NIMS NOW INTERNATIONAL

NATIONAL INSTITUTE FOR MATERIALS SCIENCE

2025 No. 1

Research Network and Facility Services Division (RNFS)

The ideal Environment for Materials Research is Here

Research Support Services in the DX Era

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NIMS boasts a collection of state-of-the-art shared equipment.
Through meticulous maintenance by skilled engineers and advanced user support,
a world-class research environment is provided for researchers both inside and outside the institution.

At the same time, NIMS has been at the forefront of driving DX* in materials development.
At NIMS, we have embarked on unprecedented missions to build a data management platform that seamlessly handles the entire lifecycle of materials data—from input (creation) to output (utilization).
By pioneering this initiative, NIMS has produced successful examples of data-driven materials development.
This effort laid the groundwork for Japan's national strategy known as the "Material DX Platform" Initiative.
Under this vision, the shared facility services have been redefined as the "frontline of data creation," uniting the shared facility services and the Material DX Platform Initiative under a common purpose.

To efficiently advance this national strategy,
NIMS consolidated engineers from both initiatives into the "Research Network and Facility Services Division (RNFS)."
Not only do they continuously refine their processing and measurement techniques,
but they also lead the way in introducing innovative data services that anticipate the needs of the times.
RNFS is turning this grand vision into reality.

*DX … Digital Transformation. It signifies a transformation in the very nature of operations through the integration of digital technologies and data utilization.

Data: Research Network and Facility Services Division

Director: Masahiko Demura

Number of Permanent Researchers & Engineers: 56

Materials Fabrication and Analysis Platform

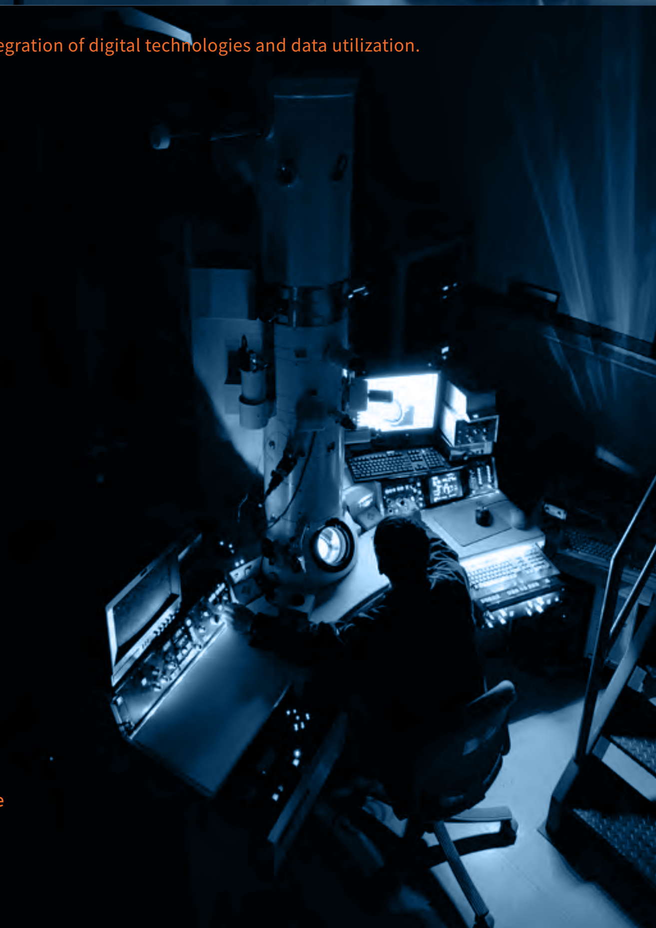
- Electron Microscopy Unit
- Surface and Bulk Analysis Unit
- High Magnetic Field Characterization Unit
- Bioanalysis Unit
- Nanofabrication Unit
- Materials Forming Unit
- Materials Melting and Manufacturing Unit
- Administrative Office

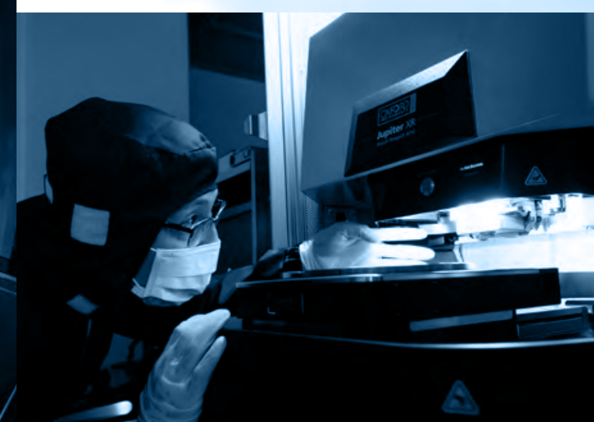
□ Central Hub of Advanced Research Infrastructure for Materials and Nanotechnology

Materials Data Platform

- Data Application Unit
- Data Infrastructure Unit
- Data Collection Unit
- Numerical Materials Simulator Unit
- Creep Data Unit
- Extreme Environment Material Data Unit
- Administrative Office

□ Data Transformation Initiative Subcommittee Administrative Office





Cover Story

Transmission Electron Microscope: "Spectra Ultra S/TEM"

The Transmission Electron Microscope (TEM) is an instrument that irradiates an ultra-thin sample, only a few tens of nanometers thick, with an electron beam of high acceleration voltage to observe its atomic arrangements and reveal the crystal structure by detecting transmitted electrons. The latest model, the "Spectra Ultra S/TEM," excels at switching acceleration voltages and stabilizing the lens and sample stage within five minutes. Many TEMs use Energy Dispersive X-ray Spectroscopy (EDS) detectors, to identify elemental distributions based on the energy of characteristic X-rays. These detectors' performance is defined by the "solid angle of detection." The Spectra Ultra S/TEM achieves an unprecedented solid angle of 4 srad, more than double the previous record of 1.9 srad in conventional TEMs. This allows for high-resolution elemental mapping in a less time and enable measurements of electron beam-sensitive materials. From 2024, NIMS is offering the Spectra Ultra S/TEM for shared use among its researchers (see p.8).

