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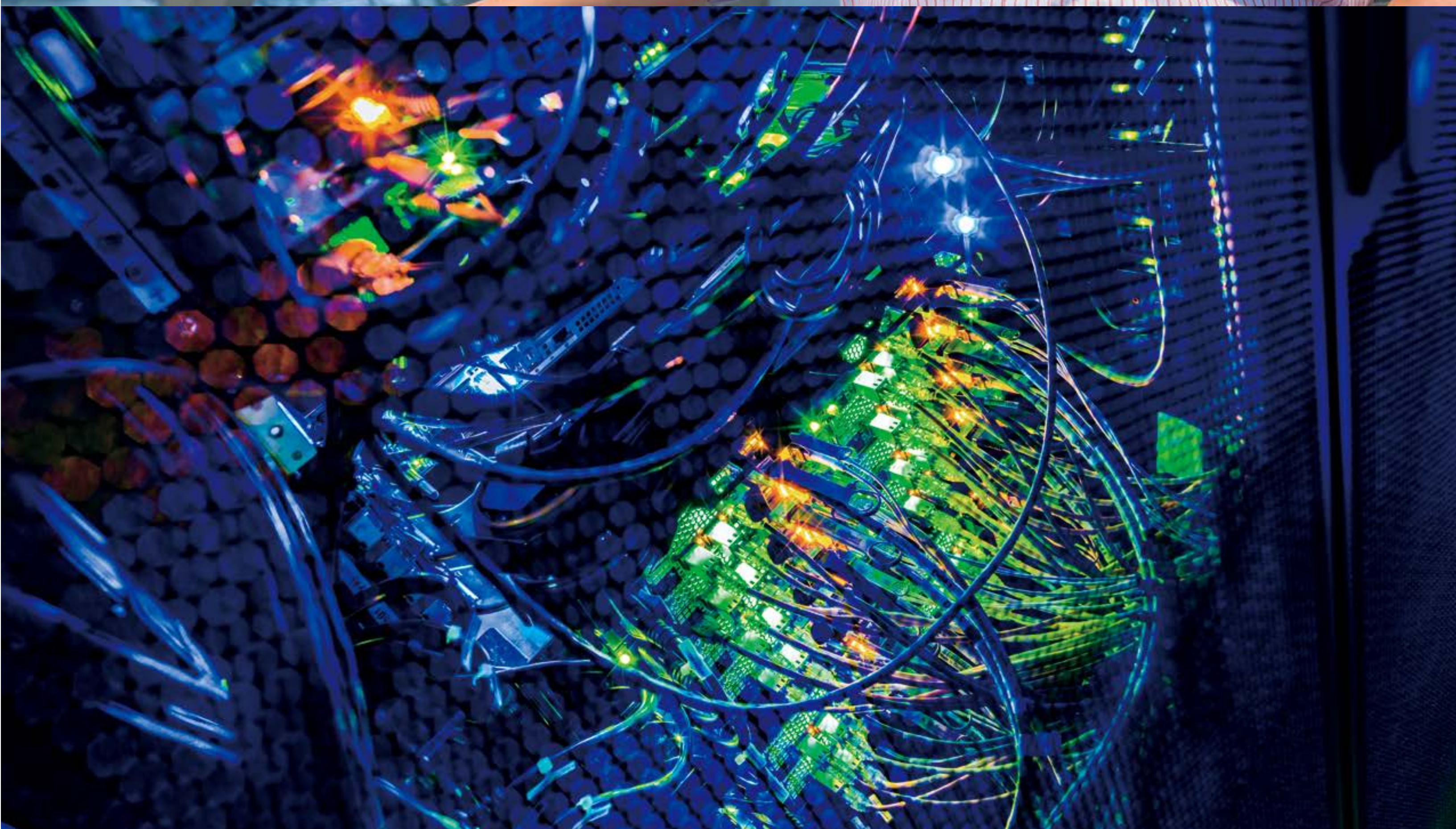
Achieving the unimaginable through data development

Data quality and quantity both crucial in materials development



Achieving the unimaginable through data development

Data quality and quantity both crucial in materials development

Materials development has traditionally been a trial-and-error process.
The rapidly growing integration of data science with the field is an emerging global trend.
This new approach, called materials informatics (MI*), uses artificial intelligence (AI) to process vast amounts of data, thereby predicting the structures of materials with desirable functions and their manufacturing processes and expediting the development of new materials.

Materials research institutes in Japan, including NIMS, have already discovered a number of new materials and generated new information using MI.
While the effectiveness of MI has been proven, an issue was also identified toward its advancement and future success: acquisition of large amounts of high-quality data.
The accuracy of AI increases as it processes and learns from more and more data.

How can we efficiently collect high-quality data?
Huge volumes of data need to be collected from the multitude of published scientific papers and readings from lab instruments. Collected data then has to be processed into MI-compatible formats.
These are very intensive tasks.
MaDIS (Research and Services Division of Materials Data and Integrated System) at NIMS has energetically pursued these labor-intensive projects.

Using the latest AI and other technologies, MaDIS is aiming to develop versatile systems capable of efficiently generating, storing, utilizing and publicizing data.
These systems may eventually enable highly streamlined materials development and the creation of materials beyond human imagination.
This NIMS NOW issue spotlights the challenges undertaken by MaDIS.

*MI is also used as an abbreviation for materials integration, as in SIP's Structural Materials for Innovation project (see p.12).

Special Talk

The power of data in the discovery of new insights

Hideyuki Yamagishi
Lead Executive Officer
Senior General Manager of Corporate Research and Development
Asahi Kasei Corporation

Yuko Nagano
Executive Vice President
Director of the Research and Services Division of Materials Data and Integrated System (MaDIS)
National Institute for Materials Science

The use of data science is the latest trend in materials R&D. The new method has already produced results and enabled some issues to be identified. What needs to be done to advance this technology? Hideyuki Yamagishi, Lead Executive Officer at Asahi Kasei, has early introduced data science within his organization by launching a new department specialized in materials informatics. Yuko Nagano, Director of the NIMS Research and Services Division of Materials Data and Integrated System (MaDIS), has strongly promoted the use of data science in materials R&D. The two discussed the current situation and future prospects of the data science approach in materials development.

