions by themselves.

Since NIMS has researchers specialized in various materials such as structural materials, functional materials, magnetic materials, battery materials and catalyst materials, I hope that they will work together to take initiatives.
(by Shino Suzuki, PhotonCreate)

MI Report-2

MI as Viewed by Businesses

What are businesses’ views on materials informatics MI?
What changes may occur to the scene of manufacturing if it is introduced?
What is required to make materials informatics work?
We asked Mr. Susumu Umemura from Toyota Motor Corporation.

Susumu Umemura
Director, General Manager,
Material Engineering Management Dept.,
Material Engineering Field,Toyota Motor Corporation

A sense of crisis to be left behind

— What do you think businesses’ views on MI are?

Umemura: My feeling is that if we do not incorporate MI into our system, we might not only be left behind in market competition but also put ourselves in challenging situations in terms of producing automobiles and surviving in the business. That is how severe my sense of crisis is.

While automobile industries are making progress toward realization of autonomous driving, more and more IT industries are moving into this area. That is really threatening to us. IT industries take actions very quickly. For example, in the automobile industry, minor model changes take place every three years or so, and major changes every six years or so. In comparison, cell phone models change every half to full year. Since customers have become accustomed to the frequent changes, we must dramatically shorten development time of new materials from the current 10 to 20 year period. I believe that MI is the key player enabling us to achieve that.

— What are the differences between the automobile and IT industries?

Umemura: IT industries collect and use big data comprising all sorts of data from around the world, thereby creating new values. We also have accumulated a large amount of data while making automobiles for over 70 years. But I cannot say that we are effectively utilizing the majority of our data. Pharmaceutical industries achieved a breakthrough in dramatically cutting down on the time it takes to develop new drugs by using “bioinformatics.” I strongly advocate the use of the same principle in materials development.

— It has been noted that Japan is behind Europe and the United States in the introduction of MI.

Umemura: That is certainly true. Toyota developed a material for an all-solid lithium-ion battery, which is long-lasting and very safe, by replacing the liquid electrolyte with a solid one. The patent granted for that invention was published in 2012. Immediately after that, Massachusetts Institute of Technology (MIT) and a South Korean firm jointly announced that they discovered a battery material with the same composition. It took us five years to develop the material by following a conventional experiment-based procedure. But I heard that it took them only about one year to discover the material using MI. I was utterly shocked. For this material, we were able to acquire the patent before them, but if we continue to practice the conventional way of materials development, I am afraid we will not survive the competition.

The meaning of Material“s” Informatics.

— What will the contribution of MI to the automobile industries be?

Umemura: The automobile industries have put forward three key terms: weight reduction, electric vehicles and smart vehicles. While we have not taken specific initiatives yet, we think that MI will contribute to the realization of these three terms.

Weight reduction is indispensable to achieve better gas mileage. Older cars were made mostly of iron, but recently, light materials such as aluminum and resin have begun to be used. Since it is not feasible to use a single material for all automobile parts, we intend to use multiple materials, that are suitable for each part. To this end, we need to develop a technology to bond and join different types of materials. We have been experimentally creating adhesives with which we successfully bonded aluminum and iron together and aluminum and resin together, but we failed to bond resin and iron together. We often encounter these sorts of unsatisfactory results, which force us to restart the adhesive development process all over again. While repeating this process over and over, 10 years seems to pass very quickly. In comparison, with the aid of MI, it is possible to predict the composition of an adhesive capable of bonding aluminum, iron and resin altogether by consulting data collected during past adhesive development projects and basic data related to materials on which information has already been released. This approach should greatly reduce development time of new materials.

I think it is meaningful that the plural form of “material” is adopted in the term “materials informatics.” MI is truly useful if datasets for many materials can be accessed and compared.

Integrating all datasets from development to commercialization

— What are your expectations regarding the contribution of MI to the development of electric vehicles?