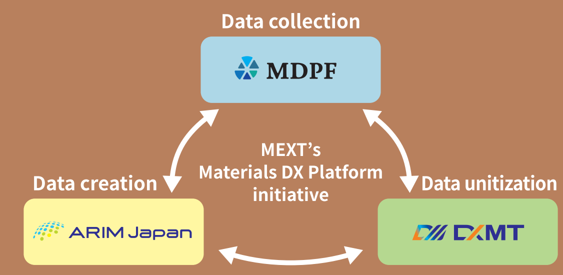
MISSION

Missions of the Research Network and Facility Services Division Platforms (RNFS)

NOTE

Materials DX Platform initiative

The initiative is to advance DX in materials research under the leadership of the Ministry of Education, Culture, Sports, Science and Technology , based on the Cabinet Office's "Materials Innovation Strategy." It aims to facilitate collection, accumulation, distribution, and utilization of materials data from industry, academia, and research institutions through a three-pronged operation model. Managed within RNFS, it ensures close collaboration in establishing operational rules and developing systems.



#1 Materials Fabrication and Analysis Platform

Platform Director
Satoshi Kawada

Breakthroughs Enabled by Advanced Shared Equipment and Robust Technical Support

The Materials Fabrication and Analysis Platform supports R&D activities of materials scientists by providing access to the wide range of cutting-edge instruments for materials fabrication, analysis and evaluation in NIMS. External users can utilize these equipment through two different services: NIMS Open Facility (NOF) and NIMS-ARIM. (Further details about these services can be found below.)

While general equipment sharing services are offered by many other organizations, NIMS stands out for the dedicated support provided by engineers with specialized expertise. This support goes beyond basic operation and maintenance—NIMS engineers tackle advanced challenges, such as developing new measurement techniques and collaborating on data analysis. As an eminent materials research facility, NIMS receives inquiries about a broad range of cutting-edge materials. To accommodate these demands, NIMS engineers continuously update their technical knowledge by keeping abreast of the latest research trends. The platform is committed to finding solutions to issues encountered by materials researchers, thereby further enhancing the quality and efficiency of their research.

NIMS Open Facility (NOF) website

The NOF website provides information on the NIMS shared equipment. Users can easily search by category for instruments suited to their objectives (e.g., intended purpose and instrument location). It also allows users to check whether instruments of interest are available through the NIMS-ARIM service.

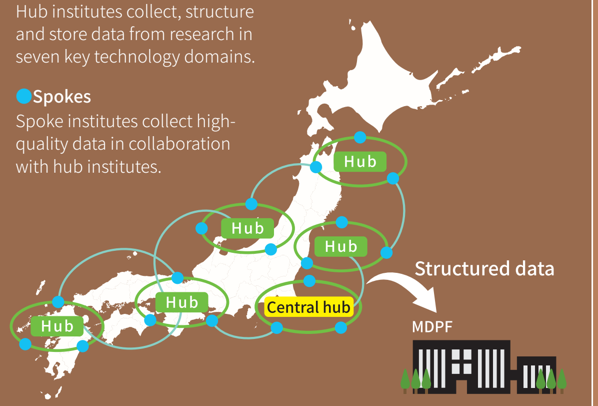
Japanese Website

Materials DX Platform project ❶

ARIM Japan

Under the government's shared equipment initiative, advanced instruments have been established at universities and research institutions across Japan. "ARIM" inherits this initiative while also collecting and accumulating materials data from these instruments. Starting in FY2025, these data will be shared. NIMS acts as the "Central Hub," overseeing operations and optimizing management. Additionally, NIMS operates "NIMS-ARIM" as the access point for its own advanced equipment.
The advantage of using shared equipment through NIMS-ARIM is that users can access the same equipment at a lower cost compared to using it through the NIMS Open Facility (NOF). However, users are required to submit usage reports via the ARIM website. Data provision is optional, but if agreed, the lowest usage fee is applied.*

* Some equipment does not support data provision.



#2 Materials Data Platform

Platform Director
Satoshi Minamoto

Dedicated research support through efficient data utilization

NIMS has been accelerating materials development through digital technology by developing a "digital ecosystem" to collect, accumulate, distribute, and utilize high-quality materials data from industry and academia. Initially operated as an internal data platform within NIMS, the system expanded, forming the foundation of "Materials DX Platform initiative" (see above), a national strategy for data-driven materials R&D in Japan. NIMS is the sole organization implementing the MDPF—one of three key projects driving this initiative. As part of this project, NIMS is enhancing MatNavi—one of the largest materials databases in the world—and developing a materials data analysis platform.

The engineers of the Materials Data Platform play a key role in the MDPF project, developing advanced systems with leading-edge data science techniques, such as machine learning and image recognition. They have been working to enhance research support by optimizing DX in materials development through close communication with researchers who generate and use the data.