Overcoming preconceptions and conventional thinking with data science

Nagano: The application of data science to materials R&D has become popular. Since 2014, NIMS has been developing materials integration systems to enable the rapid development of practical materials under the Structural Materials for Innovation project supported by the Cross-ministerial Strategic Innovation Promotion Program (SIP). NIMS has also been working since 2015 to build a research center to create functional materials using materials informatics in an effort to lead the Materials Research by Information Integration Initiative (MI^2I, see p. 12). Materials integration (see p. 13) and materials informatics share the acronym "MI." I believe that NIMS has been taking a firm lead in promoting the incorporation of data science—in the form of the two MIs—into materials development. Data driven materials research began demonstrating the power of this approach by producing a series of superb results starting in around 2017. An outstanding example of these studies is the development of an thermal insulation material composed of amorphous silicon and bismuth microcrystals—a completely unconventional combination—using machine learning (see the column on p. 13). I have heard that Asahi Kasei prioritized the early adoption of data science and has produced many excellent results.

Yamagishi: That's right. Asahi Kasei has actively adopted new techniques, such as computer simulation. We began introducing data science in around 2016 and started seeing positive results fairly quickly. For example, we produce resin compounds by combining different types of materials. To obtain the desired properties, we depended on the experience and intuition of researchers well-versed in polymer chemistry and manufacturing processes. Several formulations would need to be tested before the right one was identified. In contrast to this, data science analysis techniques can predict the correct formulation, usually requiring only a single test. The new techniques proved more effective than we imagined.

The use of data science has also enhanced the development of catalytic materials considerably. These materials are very complex because they are composed of four or five chemical elements. In the past, developing a catalyst took years of trial and error. However, by performing experiments under conditions derived from machine learning models, we were available to develop superior catalysts more quickly. What's more, the catalyst compositions obtain through machine learning models were completely different from what the experts imagined. It was exciting to see data science offer completely novel alternatives that break free from human preconceptions and conventional wisdom.

Nagano: You just gave some great examples of the benefits of data science. I believe that expedited development of high-performance materials using this approach offers a great advantage to companies seeking efficiency and cost reduction.

Yamagishi: Yes. Also, in addition to reducing development costs, these techniques make it possible to give material development projects that had been suspended due to slow progress another try. Moreover, it will be immensely beneficial for companies to preserve valuable data on substances and materials—even the knowledge and experience of researchers—in databases and learning models that can be used for future materials development. Recently, it has been becoming more and more difficult to recruit enough talented people due to Japan's shrinking and aging population. Companies must therefore find new and effective ways of passing on accumulated knowledge and skills to the next generation of workers. I believe that MI offers a solution to this issue.

It's exciting to see data science offering completely novel alternatives that break free from human preconceptions and conventional wisdom.

Hideyuki Yamagishi

Nagano: I agree with you. The use of artificial intelligence—which is capable of analyzing vast amounts of data—in combination with accumulated experience should result in research breakthroughs. Continued strategic development of MI is also vital to achieving such breakthroughs. This is why we launched MaDIS at NIMS in April 2017 and invited researchers and engineers with expertise in MI and materials data. We intended to expedite the building of an MI database and allow MI researchers to work in close collaboration.

Yamagishi: Asahi Kasei also launched the Materials Informatics Department in April 2017 to send the internal and external message that we are strongly committed to MI research. The department supports a number of research projects in different categories in which younger personnel are actively engaged.

What is Japan's status in a global society of intensifying competition?

Yamagishi: Our experience with MI has revealed a critical issue: a huge amount of data is needed to increase the reliability of predictions. Machine learning processes require inputting various parameters. In some cases, a lack of sufficient data makes it impossible to generate meaningful results. Also, database building is a fairly time-consuming and labor-intensive process. If too much effort is invested in building a database, actual materials development will bog down, defeating the entire purpose of MI. The U.S. and China are currently ahead of Japan in promoting the use of MI by their companies. Though many companies may be keen to leverage MI for rapid product development, few can afford the time and effort needed to build the necessary databases. This makes the NIMS materials database, MatNavi—which contains data organized by type of material, including polymers and inorganics—a very valuable resource.

Nagano: It would be inefficient for individual companies to make separate efforts to compile published information, such as research articles and patent publications, into databases. NIMS has released data which has been collected over many years on a diverse array of materials to a wide range of users. However, our data is still insufficient to be called "big data." Unless we continue to expand and improve the quality of our database, Japan will not be able to compete with the much larger research sectors of the U.S. and China. MaDIS therefore plans to develop one of the world's largest materials data platforms by compiling published data and high-quality experimental data. MI might appear to be cutting-edge, but its successful application will require continuous, diligent effort involving the collection of large amounts of data and structuring databases so that they are easy for data scientists to use. We are currently taking a strategic approach: standardizing terminology and creating the format used by various machines to write experimental data (see p. 8).

Yamagishi: Experimental data outputs are often inconsistently formatted and named, making them difficult for data scientists to use, so we appreciate your efforts at standardization. Once there's a standardized format for data recorded by various chemical measurement instruments, data can be expected to accumulate automatically and efficiently. Another issue is that while most studies produce large amounts of measurement data, only representative values tend to be reported, and the full data sets from studies are often not available. I have high expectations for MaDIS's ability to offer more complete databases so that the full benefit of these studies can be utilized.

Nagano: I expect that the collection and use of high-quality, reliable data will be the key to giving Japan an edge in global society. We will pursue the development of a next-generation data platform to support Japan's materials development efforts.

Tactics to establish MI

Nagano: Many countries are incorporating MI into materials development to increase their international competitiveness. For Japan to stay ahead in this competition, NIMS and the four chemical manufacturers—Asahi Kasei, Sumitomo Chemical, Mitsui Chemicals and Mitsubishi Chemical—jointly established Materials Open Platform (MOP) in June 2017. The vision of MOP is to collaborate on a national scale to solve MI-related issues common in the chemical industry. Actual collaborative activities are now in full scale operation. As a participant in the MOP initiative, what is your assessment of it?

Yamagishi: It's a groundbreaking approach for a public organization, such as NIMS, to play a central role as an impartial facilitator of research collaboration. My previous experience in science and technology policy-making in the Cabinet Office of the Japanese Government left me with a strong conviction that Japanese chemical manufacturers should collaborate to the greatest possible extent. Of course, it's not easy for companies to determine how much internal data to share with others. With NIMS at the core of the effort, I think the participating companies are collaborating smoothly in the first phase of the MOP project: building a public MI database. NIMS can continue to use its all-encompassing perspective to lead the project in the right direction. If the participating companies vie for leadership of the project, there will be no progress.

