マテリアル戦略総合シンポジウム2023

Materials Innovation Strategy Symposium 2023

Proceedings

Date

December 5th (Tue), 2023

Venue

Hitotsubashi Hall, National Center of Sciences Building 2F (Tokyo)
※Online

Organized by

Data generation and utilisation materials Research and development projects (DxMT),
Advanced Research Infrastructure for Materials and Nanotechnology (ARIM),
NIMS Materials Data Platform (DICE),
NIMS Data Transformation Initiative Subcommittee Administrative Office,
NIMS Coordination Office of Central Hub, Central Hub of ARIM

Supported by

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Data generation and utilisation materials Research and development projects (DxMT):
Tohoku University, National Institute for Materials Science, The University of Tokyo,
Tokyo Institute of Technology, Kyoto University
Advanced Research Infrastructure for Materials and Nanotechnology (ARIM):
National Institute for Materials Science, Tohoku University, The University of Tokyo,
Nagoya University, Kyoto University, Kyushu University, Hokkaido University,
Chitose Institute of Science and Technology, Yamagata University, University of Tsukuba,
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MatISS 2023

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文部科学省マテリアル戦略総合シンポジウム2023　予稿集

Materials Innovation Strategy Symposium 2023

マテリアル戦略総合シンポジウム2023

予稿集

開催日

2023年12月5日(火)
※オンライン併用開催　LIVE

会　場

一橋大学 一橋講堂（東京都千代田区一ツ橋 学術総合センター2階）

共　催

文部科学省 データ創出・活用型マテリアル研究開発プロジェクト（DxMT）、
文部科学省 マテリアル先端リサーチインフラ（ARIM）、
NIMS 材料データプラットフォーム、
NIMS データ創出・活用型データ連携部会運営室、
NIMS マテリアル先端リサーチインフラセンターハブ運営室

後　援

内閣府

参画機関

文部科学省データ創出•活用型マテリアル研究開発プロジェクト（DxMT）:
東北大学、物質・材料研究機構、東京大学、東京工業大学、京都大学、
文部科学省マテリアル先端リサーチインフラ（ARIM）:
物質・材料研究機構、東北大学、東京大学、名古屋大学、京都大学、
九州大学、北海道大学、公立千歳科学技術大学、山形大学、筑波大学、
産業技術総合研究所、早稲田大学、東京工業大学、電気通信大学、
北陸先端科学技術大学院大学、信州大学、名古屋工業大学、豊田工業大学、
自然科学研究機構分子科学研究所、大阪大学、日本原子力研究開発機構、
量子科学技術研究開発機構、奈良先端科学技術大学院大学、広島大学、
香川大学

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December 5th (Tue.), 2023, Hitotsubashi Hall
2023年12月5日(火)　一橋講堂(学術総合センター2F)

10:00–10:10 Opening Remarks　開会挨拶

10:00-10:05

Ministry of Education, Culture, Sports, Science and Technology
文部科学省

10:05-10:10

Kazuhiro Hono (President, National Institute for Materials Science, Japan)
宝野 和博（物質・材料研究機構理事長）

Session 1 10:10–11:50 Environment surrounding data-driven research
データ駆動型研究を取り巻く環境

10:10-10:40

Hiroko Takuma (Research Promotion Bureau, Ministry of Education, Culture, Sports, Science and Technology)
宅間 裕子（文部科学省研究振興局 参事官）
“Project Initiatives”
「事業の取り組みについて」

10:40-11:15　【Plenary Lecture 1　基調講演 1】

Hideo Hosono (Tokyo Institute of Technology)
細野 秀雄（東京工業大学 栄誉教授）
“Quantum Material and Catalysis”
「量子物質と触媒作用」

11:15-11:50　【Plenary Lecture 2　基調講演 2】

Thomas Schrefl (Professor, University for Continuing Education Krems, Austria)
“Materials informatics for permanent magnet design”

11:50–13:00　【Lunch 昼食】

Session 2 13:00–14:15 Collaboration of DxMT and ARIM
DxMT、ARIM の融合

13:00-13:25

Keitaro Sodeyama (National Institute for Materials Science)
袖山 慶太郎（物質・材料研究機構）
“Materials research DX activities in the Digital Transformation Initiative Center for Magnetic Materials”
「データ創出・活用型磁性材料研究拠点における材料研究DXの取り組み」

13:25-13:50

Tetsuya Shoji (TOYOTA)
庄司 哲也（トヨタ自動車株式会社）
“Toward DX　～ Common condition of Material measurement for Material map ～”
「DXに向けて　～計測の標準条件とマテリアルマップ構築に向けて～」

13:50-14:15

Yoshio Mita (The University of Tokyo)
三田 吉郎(東京大学)
“New Energy Materials and Devices Research with 1000 comrades in UTokyo”
「東大拠点1000名の仲間と拓く新規エネルギーマテリアル・デバイス研究の新展開」

14:15–14:30 【Coffee Break 休憩】

Session 3 14:30–15:50 Expectations for DPF infrastructure development for ARIM-DxMT collaboration
ARIM-DxMT 融合に向けた DPF インフラ発展への期待