Another key mission of this platform is to generate high-quality materials data. It conducts long-term and continuous tests, including creep, fatigue, and corrosion tests. In 2024, new programs were launched to test materials in low-temperature hydrogen environments. The platform also operates a supercomputer, which is essential for generating data through large-scale numerical simulations within NIMS (see the photo below). The data generated from these tests and simulations, and the digital ecosystem, have been driving DX initiatives.

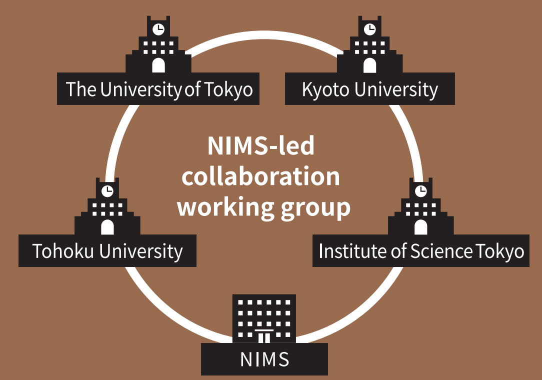
"Numerical Materials Simulator," a supercomputer for ultrahigh-speed, large-scale numerical simulations.

See p. 11 for ongoing MDPF projects

Materials DX Platform project ❷

DxMT

The DxMT was launched to facilitate materials development by leveraging and generating high-quality data. Five organizations serve as DxMT research centers: Tohoku University, the University of Tokyo, the Institute of Science Tokyo, Kyoto University and NIMS. Each center focuses on its own target materials and is conducting data-driven research.
The NIMS-led "DxMT Collabo" facilitates coordination among these five centers by identifying common issues, promoting the development and sharing of versatile data-driven techniques, and standardizing measurement conditions. The DxMT Collabo also organizes seminars and events to train researchers interested in data-driven techniques. With these activities, NIMS is driving the DxMT project, contributing to realizing the Materials DX Platform initiative .



Synergy of Technology × Technique

Engineers Empower Full Use of Leading-Edge Open Lab Instruments

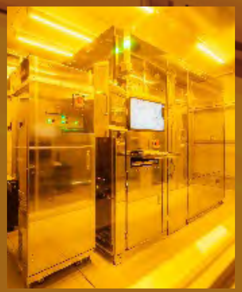
Facilitating Research on Advanced Devices by Sharing Expertise in Evolving Microfabrication Techniques

Navigator >> Eiichiro Watanabe
Nanofabrication Unit
Senior Engineer

The **Nanofabrication Unit** provides shared access to a cleanroom and over 50 microfabrication and evaluation equipment to support research on materials and processing technologies for advanced devices, primarily based on semiconductor materials. **This one-stop facility provides essential process technologies for electronic and optical device R&D,** including lithography, thin-film deposition, etching, and device performance evaluation. Among these equipment, the **electron beam lithography system (JBX-8100FS)** has gained significant attention and a strong reputation in recent years. It enables nanometer-scale patterning on semiconductors and other substrates. The primary advantages of the JBX-8100FS are advanced lithographic miniaturization, high-speed patterning, and exceptional accuracy. With a maximum acceleration voltage of 200 kV, the system achieves a finer electron beam focus than conventional models, enabling more precise patterning. Under identical conditions, it reduces the patterning time for periodic structures requiring long processing to one-fifth, significantly accelerating R&D. Additionally, in multilayer devices, alignment accuracy between layers affects performance, and the JBX-8100FS minimizes layer misalignment to within ±10 nm.

Our role as engineers is to maximize the potential of our equipment and provide the best possible support to users. For the JBX-8100FS, we continuously evaluate lithographic conditions to push the limits of miniaturization and patterning speed. In addition, all engineers in our unit undergo rigorous training to operate every equipment, **ensuring consistently high-quality service at any time.** The essence of manufacturing is in exploring the optimum equipment and processes for shaping materials, forming circuits, and building device structures. We are committed to continuously evolving as engineers who can meet user demands, staying attuned to new knowledge and technologies while honing our skills.

Equipment Data



Electron Beam Lithography System [JBX-8100FS]
Manufacturer: JEOL Ltd.
Services: Self-operation | Guided-operation | Staff-operated Service

NOF ARIM

Usage Methods for Shared Equipment

〈Inquiries for Equipment Use〉

① NIMS Open Facility (NOF): Use under Non-public Access
② ARIM: Use under Public Access

〈Usage Types〉

Self-operation
…Users independently operate the equipment and perform analysis.

Guided-operation
…Users operate the equipment with assistance and guidance from NIMS staff.

Staff-operated Service
…NIMS staff operate the equipment and perform analysis on behalf of users.

One of the World's Largest Forging Simulators: Innovative Efforts to Meet Complex Testing Demands

Navigator >> Norie Motohashi
Materials Forming Unit
Senior Engineer

The **Materials Forming Unit** supports materials research through a variety of services, including property testing, processing experimental equipment and components, designing and fabricating glassware for scientific experiments, and preparing samples. Among the various equipment, the most distinctive is the **1500-ton Forging Simulator.**

Forging is a metalworking process that involves applying pressure to metal materials to shape them into desired forms while simultaneously enhancing their strength. The metal's microstructure—and consequently, its mechanical properties—are significantly influenced by process conditions such as pressure, temperature, and cooling time. Understanding these correlations is a key research challenge. However, laboratory-scale small specimens often fail to replicate the phenomena occurring inside large metal components processed in industrial environments.