Nagano: We intend to fulfill our expected role without acting self-righteously. Our mission is to promote R&D that meets social needs in close cooperation with participating companies. We will also carefully monitor trends in MI technology and ensure that the data necessary to promote R&D is collected. We would like to work with industry, government and academia to achieve these goals.

Yamagishi: I expect that the success of this MOP project will further promote industry-academia-government collaboration. I believe that companies can work together in certain areas, such as the collection of publicized data. I am confident that Japan's MI initiatives are moving in the right direction, and I really hope that MI will become more widespread across the entire chemical industry. I look forward to continuing to work with you.

Nagano: I hope that we can work together to achieve solid results that lead to the establishment of MI in Japan. I look forward to continued partnership with you.

(by Kumi Yamada)

High-quality, reliable data will be the key to giving Japan an edge in global society.

Yuko Nagano

Materials Data Platform

[Special feature]

What is the "materials data platform"?

Brainpower enabling innovation in materials development

The Materials Data Platform Center (DPFC) was established within the Research and Services Division of Materials Data and Integrated System (MaDIS) in April 2017. The goal of the DPFC is to develop and operate a data platform to facilitate the aggregation and utilization of materials data. The quality and reliability of data gathered by the DPFC is expected to impact the success of materials informatics (MI*) research. DPFC Managing Director Mikiko Tanifuji and three group leaders of the platform development project discussed current progress and their future vision for the platform.

*MI is also used as an abbreviation for materials integration, as in SIP's Structural Materials for Innovation project (see p.12).

Masters in the use of information to become masters of materials research

The old principle that information is the key to success, is vitally important to materials research today. Significant efforts have been made in recent years to integrate information science and materials research (i.e., MI). A number of preliminary MI research projects have reported positive results, highlighting the importance of information utilization in materials research. However, materials researchers typically do not work in an environment which facilitates and promotes effective information utilization.

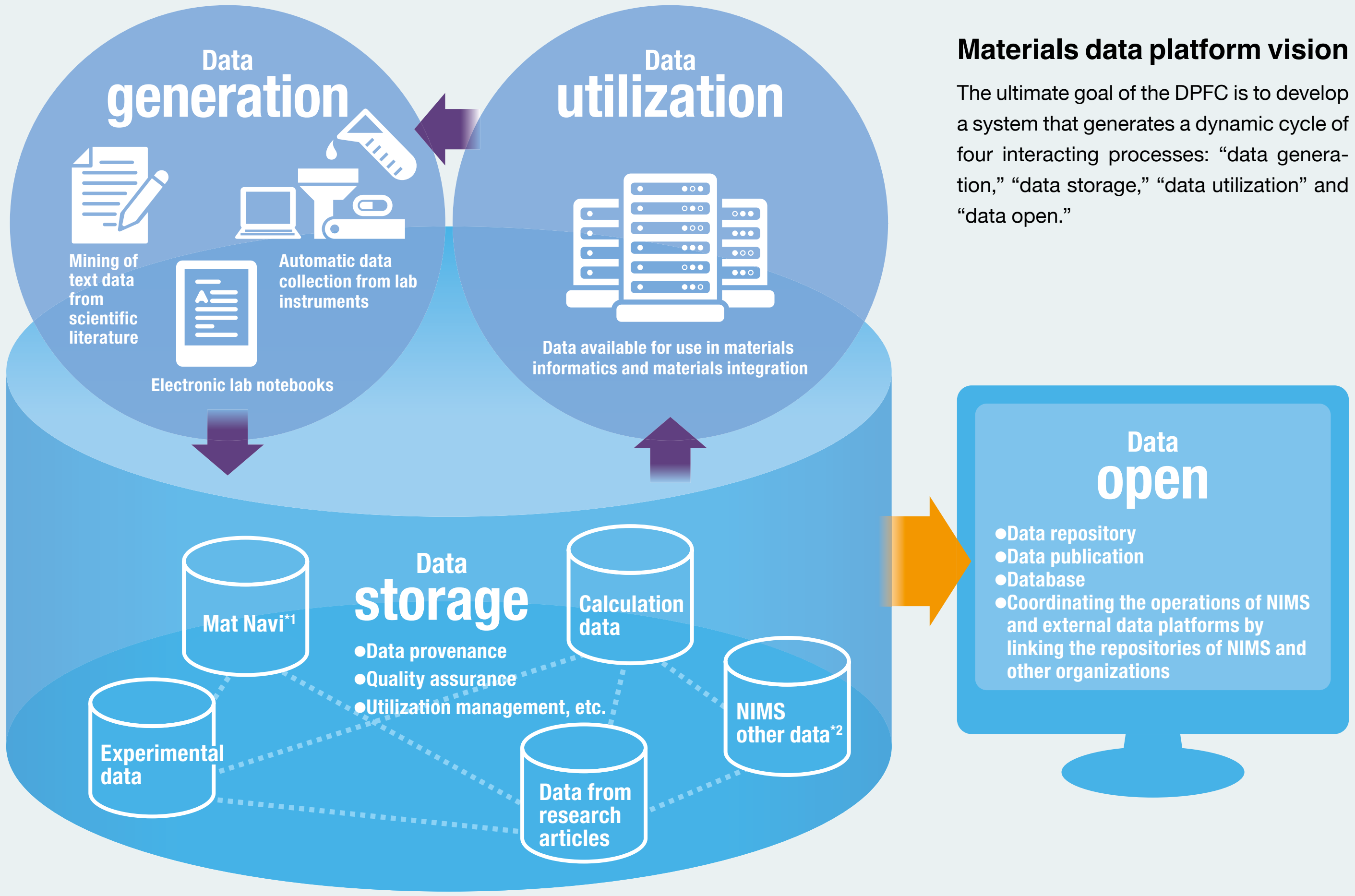
MaDIS has been carrying out systematic R&D focusing on a variety of materials since its launch, including functional, structural and organic materials. The mission of the DPFC is to aggregate the large volumes of information generated by MaDIS and other datasets that NIMS has accumulated over many years and make them available and usable for materials R&D throughout Japan. DPFC Managing Director Tanifuji characterized the significance of the Center in the following way: "When NIMS, a world-leading materials research organization, established the DPFC, it sought to bring and centralize materials information from its various sources, allowing it increase the power and synergy of this asset." NIMS, which has led materials research in Japan for more than 40 years, has taken the initiative in the systematic collection and utilization of research data.