Umemura: To reduce carbon dioxide emission, advancement has been made in R&D of electric vehicles, from gasoline vehicles to hybrid vehicles to plug-in hybrid vehicles to electric vehicles and to fuel-cell vehicles. The development of battery materials needed for the realization of electric vehicles is rapidly advancing. But I believe that the application of MI will enable us to make even greater improvement in the performance of materials. I think there are two benefits to the application of MI; first, we can reduce the time it takes to develop materials, and second, we can produce innovative materials, which would be unimaginable if we were to rely entirely on experiments and our own knowledge. MI may bring breakthroughs in the development of battery materials.

— How does the development of smart vehicles relate to materials development?

Umemura: You might think that the term smart vehicle means autonomous driving, but that is not all there is to it. We intend to collect all sorts of data while driving a car. Then, using the vast amount of data, we plan to develop materials to optimize, for example, the hardness and the type of seat materials and fragrance in the vehicle, thereby creating a comfortable driving space.

— Does MI have advantages specific to manufacturing industries?

Umemura: I think MI has a lot of potential other than its usefulness in materials development. When we develop high-performance materials, they are often found to be incompatible with the existing manufacturing process. We deal with this situation by either adjusting the manufacturing process or improving the materials. Despite these efforts, many materials ended up being wasted. We have been producing automobiles following the concept of a production management system called the Toyota Production System. We obtained a vast amount of data through this procedure. Combining this dataset with a dataset associated with car driving, we might be able to predict the relationships among the type of material used, the type of manufacturing process used, and the performance of the car produced. I envision that MI may allow us to realize this sort of great dream.

Need for database compatible with MI

— What are your expectations for the “Materials Research by Information Integration” Initiative (MI^{2}I) at NIMS?

Umemura: I am still learning what sorts of data we need to collect and what kind of database we have to set up in order to take advantage of the full functions of MI. I need to know the form of database that works most effectively with MI. Instead of the conventional practice in which each organization accumulates its own data, it is necessary for industries, universities and research institutes to share their data for the sake of producing better products faster. This sort of change in the way of thinking is vital. However, to maintain the market competitiveness of individual organizations, it is necessary to classify data so that participating organizations can make decisions as to which type and range of data should be publicized. The United States has mastered this procedure, so we should learn from it. Also, while this might be difficult to practice, the preparation of a database to be shared should involve international participants, and not just domestic participants. I think such approach may facilitate the development of even superior products.

— Regarding the introduction of MI, do you think Japan can catch up to the world leaders?

Umemura: Japan has a large amount of good-quality datasets. If we can integrate these datasets and take full advantage of them, I think Japan has a chance to outcompete other countries. This is the perfect time to take initiatives to that end.

(by Shino Suzuki, PhotonCreate)

NIMS FORUM
PANEL DISCUSSION

Japan's Leading Figures of MI talk about

A new phase of materials development brought by MI

On October 7, 2015, a panel discussion on materials informatics (MI) took place in NIMS Forum, which was held at Tokyo. Under the theme "a new phase of materials development, resulting from MI introduction," the discussion was moderated by Kiyoyuki Terakura, the project leader of "Materials research by Information Integration" Initiative (MI^{2}I), and was joined by six panelists representing industry and academia, including Professor Hideo Hosono of Tokyo Institute of Technology. Here, we report the content of the discussion.

Hideo Hosono
Professor,
Materials & Structures Laboratory / Materials Research Center for Element Strategy,
Tokyo Institute of Technology

Masato Okada
Professor,
Graduate School of Frontier Sciences
The University of Tokyo

Akira Manabe
Special researcher,
Center for Materials research by Information Integration (CMI^2), NIMS

Tomio Iwasaki
Chief researcher,
Research and Development Group,
Hitachi, Ltd.

Shinji Tsuneyuki
Professor,
School of Science,
The University of Tokyo

Toyohiro Chikyo
Principal investigator,
Nano-Electronic Materials Unit,
MANA, NIMS

Kiyoyuki Terakura
Director, Center for Materials research by Information Integration (CMI^2), NIMS

The role of MI^2 in materials development

Prior to the panel discussion, Prof. Hideo Hosono of Tokyo Institute of Technology gave a keynote lecture titled "The Development of New Materials through Pioneering Research."