The 1500-ton Forging Simulator is one of the world's largest forging testing machines, capable of isothermal hot working* at temperatures exceeding 1000°C. For instance, it can forge test specimens with diameters of up to 140 mm from materials with strengths of 800 MPa at 900°C. The simulator precisely controls strain rate, heating temperature, cooling methods, and times, enabling foundational research on materials and scientific analysis of metalworking techniques traditionally guided by skilled engineers' intuition. This understanding is essential for preserving and advancing metalworking techniques. Custom-built with a hydraulic press, heating furnace, and cooling systems, **this unique equipment is exclusively operated by our unit's engineers.**

Beyond simply operating the equipment, we continuously innovate by refining temperature control systems to enable more advanced isothermal forging tests. These efforts were recognized with the Research Support Award from the Minister of Education, Culture, Sports, Science and Technology for fiscal year 2023.

The simulator is also capable of processing metals into complex shapes. **When researchers request unprecedented testing conditions, we adapt the equipment, design custom fixtures, and pursue the best possible solutions.** During testing, we work closely with researchers in the field, reviewing and adjusting conditions as needed to meet specific research demands with precision.

*Isothermal Hot Working: A method where both the metal and the die are kept at a constant temperature during processing.

Equipment Data

1500-ton Forging Simulator
Services: Staff-operated Service

NOF

State-of-the-Art Instruments and Skilled Engineers Enable Advanced Nanostructure Analysis

Navigator >> **Jun Uzuhashi**
Electron Microscopy Unit
Principal Engineer

The **Electron Microscopy Unit** provides researchers with expert support for observing materials and devices using scanning electron microscopy (SEM) and transmission electron microscopy (TEM), as well as for preparing specimens with focused ion beam (FIB) systems. While the performance of these instruments continues to improve significantly, fully utilizing them requires specialized expertise. TEM techniques, for example, offer multiple imaging modes and a variety of optional functions. Selecting the appropriate equipment and optimizing its settings demand deep, up-to-date technical knowledge. Our experienced engineers offer high-quality support to ensure accurate and reliable nanostructure analysis results.

A key focus of the unit is to enhance its services by adopting cutting-edge technologies. In 2024, the **Spectra Ultra S/TEM** was introduced to NIMS for internal research use. One key innovation of this instrument is its high-speed accelerating voltage switching, enabling rapid optimization of the voltage for specimen observation. Seamless transitions between voltages within a single session enhance flexibility in imaging and spectroscopy. Additionally, the world's highest-performance elemental analysis system allows for fast, high-resolution elemental mapping (see p. 3 for details). External researchers can access this cutting-edge tool through collaborative research with NIMS researchers.

However, TEM has limitations, particularly in the quantitative analysis of light elements and the detection of trace elements as rare as one atom among millions. These challenges can be addressed by three-dimensional atom probe (3DAP), which enables 3D elemental mapping of materials and devices. By using TEM and 3DAP complementarily, highly advanced nanostructure analysis can be performed . In October 2024, a cutting-edge 3DAP instrument, the Invizo 6000, became available at NIMS for shared use. **As one of the few engineers proficient in both TEM and 3DAP**, I am committed to advancing nanostructure analysis and contributing to the development of innovative materials and devices.

Equipment Data

Spectra Ultra S / TEM
(for internal use within NIMS only)

For external-use equipment managed by the Electron Microscopy Unit, scan the QR code.

Understanding the Essence: Pride in Designing Approaches for High Magnetic Field Measurements

Navigator >> **Shigeki Nimori**
High Magnetic Field Characterization Unit
Chief Engineer

The **High Magnetic Field Characterization Unit** supports research activities by developing advanced measurement technologies utilizing superconducting magnets and nuclear magnetic resonance magnets, while ensuring a stable supply of liquid helium to researchers at NIMS. One of the key instruments under our management, the **"Physical Property Measurement System,"** is an advanced device designed to automatically measure fundamental physical properties crucial for material evaluation under high magnetic fields, which is up to 16 tesla, the highest level among general-purpose physical property measurement instruments. It also features exceptional expandability, offering a wide range of optional equipment to enable the measurement of various physical properties. **To accurately interpret the meaning of the data, it is crucial to have a deep understanding of the sample's characteristics and the principles behind the measurement.** Leveraging broad research experience in magnetic materials, superconductors, and semiconductors, I collaborate with researchers to propose the most optimal approaches. I place great value on maintaining a curious mindset and continuously learning the latest insights.

Equipment Data

16T Physical Property Measurement System
Manufacturer: Quantum Design Japan, Inc.
Services: Self-operation | Guided-operation | Staff-operated Service

NOF

Commitment to Users: Advancing R&D of Biomaterials

Navigator >> **Shinya Hattori**
Bioanalysis Unit
Engineer

The **Bioanalysis Unit** provides experimental environments, such as cell culture and genetic analysis, as well as equipment for the analysis and evaluation of biomaterials. For biomaterials interacting with biological systems, understanding their "interaction with biological systems" is a key theme. For example, information on how proteins in cells change after contact with a material is essential for evaluating the material's performance. The **"Liquid Chromatography-Mass Spectrometry (LC-MS)"** I manage identifies substances by measuring the mass of sample components. The newly introduced "LC-MS (OE480)" is capable of detecting a wider range of proteins with greater speed and precision than its predecessors. My policy is to **fully engage with clients' needs.** In our unit, a single engineer typically handles all aspects of the process for a client—from scheduling and operation to data analysis—fostering long-term relationships. **Familiarity with their research history allows me to understand their intentions and propose alternative methods beyond initial requests.** Receiving feedback like "our research has progressed" gives me great fulfillment.