Preparing adequate data essential to platform success

To promote materials R&D, a platform must be designed to cover all aspects of data utilization. Collected data must first be processed into a user-friendly format ("Data generation"). To achieve this goal, the DPFC is developing data processing methods that use both qualitative and quantitative approaches in which data quality is ensured by human experts while data extraction and formatting are performed automatically using artificial intelligence (AI) and machine learning.

In addition to data processing mechanisms, "data storage" mechanisms must be built into the platform. "Aggregating datasets from different sources, for example the NIMS-managed MatNAVI materials database and data generated in real-time through experiments and simulations, at one location and linking them together are vital platform functions," Tanifuji said.

Data accumulated under the platform in this manner will be used in MI research to generate novel data that will be added to the database, creating a virtuous cycle. In addition, the DPFC plans to increase the efficiency of this cycle by incorporating a publication function that will provide data reference and citation services to the public. This approach will be important for achieving efficient and sustainable MI development. Tanifuji has been leading these efforts as the DPFC Managing Director since April 2018. Let's look at some specific activities carried out at the Center.



Materials data platform vision

The ultimate goal of the DPFC is to develop a system that generates a dynamic cycle of four interacting processes: "data generation," "data storage," "data utilization" and "data open."

*1 NIMS' materials database
*2 Accident investigation records and researcher profile data, etc.

One type of materials data is experimentally obtained data. Hideki Yoshikawa (DPFC Deputy Managing Director and Leader of the Materials Data Analysis Group) said, "The current trend in materials research is to find ways of leveraging huge amounts of specific types of data, called 'big data.' Big data specific to materials research does not currently exist. I believe that we can create it by collecting all of the experimental data NIMS generates daily." The data published in research articles is a tiny fraction of the original experimental data. Most original data goes unnoticed and unused. However, if the large amounts of original data that are currently disregarded due to disappointment or incuriosity on the part of researchers during studies can be recovered and incorporated into a big data platform, they may become valuable MI research assets.

Data aggregated from various sources must be processed into a user-friendly format before storage. However, this is challenging, because a wide range of research fields and lab instruments generate valuable data. Even if you had access to these various types of data in their original form, you would almost certainly be unable to interpret them, Yoshikawa said. This is because metadata (i.e., data that contextualizes other data) is necessary to understand the original data. Research data must be accompanied by its associated metadata, which provides context of who collected it and how it was collected. This time-consuming requirement often discourages researchers from providing their data to large centralized platforms. Yoshikawa is considering offering services (e.g., greater access to special analytical software) to data creators who meet the requirements to highlight the importance of the associated metadata for the data platform.

In addition, Yoshikawa has negotiated with lab instrument manufacturers to obtain information on the formats and terminology used in experimental data generating instruments to make data provision more convenient. Yoshikawa is also developing software capable of automatically extracting metadata from original experimental data that includes metadata. (see the top of p. 11). As a result of these efforts, major manufacturers of instruments including X-ray photoelectron spectrometers and X-ray diffractometers, have been cooperating with the DPFC in preparation for the general release of software which will automatically translate original data into interoperable data with well-organized metadata.

Automatic extraction of key data from research articles using AI

In addition to gathering materials research data generated by NIMS, the DPFC is working to extract and process information from published documents, including research articles, into useable formats. Text data mining is a data extraction technique commonly used by the Materials Database Group. Group Leader Masashi Ishii said, “Research articles contain crucial information that we want to know, such as the data analysis and interpretation. However, the amount of research article information is estimated to have increased 100-fold over the last 50 years and continues to steadily increase. Because humans have a limited capacity to manually review documents, our group focused on the use of AI, the performance of which has been rapidly improving. We are taking the approach of having AI read and analyze patterns and rules within text. However, because AI is initially unable to recognize and extract key data and information from papers, we first need to repeatedly teach it what information is important. Authors of research papers claim their research to be novel using a variety of expressions, making it very difficult for AI to discern the relative importance of information. When we teach AI about magnets, for example, we first need to teach it the concept that a magnet has north and south poles and that its magnetic field originates from electron spins in atoms. This is similar to what parents do in raising their children.” Ishii is currently working to improve the precision of automatic data extraction using AI. He is targeting over 100 material properties, mainly for polymers. (see the middle of p. 11). Efforts like these are producing steady progress in the development of data extraction capabilities.

A user-friendly data system

Finally, a repository is needed to store data collected and extracted using the techniques developed by Yoshikawa, Ishii and others. The Data System Group has been carefully designing the specifications for such a data repository. Group Leader Takuya Kadohira said, “We anticipate situations in which AI is used to analyze large amounts of data collected from lab instruments. Therefore, the repository needs to mechanisms to facilitate transfers of data to or from the AI.”

For example, assigning proper metadata or distinctive IDs to collected data will enable more efficient data searches and downloading. The group is also considering the development of other mechanisms capable of recording data provenance, managing data user information, and assisting data review by third party researchers, thereby increasing data reliability. These added capabilities will significantly improve the convenience of using (“Data utilization”) and publishing data from the repository (“Data open”).

The above-mentioned platform functions have been developed with an eye toward long-term sustainability. The Data System Group is expected to play a major role in developing a platform that can effectively process and store data and allow users to efficiently utilize and open data as envisioned by Tanifuji (see the bottom of p. 11).

Teamwork to overcome platform development challenges

“All of our projects are new challenges for us, and we all feel like we are climbing a mountain with a summit no one has yet succeeded in reaching,” Tanifuji said. “We appreciate the opportunity to lead a national project whose sole purpose is to advance science and technology, allowing us to focus on these exciting missions. If we are to successfully surmount this seemingly invincible peak, it will be absolutely essential that everyone at the DPFC contributes. We have developed supportive relationships, so that when one of us loses his or her footing and is about to fall, the rest of us can throw him or her a lifeline and we can discuss solutions as a team. I believe that the progress we have made so far has been made possible by the combined efforts of the DPFC’s members striving to complete their tasks with conviction and a clear vision of the future.”