At the beginning of his lecture, Prof. Hosono explained that there are three interconnected approaches to materials development: search (intuition), theories and models (brain), and processes (physical work) (Fig. 1). He stated that applying MI between the "theories and models" and "processes" is very useful, as doing so may reduce the developing time by half.

On the other hand, "search" to discover new revolutionary materials requires keen observations involving all five human senses and inspiration gained from excellent researchers. These elements are irrelevant to MI. He concluded his lecture by suggesting that materials researchers should focus their efforts on "search," which cannot be achieved by MI.

Then, Prof. Masato Okada of The University of Tokyo, who is a physicist and data scientist, gave a lecture. In his speech, he stated, "MI is a means to identify automatically how the essential characteristics of materials is determined by the feature quantity, using data. In other words, MI makes our regular efforts more efficient."

The next speaker, Akira Manabe of NIMS, who previously worked on materials development at Toyota Motor Corporation, gave a brief lecture titled "MI^2 as viewed from the application: expectations and issues." He stated that at present, industrial people have three concerns about MI^2: "Will the use of MI^2 really speed up R&D?," "Will the use of MI^2 require/allow data sharing?," and "What is the first thing they have to do using MI^2?" To address these questions, Dr. Manabe divided the process of materials development—from the discovery of new materials to their practical use—into four stages: 1) creation of new materials, 2) identification of extreme values for materials physical properties, 3) optimization of materials, and 4) applied research and development (Fig. 2). Dr. Manabe explained that answers to the questions above vary depending on the stages.

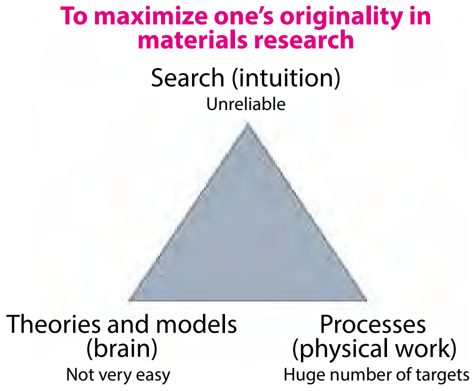


Figure 1

Computational science as a contributor to materials R&D

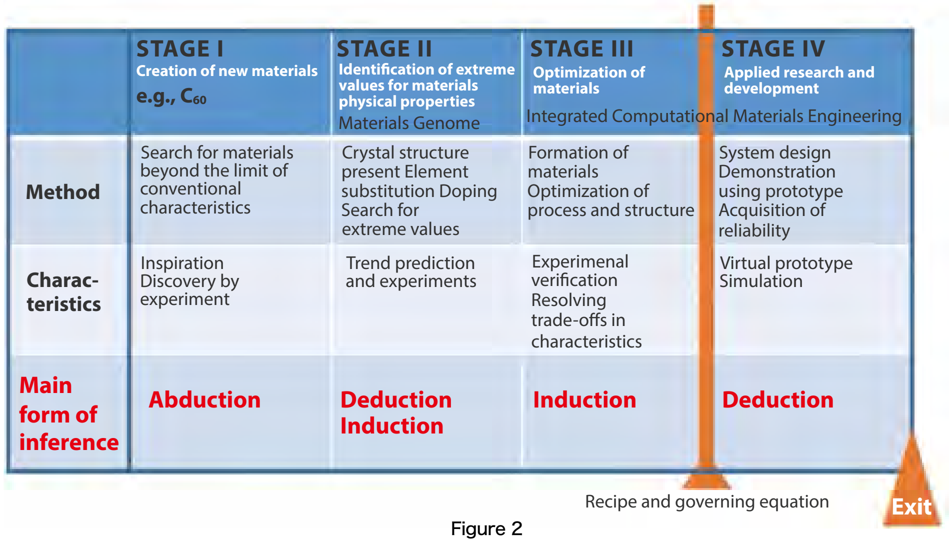
After the lectures above, Tomio Iwasaki of Hitachi, Ltd., Prof. Shinji Tsuneyuki of The University of Tokyo, and Toyohiro Chikyow of NIMS joined for a panel discussion. Kiyoyuki Terakura, the director of CMI^2 served as a moderator.