Equipment Data

Liquid Chromatography-Mass Spectrometry [OE480]
Manufacturer: Thermo Fisher Scientific Inc.
Services: Self-operation | Guided-operation | Staff-operated Service

NOF ARIM

Providing the Tacit Knowledge of Manufacturing: Where Cutting-Edge Superalloys Are Born

Single-crystal superalloy (Right) and its casting mold (Left)

Navigator >>

Yuji Takata
Materials Melting and Manufacturing Unit
Senior Engineer

The **Materials Melting and Manufacturing Unit** provides metal processing technologies, including melting, plastic working, and heat treatment. **This work demands advanced technical skills and a deep understanding of materials** to handle elements that are difficult to quantify. My main role is producing heat-resistant materials, focusing on single-crystal nickel-based superalloys developed at NIMS. I manage the entire process, from crafting spiral-structured molds for crystal orientation control to casting in melting furnaces, followed by heat treatment and property evaluation. Few engineers specialize in all these processes, and **my strength is rapidly prototyping alloys tailored to researchers' needs.** Recent advances in computer simulation have enhanced guidelines for element composition and heat treatment temperatures. However, factors such as heat distribution affected by mold thickness and the sequence and timing of adding over ten elements to the melting furnace still demand careful attention. This is where engineering expertise plays a crucial role. Most requests currently come from NIMS researchers, but we also accommodate external inquiries, aiming to strengthen Japan's materials development.

※For external-use equipment of the Materials Melting and Manufacturing Unit, scan the QR code on the right.

No Compromise on Accuracy: Identifying the Chemical Composition of Materials

Navigator >>

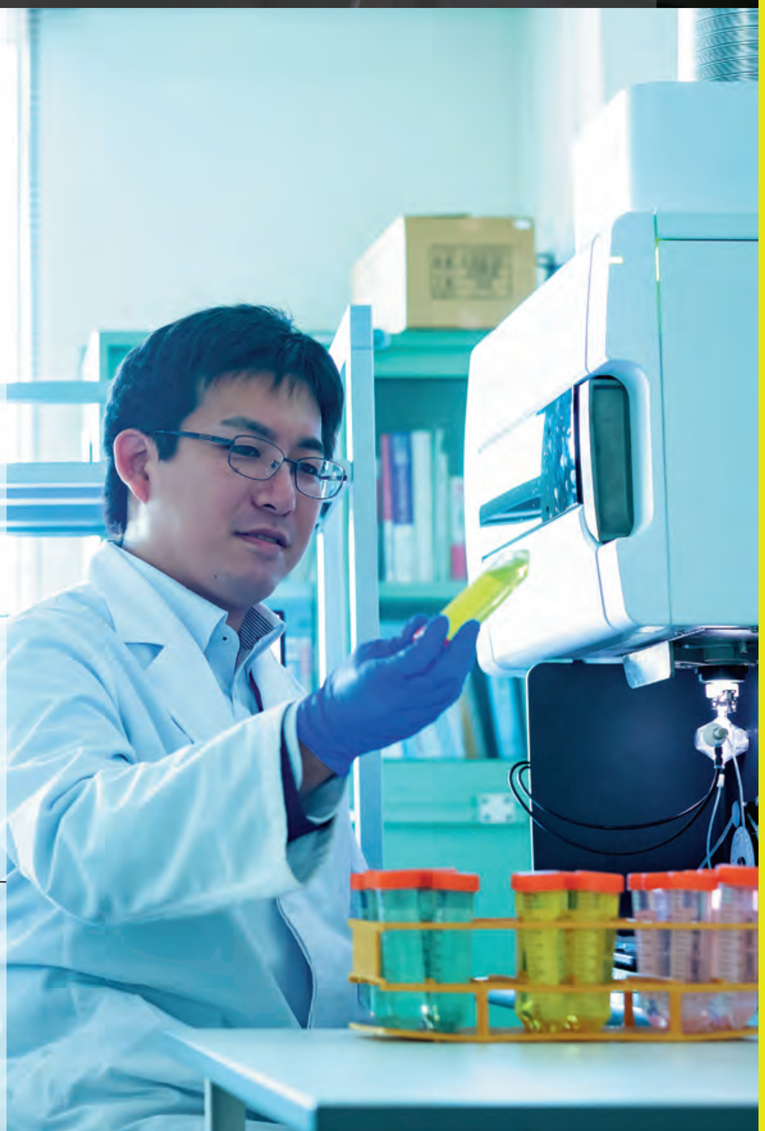
Yu Fujii
Surface and Bulk Analysis Unit
Engineer

The **Surface and Bulk Analysis Unit** utilizes a variety of analytical instruments to investigate chemical composition, crystal structure, and electronic properties of the samples . My expertise lies in chemical analysis, and one of the instruments I manage is the **Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES)**, which can quantify more than 70 elements simultaneously. When analyzing solid samples with ICP-OES, the sample needs to be completely dissolved in a solution as a pre-treatment. This process ensures that the elements from the solid are fully dissolved and uniformly distributed in the solution, allowing for an accurate assessment of its overall elemental composition. **Even with highly chemical-resistant samples, we draw upon years of accumulated knowledge to devise optimal decomposition methods, ensuring complete dissolution.** To ensure analytical accuracy, we compare the obtained values with the certified reference materials, which serve as our benchmark for reliability. Some elements are difficult to detect due to spectral interference from other elements or extremely low concentrations, requiring careful evaluation. I will continue honing my skills to adapt to cutting-edge materials and future challenges.