Yoshikawa said, “We have become increasingly motivated to recover unused and buried research data produced by industrial organizations.” He believes that manufacturers are gradually coming to an understanding of his group’s efforts to effectively use materials research data and develop a data platform. “If AI gains the capability to properly interpret research articles, it might even be able to give scientists research advice,” said Ishii, who envisions novel ways of conducting materials research driven by AI. Finally, Kadohira said with passion. “I hope to create a user-friendly data platform that will be perceived by many researchers as a valuable resource.”

Tanifuji concluded the interview with the following remarks. “When we hear researchers say that the materials data platform is a useful and powerful tool, and start voluntarily providing their data to it, we are close to achieving our objective. Our mission is to pass on a functional data platform and our accumulated data to the next generation. If researchers are able to produce outstanding results using the database we are building, we will have accomplished our mission.”

(by Akiko Ikeda, Sci-Tech Communications)

Materials Data Platform Center (DPFC)
Research and Services Division of Materials Data and Integrated System (MaDIS)

From left

Masashi Ishii
Group Leader, Materials Database Group

Mikiko Tanifuji
Managing Director, Materials Data Platform Center

Hideki Yoshikawa
Deputy Managing Director,
Materials Data Platform Center Group Leader,
Materials Data Analysis Group

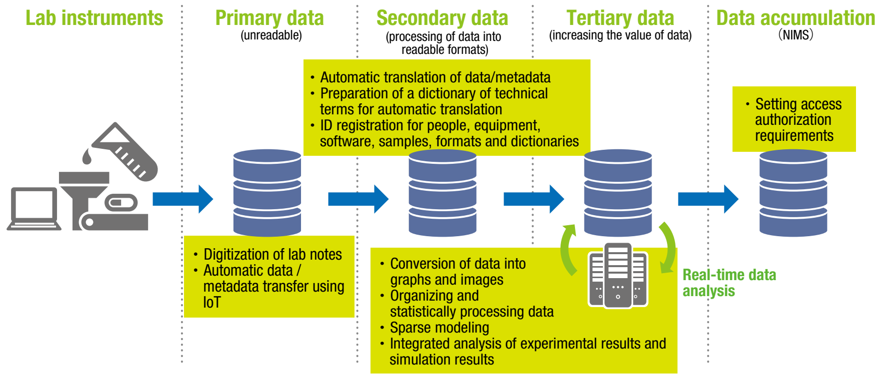
Takuya Kadohira
Group Leader, Data System Group

Three groups developing the materials data platform

Materials Data Analysis Group / Group Leader, Hideki Yoshikawa

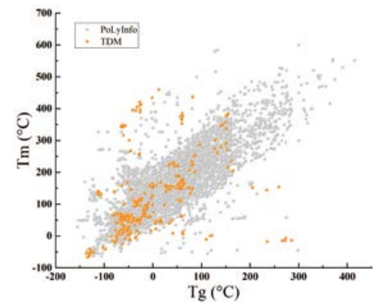
The mission of the Materials Data Analysis Group is to collect data currently possessed by researchers—expected to be a large amount—and increase its value. To accomplish this, we are working to establish a series of procedures that can be used to collect data recorded by lab instruments and process it into readable formats for general purpose computers, rather than the specialized computers directly associated with these instruments (e.g., computers with advanced data analysis functions, including machine learning functions; Figure). The collection of vast amounts of data requires high-speed, real-time data collection techniques, which has inspired us to pursue innovation in data collection. We developed an IoT system capable of directly collecting data from a variety of lab instruments—whether old or new, at NIMS or elsewhere—without posing an information security risk. We also developed and are promoting the wider use of “electronic lab notebooks” in an attempt to unobtrusively collect data from lab notes taken by researchers during their experiments.

Experimental data processing flow



Materials Database Group / Group Leader, Masashi Ishii

The Materials Database Group has been developing techniques to extract key information as “knowledge” from the multitude of research articles published over the decades and compile the data into databases. Because manual extraction is impractical due to the large volume of articles, this group has been using AI. Specifically, they are using text data mining techniques capable of exhaustive text analysis. The AI learns rules and patterns in research articles, such as context associated with specific terms and the relationships between the terms. Initially, data extracted by the AI must be checked by humans for errors, and if the AI extracts incorrect data, we subject it to repeated learning. Ultimately, the AI will become capable of extracting the correct data independently. In 2018, our group, RIKEN and the Nara Institute of Science and Technology jointly analyzed approximately 60,000 research articles regarding polymers and succeeded in automatically extracting approximately 7,500 points of data on glass transition temperature and approximately 5,500 points of data on melting point. “This extraction was completed in only a matter of several days, including the time required to train the AI,” Ishii said. “The use of AI has dramatically expedited database building processes when compared to manual procedures.”



Graph showing data from polymer material research articles extracted automatically using AI.

Data System Group / Group Leader, Takuya Kadohira

To realize the DPFC’s vision, the Data System Group has engaged in systems design and development, including the development of a hardware platform, with the goal of coordinating multiple software programs with specific functions, related to data storage, that direct the underlying hardware to perform certain tasks. We are currently developing an environment conducive to the safe operation of a system that includes data protection, quality assurance, management, and other functions. In addition, to organize the collected data into publishable forms, we have increased its value by transforming numerical data into graphs to enable easy visualization and have linked the DPFC data repository with the data repositories of other organizations. Moreover, to promote the use of the data platform by a wide range of users, we are considering new public services compatible with the operation of the system, such as launching a scientific journal specializing in data-related topics. We encourage platform users to provide feedback that we can use to improve the data system, generating a virtuous cycle, and attracting more users. As the main group pursuing the DPFC’s vision, we will continue to flexibly respond to various situations and requests.

(by Akiko Ikeda, Sci-Tech Communications)

Pioneering projects where data science meets materials science

The MI^{2}I and SIP-MI projects: past, present and future

NIMS is currently leading two national research projects that integrate data science with materials development: Materials Research by Information Integration Initiative (MI^{2}I)—aimed at discovering new functional materials—and the development of a materials integration system (SIP-MI) aiming to expedite the development of structural materials in the Structural Materials for Innovation project of the Cross-ministerial Strategic Innovation Promotion Program (SIP). We asked Satoshi Itoh, an MI^{2}I project leader, and Masahiko Demura, a SIP-MI project leader, about their past accomplishments and the future prospects for their respective projects.