Facilitator（ファシリテーター）

Takuya Kadohira (National Institute for Materials Science)
門平 卓也（物質・材料研究機構）

Panelists（パネリスト）

Katsufumi Ohsumi (Nagoya University)
大住 克史（名古屋大学）

Tadashi Furuhara (Tohoku University)
古原 忠（東北大学）

Yu Hoshino (Kyushu University)
星野 友（九州大学）

Shoichi Matsuda (National Institute for Materials Science)
松田 翔一（物質・材料研究機構）

Toshio Kamiya (Tokyo Institute of Technology)
神谷 利夫（東京工業大学）

Mitsuaki Kawamura (The University of Tokyo)
河村 光晶（東京大学）

Taro Takemura (National Institute for Materials Science)
竹村 太郎（物質・材料研究機構）

Tetsuya Shoji (TOYOTA)
庄司 哲也（トヨタ自動車株式会社）

Koichiro Kato (Kyushu University)
加藤 幸一郎（九州大学）

Toshiyuki Tsuchiya (Kyoto University)
土屋 智由（京都大学）

15:50–16:00 【Coffee Break 休憩】

Session 4 16:00–17:20 Poster Session
ポスターセッション

17:25–17:30 Closing Remarks 閉会挨拶

17:25-17:30

Satoshi Itoh (Sub Program Director, DxMT and ARIM)
伊藤 聡（DxMT、ARIMサブプログラムディレクター）

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Session 1

Environment surrounding data-driven research

データ駆動型研究を取り巻く環境

【Plenary Lecture 1 / 基調講演 1】

“Quantum Material and Catalysis”
「量子物質と触媒作用」

Hideo Hosono (Tokyo Institute of Technology)
細野 秀雄（東京工業大学 栄誉教授）

Quantum Material and Catalysis
量子物質と触媒作用

[1,2]Hideo　Hosono
[1]Tokyo Institute of Technology, 4259 Nagatsuta, Midori, Yokohama 226-8503, Japan
[2.] National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

Abstract
Last decade our group has concentrated on application of quantum materials to catalysis, seeking unique catalytic activity for demanding chemical reactions. The quantum materials chosen are electride and topological insulators, and the chemical reactions focused are ammonia synthesis (N_2 activation) and organic urea synthesis at mild conditions, and efficient H_2 ortho-para conversion. This talk reports recent results on these researches along with the approach.

I. Introduction
Quantum materials and catalysis have been studied in the different academic discipline, i.e., condensed matter physics and chemistry. The role of catalysts is of quite importance for resolving energy and zero-carbon emission, and innovative idea for novel catalysts is required to meet these issues.　Although traditional material combined with transition metal have extensively studied to date, I think introduction of non-traditional materials is pivotal for realizing innovative catalysts for the above targets

II. Electride catalysts for green NH_3 synthesis [1]
Electride is a material in which electrons serve as anions, and is a novel conceptional solid. Various types of electride materials have been synthesized since our first report on RT stable electride, C12A7:e, in 2003. A unique property of our electride materials is to have both low work function and chemical/thermal stability unlike alkali metal. We utilized transition metal (TM)-loaded electride as catalyst for NH_3 synthesis at mild conditions toward green NH_3 synthesis. Strong electron-donating power of electride combined with the ohmic contact nature (contact of TM/conventional support is Schottky-type) with TM nanoparticles successfully activates N_2 adsorbed and the activation barrier for N_2 dissociation is reduced to almost the half of the previous catalysts. Fig.1 summarizes our progress in electride materials and electride-based catalysts.

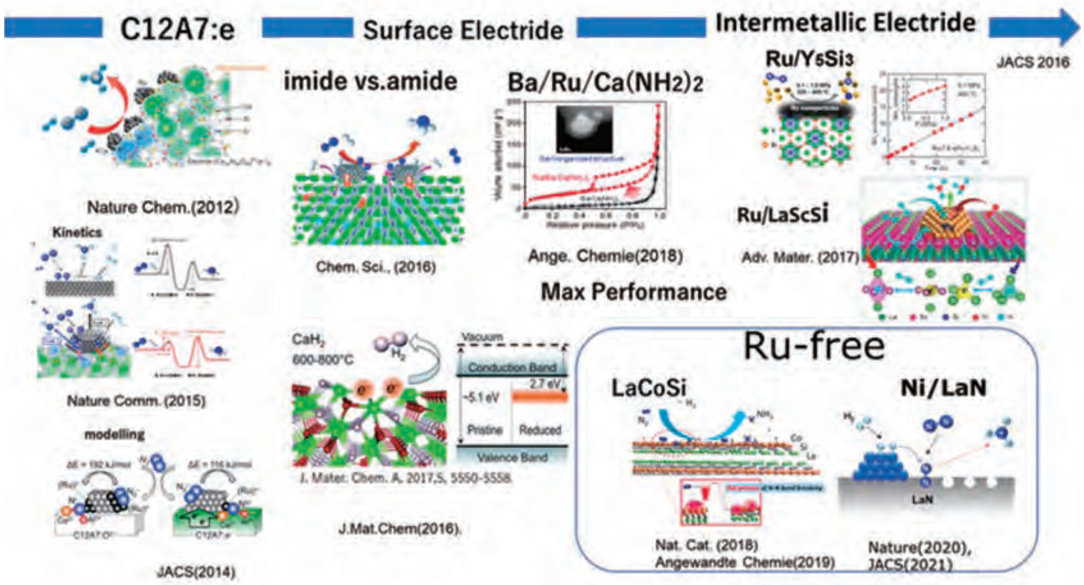


Fig.1. Progress in electride-based catalysts for NH_3 synthesis.