Equipment Data

Inductively Coupled Plasma Optical Emission Spectrometry [Agilent5800]
Manufacturer: Agilent Technologies
Services: Staff-operated Service

NOF ARIM



Special Roundtable

Pioneering Material DX

Conquering the Challenging Path to Success

Takuya Kadohira
Materials Data Platform
Deputy Platform Director /
Data Infrastructure Unit
Unit Leader

Satoshi Minamoto
Materials Data Platform
Platform Director /
Data Application Unit
Unit Leader

Isao Kuwajima
Materials Data Platform
Data Collection Unit
Unit Leader

The Ministry of Education, Culture, Sports, Science and Technology (MEXT) is promoting the development of the "Material DX Platform" through the integrated efforts of three interlinked initiatives: the Advanced Research Infrastructure for Materials and Nanotechnology in Japan (ARIM), the Materials Data Platform (MDPF), and the Data-creation and Application-oriented Materials Research and Development Project (DxMT) (explained on p.5). Among these, NIMS serves as the sole implementing organization for the MDPF initiative, responsible for collecting and accumulating materials data from across Japan and developing the necessary infrastructure and frameworks for its utilization. In this interview, Satoshi Minamoto, Takuya Kadohira, and Isao Kuwajima, who oversee the MDPF initiative, share insights into its current status and future prospects.

The Core of the Data Strategy: The Role of MDPF

— Could you tell us about the MDPF, one of the key pillars of the Material DX Platform development?

Minamoto: At MDPF, our goal is to collect, accumulate, distribute, and utilize high-quality materials data. We are expanding various data services while developing the necessary infrastructure. Our concept is to seamlessly manage the entire process—from data input (creation) to accumulation (collection) and output (utilization).

Kadohira: Since the mid-2010s, NIMS has been implementing an internal cycle of "creation, collection, and utilization" of materials data. Entering the 2020s, under the Material DX Platform initiative, we have expanded this cycle to form a broader network that includes research institutions and universities across Japan. We are currently focused on developing and implementing the necessary steps to realize this vision.

Kuwajima: Within MDPF, I lead the Data Collection Unit, which is responsible for gathering materials data. Dr. Kadohira manages the Data Infrastructure Unit, overseeing the infrastructure development, while Dr. Minamoto leads the Data Application Unit, promoting the practical use of material data. However, in practice, our units aren't strictly divided. We all share the common goal of advancing MDPF through cutting-edge innovation while ensuring stable operations. We work together as a unified team towards this objective.

"MDPF is deliberately taking a challenging path. That's precisely why a national research institute should play a central role in DX."
— Satoshi Minamoto

— The first step in the data strategy is to collect and accumulate materials data. How is this progressing?

Kuwajima: Since 2003, NIMS has been developing MatNavi, one of the world's largest materials databases, comprised of over a dozen databases and several applications covering inorganic materials, metallic materials, polymers, and more. The Data Collection Unit extracts relevant data from research papers, integrates experimental results from NIMS, and performs calculations when necessary. The data are then standardized and registered in the databases. Expert curation ensures the accuracy of information from papers, while materials testing—such as creep testing—are conducted according to consistent standards at NIMS. This maintains MatNavi's exceptional data quality, making it one of the core services of MDPF.

Kadohira: Alongside the development of MatNavi, MDPF has also been enhancing data collection through a service called RDE (Research Data Express). RDE is a system designed to transfer data directly from remote experimental instruments and store it in a format optimized for AI-based analysis. Conventionally, data output from experimental instruments varied in terminology and format, making it difficult to integrate into a unified database. However, RDE features an automated structuring function that translates terminology, assigns metadata, and converts formats. This enables real-time data archiving in MDPF's shared database.

Initially, RDE was operated within a closed environment at NIMS to establish an internal data service cycle. In January 2023, RDE was officially incorporated into the MDPF service lineup, and MDPF's system infrastructure was migrated to a public cloud. This transition enabled experimental instruments from research institutions and universities participating in ARIM to transmit data online via RDE, centralizing data collection and storage. This integration established the full-scale collaboration of ARIM, MDPF, and DxMT into an interconnected system.

Promoting Data Utilization: The New Service "pinax"

— Now that the infrastructure for collecting and accumulating materials data is in place, the next phase is full-scale data utilization. How does MDPF envision utilizing these data?

Minamoto: We have long debated the best ways to utilize the vast amount of data accumulated. Materials development is currently undergoing a transitional phase in its digital transformation (DX), and there is no definitive answer on the optimal method for leveraging these data. AI-driven data analysis is among the most promising approaches, but building predictive models requires trial and error. For example, should temperature be included as a parameter in the analysis, or is it better left out? Various scenarios need to be tested.

Kadohira: Since the inception of our data services, we have discussed the need for a platform to facilitate AI-based analysis. With this goal in mind, Dr. Minamoto initiated the development of "pinax" in 2022. Simply put, pinax is a system that enables users to develop various predictive models and conduct analyses using datasets provided by MDPF. We have already started offering the system to researchers at NIMS and are preparing for a wider rollout.