First, Dr. Iwasaki explained material design using computational science, which he has been performing since he joined Hitachi, as a practical example of an MI method called a response surface methodology. Dealing with electronics products, Dr. Iwasaki has been using computational science for such purposes as the determination of optimum material combinations and the selection of additives to achieve desirable performance. For example, he was able to determine the best substrate metal to be used for electronic parts by calculating adhesion strength between copper wiring and substrate metals.

Prof. Tsuneyuki is serving as a project director for MI research supported by the Japan Science and Technology Agency PRESTO program, and for research using the K supercomputer as well as the successor of the K supercomputer. He stated that addressing the question of whether computational science could contribute to materials research was his major research objective for many years. According to Prof. Tsuneyuki, computational science has strong applicability in the visualization of materials at the atomic level using simulations, virtual experiments to test certain ideas, and the prediction of characteristics of new materials. On the other hand, he pointed out that computational science has some weakness, such as that simulations with high degrees of freedom and multiscale simulations do not perform sufficiently, and that it is difficult to discover new materials with the desired performance or functions. He plans to solve these issues by incorporating MI in the PRESTO project.

Dr. Chikyow at NIMS conducts high-throughput synthesis and measurements to process a large amount of materials using a combinatorial method. He has accumulated data of synthesis and measurements using real materials based on material design driven by computational science. He mentioned the possibility of adding these data to NIMS materials database "MatNavi" in the future. As an experiment specialist, Dr. Chikyow stated that his contribution to MI^2 is two-fold: he will verify the results predicted by computational science through experiments and measurements, and provide data valuable to MI^2. He also shared his experience that seemingly uninteresting measurement data at first sometimes turned out to be appealing to materials researchers' instincts and led to the discovery of new materials, only after visualizing the data using computational science.

To which materials development stage will MI^2 contribute?



	STAGE I Creation of new materials e.g., C_{60}	STAGE II Identification of extreme values for materials physical properties Materials Genome	STAGE III Optimization of materials	STAGE IV Applied research and development
			Integrated Computational Materials Engineering	
Method	Search for materials beyond the limit of conventional characteristics	Crystal structure present Element substitution Doping Search for extreme values	Formation of materials Optimization of process and structure	System design Demonstration using prototype Acquisition of reliability
Charac-teristics	Inspiration Discovery by experiment	Trend prediction and experiments	Experimenal verification Resolving trade-offs in characteristics	Virtual prototype Simulation
Main form of inference	**Abduction**	**Deduction** **Induction**	**Induction**	**Deduction**

Figure 2

Prof. Terakura asked Prof. Tsuneyuki about the importance of MI^2 in relation to the successor of the K supercomputer. Tsuneyuki replied, "Expectations are high for the successor computer to be used in the wide range of materials research field, to address and cope with social issues. We believe that the role of MI^2 is vital especially in relation to magnetic and structural materials."

Dr. Iwasaki commented on the four stages in materials development explained by Dr. Manabe, saying, "In the industrial sector, the needs for computational science are high in terms of its application to stages 2 and 3. Similarly, MI^2 is also expected to be useful in these stages."

Dr. Okada added, "MI^2 is not meant to be a magic wand that will undertake all the work currently performed by people. So, as Prof. Hosono noted earlier, stage 1 would be the last phase to which MI^2 can contribute."

Prof. Hosono agreed with Dr. Iwasaki and Dr. Okada, stating, "Currently, stages 2 and 3 in materials development are the focus of discussion, and I expect MI^2 to play a major role in reducing the development period and cost by half in these stages." He added, "For example, if we want to create ferroelectric materials with a perovskite crystal structure, the only way to achieve the optimum results at present is to conduct experiments to test every possibility. For university researchers, discovering a couple of new materials and publishing papers on them would be satisfactory. However, that is insufficient for industries. If the application of MI^2 can reduce development period and cost, that will be very significant accomplishments."