Two projects that have revolutionized materials development

The use of data science to accelerate materials development is drawing global attention amid intensifying competition in the field. While various countries are racing to develop effective methods, NIMS in Japan quickly undertook two initiatives: the SIP-MI and MI^{2}I projects.

SIP-MI was launched in 2014 to develop materials integration systems that enable the creation of structural materials vital to social infrastructure and capable of solving environmental and energy issues. MI^{2}I was initiated in 2015 to promote materials informatics research focused on the development of functional materials indispensable to our everyday lives, such as rechargeable battery materials, magnetic materials, materials that control heat transfer and thermoelectric materials. While these initiatives—whose names both contain “MI,” meaning materials integration and materials informatics—share the common objective of developing new data driven R&D techniques, they intend to use these techniques for different purposes: discovering new materials and putting materials into practical use. These five-year projects, now entering their final phases, have produced a number of positive results.

Satoshi Itoh

Director,
Center for Materials Research by Information Integration (CMI^2)
Research and Services Division of Materials Data and Integrated System (MaDIS)

MI^{2}I enables materials searches by solving “inverse problems”

Let’s first look at the MI^{2}I, which has pursued the development of methods of searching for novel materials. The conventional approach to the quest for materials with new functions usually involves a trial-and-error process: experts use their experience and intuition to find the right combinations of chemical elements. This process is commonly referred to as “solving a forward problem.” This approach to materials search, however, is expensive and time-consuming because it requires exhaustive examination of all combinations of chemical elements to be used. By contrast, first determining a desirable function to pursue and then searching for combinations of chemical elements that may exhibit it is casually called “solving an inverse problem.” The use of data science to solve inverse problems can dramatically increase the speed of materials searches. This approach may also lead to the discovery of new theories and principles in materials science. These activities are the focus of the MI^{2}I.

“When the MI^{2}I project was launched, no method was available that allowed the use of data science in materials searches,” Ito said. “My first task was therefore to develop an effective methodology. Because NIMS did not have any proficient data scientists at the time, I invited data scientists from the field of bioinformatics—which had become popular before materials informatics—to our project. We carried out in-depth studies to find ways of applying data science to materials research.”

“The underlying philosophy of a data driven approach is to first understand the mechanisms behind a desirable material function before searching for it, rather than searching for desirable functions through trial and error without a solid logical basis, hoping for accidental discoveries,” Itoh said. In agreement with this philosophy, MI^{2}I researchers have been investigating the relationship between materials and their functions and developing an effective methodology using computational science techniques typically involving computer simulations, such as machine learning and sparse modeling.

The theoretical discovery of promising materials with desirable functions may prove fruitless if they cannot actually be synthesized. MI^{2}I researchers are aware of this issue and focus a great deal of effort on the actual fabrication of materials after predictions are made.

“In 2017, we succeeded in creating a material with the world’s highest thermal insulating performance,” Ito said. “We were able to achieve this rapidly by identifying key chemical elements and using them to narrow several thousands of candidate materials down to a small number of promising materials (see the COLUMN above). Through this success, we were able to demonstrate the effectiveness of our method.”

Optimization of manufacturing processes and materials’ performance through SIP-MI

The SIP-MI project, on the other hand, aims to speed up the development of practical materials. Atomic-level examination of materials already in actual use has revealed that their crystalline structures are non-uniform and contain various defects. These “microstructures”—a term used in materials science and engineering—are greatly influenced by “manufacturing processes,” such as casting and welding, and control materials’ “properties” (e.g., strength) and “performance” (e.g., durability).

These four factors are of fundamental importance in materials engineering, and their correlations and cause-and-effect relationships need to be understood and controlled to permit the successful development of practical materials. However, no comprehensive method was available that enabled the prediction of performance from manufacturing processes through microstructure and property. For this reason, the determination of optimum manufacturing processes had in many cases required very costly, labor-intensive and time-consuming experimentation.

To overcome this issue, the SIP program proposed a new materials integration concept that promotes the development of systems capable of computaitionally linking among the four factors mentioned above by integrating experiments, theories, empirical formulae and numerical simulations using data science. The SIP-MI project was launched to put this concept into practice, with NIMS and the University of Tokyo serving as core organizations.

The SIP-MI project initially focused on the development of a prediction system targeting welded steel. This subject was chosen because the microstructure of steel requires highly advanced control during its formation, and the welding process—from melting to solidification—often degrades it. Researchers assumed that a system capable of handling this complex subject would also be applicable to a wide range of other materials. They chose metallic fatigue, creep damage, brittle fracture and hydrogen embrittlement as the performances to predict.

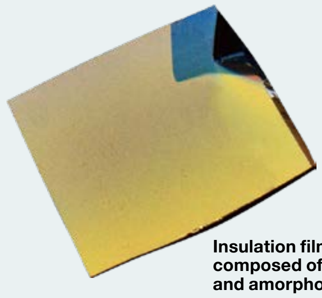
Masahiko Demura

Deputy Director,
Research and Services Division of Materials Data and Integrated System (MaDIS)
Group Leader, Materials Integration Group
Materials Data Platform Center (DPFC)

COLUMN MI^{2}I produces the world’s highest performance thermal insulation films

Thermal insulation materials are capable of resisting temperature changes. They are used, for example, in automobile engine compartments to block radiant heat from high temperature fuel combustion, increasing energy efficiency. The use of superior insulation materials would further increase the energy efficiency of engines. However, because the materials recorded to have excellent insulation potential number in the thousands, it would be difficult to carry out exhaustive analyses on all of them to select the most effective materials. Using data science and artificial intelligence (AI) as an alternative to this exhaustive analysis, an MI^{2}I research group led by Yibin Xu succeeded in fabricating a film material exhibiting the highest insulation capacity ever reported.

Xu’s group first selected several insulation-related parameters from 80 research articles on insulation materials and entered them into the AI. The group then allowed the machine learning function to identify a parameter most closely linked to thermal insulation and used it to narrow thousands of chemical element combinations with insulation potential down to several hundred more promising combinations. From these combinations, the group selected a combination of silicon (Si) and bismuth (Bi) because these elements are relatively easy to use in the synthesis of materials and fabricated a film material from them. A total of 28 film samples were prepared under slightly different synthesis conditions. The group measured the insulation performance of these samples and found that the thermal conductivity of one sample was 0.16 W/mK, representing the world’s highest insulation performance. The group is currently optimizing fabrication conditions for this film using machine learning.