Minamoto: With pinax, users have access to a cloud-based virtual desktop environment for their personal workspace. There, they can develop custom predictive models and conduct AI-based analyses using pre-installed programming languages and shared analytical tools. We also implemented a traceability system that records the data source and development process of predictive models. This enables users to gain insights into the key factors that contributed to enhancing model accuracy. Our core principle in developing pinax was to build a system that answers the "why" questions analysts encounter.

Kuwajima: Users can leverage not only MDPF-provided datasets, such as MatNavi, but also their own proprietary data from research institutions and universities, uploading them into their private workspace within pinax for analysis.

Additionally, predictive models created within pinax can be shared with designated members. We want to emphasize that pinax serves as a secure and flexible sandbox for users. From my perspective as the one responsible for data collection, I strongly hope that researchers will fully utilize pinax to unlock the true potential of materials data in their research—that is our ultimate goal.

Harnessing System Integration to Solve the "Inverse Problem"

— What kind of advancement do you anticipate arising from the use of MDPF's various services?

Kadohira: At present, our primary goal is to demonstrate practical applications of data utilization through MDPF's services, and one key approach is experimenting with system integration.

For example, there is a system called "MInt." This system is designed to establish strong correlations between the four key elements of materials engineering—manufacturing processes, microstructure, properties, and performance—allowing for seamless predictive modeling. Originally, it was developed under the Cabinet Office of Japan's "SIP" project, focusing on structural materials. Following the project's completion, Dr. Minamoto led efforts to broaden its scope to encompass all types of materials. MInt incorporates various computational tools known as modules, which can be linked to form workflows. By tracing these workflows, it becomes possible to clearly describe correlations, such as how increasing temperature leads to grain growth, thereby enhancing material strength. Then, it naturally leads us to consider integrating predictive models developed in pinax as computational modules within MInt.

Minamoto: One of the groundbreaking features of MInt is its ability to provide a method for solving inverse problems. In conventional materials development, the process begins with manufacturing steps, followed by analyzing microstructure, and then determining the properties and performance—this is known as the forward problem. Conversely, the inverse problem starts with the desired performance, identifies the required microstructure, and then determines the manufacturing process needed to achieve it. Solving inverse problems could dramatically reduce trial and error, which has long been a major goal for materials scientists. However, it remains an extremely challenging, and MInt offers one potential solution.

A major challenge now is expanding the range of solvable problems. Currently, solving inverse problems with MInt involves running numerous predictions using forward problem calculation modules, then analyzing the collective results. However, developing and implementing forward problem modules within MInt is a complex and time-consuming process. In contrast, building machine learning–based predictive models in pinax is significantly easier. If these models from pinax could be leveraged as computational resources within MInt, it would greatly expand the range of problems MInt can handle. Moreover, since machine learning models require less complex calculations, they can enhance computational speed even in forward-problem scenarios. This illustrates how system integration can solve challenges that MInt alone could not overcome.

Kadohira: We are also enhancing pinax's integration with RDE and MatNavi to facilitate the use of experimental and simulation data essential for developing predictive models in pinax. This not only accelerates the development of predictive models but also consequently expands the scope of solvable inverse problems. Ultimately, we aim to drive a transformative shift in materials development, much like how AI revolutionized strategies in shogi.

Minamoto: Currently, MInt is being used within NIMS and by a select group of companies involved in the Structural Materials DX-MOP project. Moving forward, we aim to lead in exploring new avenues for data utilization and developing innovative services.

Making "Material DX" from Trend to Standard

— As you continue developing various services and driving DX, what key considerations guide your approach? Additionally, could you share your vision for the future?

Kadohira: Earlier, I emphasized the need for a "platform" for AI-based analysis. However, if AI analyses alone were the goal, existing systems like those offered by Google could fulfill that need. The reason NIMS is developing our own system lies in our approach to system design, which incorporates a materials science perspective. For example, by pre-labeling data as related to manufacturing processes or crystal structures, correlations across datasets become clearer, making it easier to

"Promoting DX in materials development is about fostering a new culture."
— Isao Kuwajima

"I want to bring about a transformative shift in materials development, much like how AI revolutionized strategies in shogi."
— Takuya Kadohira

generate insights and suggestions for other users. Our strength is in designing systems tailored to the unique needs of materials research, ensuring seamless data workflow.

Kuwajima: How data is handled in each system directly impacts data collection strategies. Depending on its usage, we may need to adjust labeling methods or data structuring formats. In some cases, we even need to question the adequacy of existing databases, prompting us to rethink our approach from the ground up. This is why the three of us frequently discuss optimizing data collection methods. Moving forward, we plan to actively incorporate new approaches that enhance both quality and efficiency, such as using AI-based text mining to extract information from research papers.

When I give lectures at research seminars, I often see a clear divide: some researchers are highly interested in data-driven research, while others are not. I believe that DX in materials development is about fostering a new research culture. For researchers who have already established their own research styles, adapting to data-driven methods means embracing a completely different culture—a significant challenge. While overcoming this hurdle won't be easy, we will continue refining our services to ensure that more researchers can fully utilize MDPF's offerings and appreciate their value.

Kadohira: Some may feel that inputting research data into databases introduces new tasks that didn't exist before, seemingly contradicting the goal of "achieving research results as quickly as possible." However, by steadily advancing DX in materials research, I anticipate a paradigm shift—a moment when the underlying assumptions change, enabling researchers to achieve their desired outcomes at unprecedented speeds.