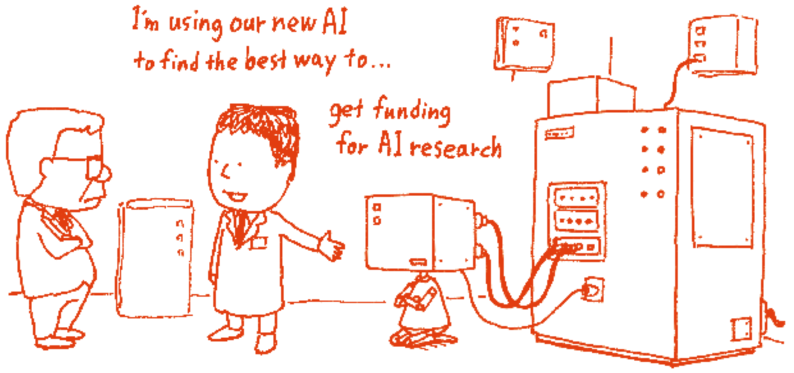
In addition, Dr. Chikyow stated, "Most high-throughput synthesis and measurements take place in stages 2 and 3. I believe that if these synthesis and measurement data are made available in an easy-to-understand way, they would provide helpful hints concerning stage 1."

In the conclusion of the panel discussion, Dr. Manabe stated, "For industries, stage 3 is of critical importance, and I felt very reassured to hear that MI^2 is expected to be very beneficial in this regard. I also hope that MI^2 will serve as the most useful tool by complementing human intuition or hunches used in stage 1 of materials development."

(by Kumi Yamada)

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

Will AI surpass the human brain?



It was back in 1956 when the term "artificial intelligence (AI)" was coined. The term was used for the first time in a proposal presented at the Dartmouth Conferences, which involved the participation of such figures as Claude Shannon and Marvin Minsky. There were high expectations that computers would become capable of recreating human intelligence, although their capability at that time was far insufficient to achieve such a feat.

AI received public attention again in the 1980s. The "Fifth-generation computer systems" initiative by Japanese government led the second AI boom. While some accomplishments were made, Japan's movement was viewed as a major failure by the international community due to the slow progress made in the development of AI.

And the third AI boom is currently ongoing. Unlike the previous two booms, the people's enthusiasm toward AI this time does not seem like it will easily fade away, due to the advancements made in network society, which makes possible data collection from all around the world, and the dramatic improvements made in the performance of computers.

A number of automobile firms are making efforts toward the realization of autonomous driving, and they are just a step away from achieving that goal. In the United States, Watson, a computer system developed by IBM, has beaten human opponents on the quiz show called Jeopardy!. In addition, a robot designed to pass the entrance exam for the top university in Japan is expected to achieve the goal in two or three years.

A method called deep learning, which has been drawing much attention, is said to be the core of the third-term AI boom, and is outstanding in image recognition capability due to increased computing capability (e.g., speed of calculation) and the introduction of big data.

The term "deep learning" reminds me of Professor Minsky who died recently at the age of 88. I met him, who was also known as the father of AI, for the first time in 1990 when he was visiting Japan to receive the Japan Prize. At that time, cellphones were still unavailable and public interest in AI was limited. However, to make machines learn more by themselves, Minsky proposed at the award ceremony that in addition to the development of the theory and practical application systems, it is necessary to study the human mind including emotions and self-consciousness. Given that the network society, which makes possible data collection from every part of the world, has made great progress and that the performance of computers has remarkably improved, I feel that Minsky's statement still has power today.

While the capabilities of AI are still restricted to certain fields, researchers are steadily working to develop versatile AI. Then, when will AI catches up with and exceeds human intelligence?

That hypothetical moment can be described by a term called the technological singularity. Based on the current trends of AI research, some researchers predict that the singularity will be reached in several decades. Some of them envisions that that point will arrive at year 2045.

It's said that no one can envisage with certainty what the future of humankind and the world would be like beyond the occurrence of the singularity.

However, I don't believe that computers can easily acquire intellectual capacity superior to the human brain. Even if computers become able to process an incredibly large amount of data very quickly, they still lack the creativity and imagination that humans possess. I believe that we will be able to maintain human-led society using wisdom derived from such qualities unique to humankind even if the technological singularity indeed takes place.

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.

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