Insulation film material composed of Bi and amorphous Si

The prediction of them requires understanding of a series of phenomena that occur over a wide range of spatial scales, from micro to macro. A system capable of accurately predicting them should be applicable not only to structural materials—the current target of the SIP-MI project—but also to various other materials.

Demura explained the key steps in the system's development. "First, numerical models need to be constructed that describe physical phenomena occurring in materials in terms of mathematical equations. We have developed a group of such models—or what we in the SIP-MI project call 'modules'—capable of predicting the fatigue life and creep life of materials. We then developed other capabilities by connecting multiple modules: prediction of performance from manufacturing processes through microstructure and property. A sequence of steps executed in a certain order across these modules is called a 'workflow.' We made workflows possible by developing various techniques to connect modules." Data science played an important role in this effort.

"Simulation results and experimental results sometimes differ considerably," Demura said. "Data assimilation techniques are effective in filling the gaps between them. They are used to adjust the parameters of numerical models so that their conformity with experimental data increases. In addition, sparse modeling is a very useful model selection technique when multiple model options exist."

Demura finally explained the current status of SIP-MI activities. "We are in the final stage of the development of the SIP-MI system and we expect to complete it by March 2019. Companies participating in the SIP-MI project are set to begin test use of the model."

MaDIS framework brings synergy

Since April 2017, the MI^{2}I project—which aims to search for new materials—and the SIP-MI project—which aims to accelerate the development of practical materials—have been carried out collaboratively under MaDIS. This arrangement is expected to promote synergy between the two projects, leading innovation in materials R&D. "Through the MI^{2}I project, we were able to identify many materials with the potential to exhibit superb properties using the prediction system we developed," Itoh said. "However, some of the materials identified are difficult to fabricate. I am hopeful that the manufacturing process module developed in the SIP-MI project will provide a breakthrough solution to this issue." Demura also expressed his expectations for the corroborative framework. "As has been the case with the MI^{2}I project, we plan to take an inverse design approach in our next SIP-MI project (see the TOPIC below). The methodology developed in the MI^{2}I project will be of great help to us."

These projects have also identified common issues. It is critical that we accumulate high-quality data and improve its usability for the steady promotion of the two MIs. Thus, the two projects plan to closely coordinate with the materials data platform (see p. 8) under development by MaDIS and develop efficient MI workflows. Expectations are growing for the collaboration among the three projects under the MaDIS framework. (by Kumi Yamada)

TOPIC A new project launched in the second term of the SIP program

Establishment of the Inverse Design MI Basis for Advanced Structural Materials and Processes

Principal Investigator: Masahiko Demura (MaDIS Deputy Director)

* MI is an abbreviation for materials integration.

The second term of the SIP program has started. The program has approved an R&D project entitled "Establishment of the Inverse Design MI Basis for Advanced Structural Materials and Processes" in which Demura serves as a Principal Investigator. This project is under the SIP category entitled "Materials Integration for Revolutionary Design System of Structural Materials" (Program Director: Teruo Kishi, Professor Emeritus of the University of Tokyo). The project is slated to last approximately five years from November 2018. Its goals are to increase the sophistication and versatility of the SIP-MI system developed during the first term of the SIP program and to develop a new industry-academia-government collaboration framework.

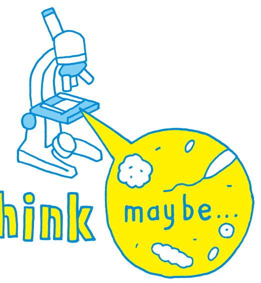
Researchers participating in this project intend to increase the sophistication of the SIP-MI system by developing an analytical method that employs an "inverse problem solving" approach, the opposite of the analytical method that uses a forward problem solving approach developed during the first term of the SIP program. In this new analytical method, the desirable "performance" of materials is first determined, the "microstructures" and "properties" of materials necessary to generate the target performance are then entered into a prediction system and the system is allowed to predict optimum "manufacturing processes" capable of producing materials with these characteristics. Development of this method is expected to be very challenging.

The researchers plan to expand the applicability of the SIP-MI system to a wide range of advanced structural materials and manufacturing processes in addition to welded steel, which was the initial focus during the first term of the SIP program. New target materials include carbon fiber-resin composites, heat-resistant metallic powders and ceramic matrix composites—key materials in solving environmental and energy issues.

Concurrent with this effort, the researchers will also design formats to be used in recording material data—a very unique aspect of this project. They plan to develop an SIP-MI System 2.0 that integrates computer science and materials science by creating an environment conducive to more advanced data use in close coordination with the material data platform project.

SIP-MI System 2.0 will be developed through close collaboration between industry, academia and government. This multi-sectoral group will first identify target issues to be addressed through an inverse problem solving approach. Individual sectors will then be assigned to separately develop components of the system (e.g., modules and workflows). Participating companies will be allowed to use output data generated by the system for their own specific purposes. In addition, output data will continuously be accumulated in the SIP-MI system to increase the efficiency of future multi-sectoral collaboration. Through these activities, the project participants intend to develop collaborative R&D frameworks unique to Japan, i.e., a combination of multi-sectoral collaborative R&D efforts and those of individual companies.

Science is even more amazing than you think



The threat of methane gas

Text by Akio Etori
Illustration by Joe Okada (vision track)

Carbon dioxide (CO_2) is a major global warming contributor. The atmospheric CO_2 level at the beginning of the Industrial Revolution is estimated to have been 280 ppm, but it has since risen by over 40% to more than 400 ppm as a result of the burning of fossil fuels, such as coal and petroleum, steadily warming the planet.

CO_2 is not the only gas that contributes to global warming, however. In addition to CO_2, which currently makes up the bulk of atmospheric greenhouse gases, other gases, such as methane, nitrogen oxide and chlorofluorocarbons (CFCs), also act as greenhouse gases.

CFCs are man-made chemicals and are not naturally occurring. Although they were in the past used widely as coolants in refrigerators and for other purposes, their production and use was banned after they were found to damage the ozone layer. Thus, their atmospheric levels are unlikely to rise significantly in the future. I expect methane to be more problematic.

Composed of carbon and hydrogen, methane (CH_4) is an excellent fuel. As many of you know, methane is the primary component of natural gas.