Minamoto: By then, the term "Material DX" will likely be obsolete. People might even say, "Oh, that was a thing once!" Right now, we are in a phase where we need to steadily demonstrate the benefits of data utilization and firmly establish them within the research community.

Even with pinax, integrating materials science–oriented features into the system makes its development and maintenance increasingly complex. Additionally, as the system scales up, updating the OS and protecting against cyberattacks become more demanding. In this sense, MDPF is deliberately taking on a challenging path. Yet, this is precisely why it makes sense for a national research institute to play a central role in DX. Even if it's labor-intensive, we are committed to doing what needs to be done. This commitment is shared by all members of MDPF, and we are deeply united as one team in achieving DX in materials development.

Special Roundtable
Pioneering Material DX
Conquering the Challenging Path to Success

Materials Data Platform

TOPICS

1 Advancing the Hydrogen Society: New Testing Facility for Hydrogen-Compatible Materials Completed

In October 2024, NIMS launched a facility to evaluate the mechanical properties of materials in a hydrogen environment under low-temperature and high-pressure conditions. This facility replicates temperatures from 20 K (-253°C) to 193 K (-80°C) and pressures from atmospheric levels to 10 MPa, covering an unprecedented range worldwide.

This facility enables the simulation of conditions essential for transporting and storing liquefied hydrogen. It allows the evaluation of material durability against liquefied hydrogen and low-temperature hydrogen gas, along with data on tensile and fatigue properties, and fracture toughness. Expanding material options for hydrogen infrastructure could reduce supply costs, a key barrier to widespread adoption of hydrogen energy. Material selection for hydrogen applications must consider hydrogen embrittlement in hydrogen gas environments and low-temperature embrittlement in liquefied hydrogen environments. However, few materials withstand these extreme conditions, making it difficult to achieve substantial cost reductions in hydrogen infrastructure. NIMS is currently refining facility operations, aiming to begin full-scale acquisition and provision of mechanical property data by the 2026 fiscal year. By supporting material development through evaluation testing, NIMS will play a crucial role in laying the foundation for a hydrogen-powered society.

*Press Release 2024.10.28
https://www.nims.go.jp/eng/press/2024/10/202410280.html

2 Improving the Reliability of Domestic Heat-Resistant Metallic Materials: Three Entries Related to the Creep Data Sheet Project Added to the "MIRAI Technology Heritage"

NIMS' "Creep Data Sheet Project," initiated in 1966, has been crucial in establishing the reliability of steel materials. The long-standing achievements of the project have earned recognition, with related materials registered as "Essential Historical Materials for Science and Technology※" (MIRAI Technology Heritage) for the fiscal year 2024.

In Creep Testing, steel test specimens are subjected to constant tension from both sides under high temperature, with deformation and fracture time measured. The results, published as "Creep Data Sheets," serve as key references for designing equipment that requires extremely high safety standards, such as thermal power plants.

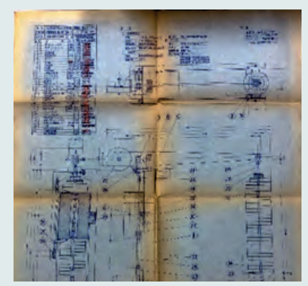
The registered materials include 1) the minutes and related documents of the Creep Committee of the Iron and Steel Institute of Japan, 2) the creep machine and its design drawings, and 3) the creep data sheets, test records, and creep fracture specimens. Notably, the creep machine, still in operation, is the first such equipment to be registered. The accompanying test records are highly detailed, noting specimen dimensions before and after testing, as well as incidents (e.g., power outages or earthquakes), showing rigorous management behind the process.

Thanks to the tireless efforts of engineers, the Creep Data Sheet Project has built unwavering trust. NIMS will continue to carry the torch for this vital work.

※Essential Historical Materials for Science and Technology … The National Museum of Nature and Science selects these materials annually to preserve and pass on the history of science and technology to future generations, under the nickname "MIRAI Technology Heritage."

*Press Release 2024.9.12
https://www.nims.go.jp/eng/news/2024/09/202409120.html

Minutes from the first "Creep Committee" meeting, the only document that outlines the origin of the project.



Blueprint of the creep machine. The frame of the 500 units still in operation remains the same as the original design.

Approximately 12,000 creep fracture test specimens, stored in a condition that allows identification by markings.

Launch of the Online Edition of NIMS NOW

Thank you for your continued readership of NIMS NOW, the public relations magazine of NIMS.

We are pleased to announce that NIMS NOW will launch its online edition in July 2025, making it more accessible to a wider audience. The online edition will be available in both Japanese and English, featuring not only the latest articles but also an archive of past issues, which will be gradually released for on-demand access at any time.

With the transition to the online edition, the print version of *NIMS NOW International* will be discontinued.
We kindly ask you to switch to the online edition.

Update info for the online edition will be announced through the NIMS official website, NIMS e-Newsletter, and NIMS social media accounts.

—— NIMS NOW Editorial Team

NIMS Official X

NIMS e-Newsletter

NIMS NOW International 2025. Vol.23 No.1
National Institute for Materials Science
https://www.nims.go.jp/eng/nims/publicity/publication/nimsnow/

Photo by Michito Ishikawa (cover, p.2-14) Writing by Kumi Yamada (p.6, p.8, lower half of p.9, upper half of p.10, p.11-14), Bifue Ushijima (p.7, upper half of p.9, lower half of p.10)
Editorial design by Barbazio Inc.
On the cover: Spectra Ultra S/TEM (see p.3 for details)

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ISSN 2436-3510