Once it is released into the atmosphere, however, methane can be harmful to the environment. It is 21 to 72 times more potent as a heat-trapping gas than CO_2.

Methane emissions had not been considered a serious issue because the atmospheric methane level is much lower than that of CO_2. However, some countries are concerned about the effect that the digestive processes of farm animals, such as sheep and cattle, may have on global warming. These animals have methane-producing anaerobic microorganisms in their intestines and are significant sources of methane emissions, and some countries warn that such farming should be curtailed.

More surprisingly, some scientists have reported that vast amounts of methane gas produced underground may be released into the air.

Research in Alaska and Siberia detected the slow release of gases stored underground into the atmosphere as frozen soil melts in response to slight increases in atmospheric temperature. Further recent research reported releases of large amounts of underground methane in the Arctic.

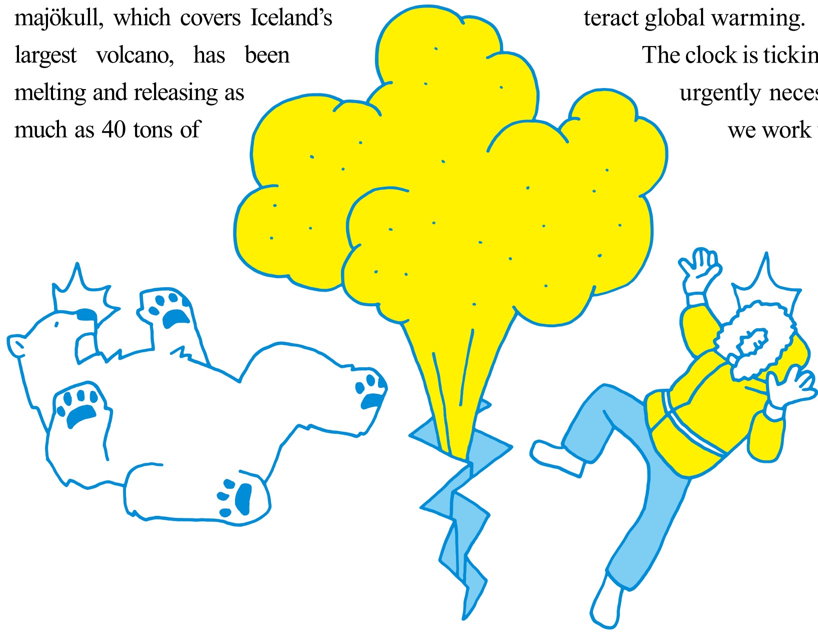
According to an article in Scientific Reports, a huge glacier called Sólheimajökull, which covers Iceland's largest volcano, has been melting and releasing as much as 40 tons of methane gas a day. This is a difficult problem due to the close glacier-volcano association.

The meltwater under this glacier is oxygen deficient and rich in nutrients derived from volcanic gases. It also contains a large number of anaerobic microorganisms that produce large quantities of methane gas, which dissolves in the water and is eventually released into the air.

Professor Peter Wynn of Lancaster University in the UK, who led this research project, said that it is highly probably that other areas in which glaciers and volcanoes interact are emitting methane gas. If similar conditions prevail in Antarctica, where many volcanoes exist, this may pose a serious risk of worsening global warming.

We appear to be falling into a vicious cycle: global warming melts glaciers, which then unlocks subglacial methane into the air, intensifying global warming, which then aggravates glacial melting. To stop this cycle, I believe that each one of us must make a conscious effort to counteract global warming.

The clock is ticking and it is urgently necessary that we work together.



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 Eleven NIMS members recognized as “Highly Cited Researchers 2018”

Clarivate Analytics selected 11 NIMS members as its “Highly Cited Researchers 2018.”

“Highly Cited Researchers” are authors of scientific papers that are in the top 1% in number of citations in a given research field based on Clarivate Analytics’ Essential Science Indicators database.


Katsuhiko Ariga


Yoshio Bando


Dmitri Golberg


Kazuhito Hashimoto


Jonathan P. Hill


Takashi Taniguchi


Kenji Watanabe


Yusuke Yamauchi


Jinhua Ye

Satellite Principal Investigator


Thomas E. Mallouk


Zhong Lin Wang

※Listed in alphabetical order

2 RCFM Director Naoki Ohashi awarded the French National Order of Merit

Naoki Ohashi, Director of the Research Center for Functional Materials (RCFM) was awarded L’Ordre National du Mérite (the French National Order of Merit) with the title of Chevalier for his significant contributions to research exchange and cooperation with France.

Director Ohashi has led the way in international industry-academia collaboration between France and Japan by forming and operating a joint research unit composed of representatives from NIMS, the CNRS (the French National Center for Scientific Research) and Saint-Gobain, a French private company. France has recognized these and other efforts made by Director Ohashi to increase bilateral research exchange and collaboration. The conferment ceremony was held on January 15, 2019 at the French ambassador’s residence in Minami-Azabu, Tokyo and the French Ambassador to Japan, Mr. Laurent Pic, presented the award.

Ohashi says, “I would like to continue contributing to academic exchange between France and Japan”.


RCFM Director Naoki Ohashi (left) receiving the Order of Merit from the French Ambassador to Japan, Mr. Laurent Pic (right). Prior to this decoration, RCFM Director Ohashi received 'Le Doctorat Honoris Causa' from the University of Rennes 1 in France.

Hello From NIMS

Bonjour, I’m Victor, born in Canada from Franco-Belgian parents. After finishing my bachelor in physics engineering in Montreal (CAN) and my master in Toulouse (FR), I decided to undergo a Ph.D in Wollongong (Australia), where I met my wife (whose Indian). It gets more and more difficult to answer the simple question: Where are you from?

My generation have seen the emergence of nanotechnologies, which always seemed very exciting to me, especially the physical aspects. I decided, however, to focus my research towards the chemical fabrication of nanocrystals as it appeared more viable for future industrial applications. After conducting my doctoral research on colloidal quantum dots-based solar cells, I also started having interest towards mesoporous materials. This brought me to NIMS in 2014 where I had the chance to work under Prof. Yamauchi. Since then I have enjoyed carrying on my research thanks to a fruitful environment. Japan has been very welcoming and keeps surprising us with so many interesting places to visit, while providing a safe and warm atmosphere for our family.


Visiting Fukushima prefecture in autumn.

Victor Malgras
(French/Canadian)
ICYS Research Fellow

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