III. Topological catalyst for RT organic urea synthesis

The unique quantum properties of Bi_2Se_3 make it a promising catalyst for the synthesis of organic ureas, Thanks to its topological surface states, the proposed catalyst exhibits remarkably high catalytic activity and durability when used for the synthesis of various urea derivatives, which are usable as nitrogen fertilizers. We found that the spin state of the O_2 molecule is changed from triplet to singlet by the local magnetic field arising from the strong spin–orbit interaction of Bi and the singlet O_2 with much higher reactivity pulls hydrogen out from the amine, reducing energy barrier for the desired reaction. This catalytic effect is a result of the unique features of topological materials and the appropriate element choice of Bi and Se for this reaction.

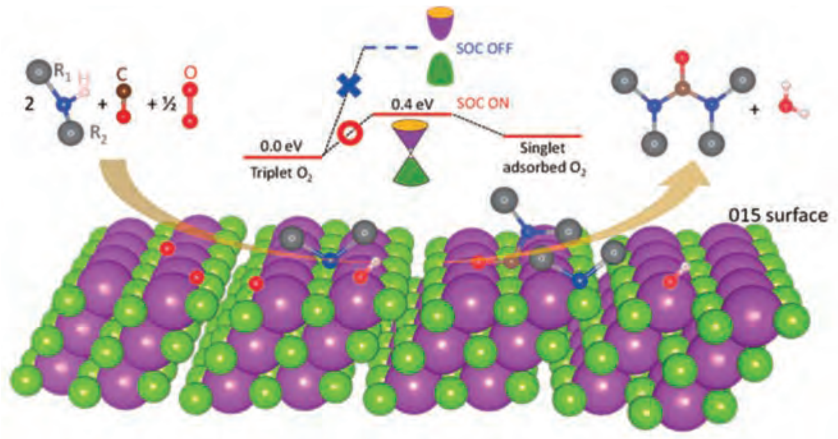


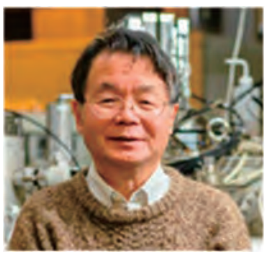
Fig.2 Reaction mechanism for organic urea synthesis from amine, CO and O_2 on Bi_2Se_3 (015) surface. Singlet O_2 is stabilized on Bi and extracts H from amine adsorbed on Se to give rise to urea bonding.

III. Exploration for catalysts for H_2 ortho-para conversion [3]

Research on H_2 o-p conversion catalyst has a long history but the designing concept is still unclear. We performed extensive catalyst screening of ~170 materials ranging non-magnetic insulating oxides to magnetic metals. The results show magnetic metals do not exhibit high activity, suggesting the most influential factor is electric field gradient around H_2 adsorbed on insulating material.

References

[1]Review: Hosono and Kitano, *Chem. Rev*. 121, 3121–3185(2021); Hosono, *Faraday Discuss*., 243, 9-26(2023),
[2] Li, Wu, Tada, Kitano ---,and Hosono, *Sci. Adv*. 9, eadh9104 (2023).
[3] Abe, Mizoguchi, Eguchi and Hosono, *Exploration*, in press.



<CV> Hideo Hosono is an honorary and institute professor of Tokyo Institute of Technology and a distinguished fellow and a group leader at National Institute for Materials Science. He received a Ph.D. from Tokyo Metropolitan University in 1982, and became a professor of Tokyo Tech in 1999 via Nagoya Tech, Institute for Molecular Science and Vanderbilt University. His research focus is creation of novel functional materials based on own design concept. The representative achievements so far are material design of transparent oxide semiconductors such as IGZO and their TFT applications for the state-of the art displays (OLED-TVs are driven by IGZO-TFTs), creation of stable electrides and discovery of high-Tc iron-based superconductors. He is a recipient of various honors including the Japan Prize, von Hippel Prize (MRS), J. McGroddy Prize (APS), Karl Brawn Prize (SID), Eduard Rhein Award, Imperial Prize (the Japan Academy), and is a Thomson Reuter Citation Laureate and a foreign fellow of the Royal Society.

【Plenary Lecture 2 / 基調講演 2】

“Materials informatics for permanent magnet design”

Thomas Schrefl
(Professor, University for Continuing Education Krems, Austria)

MATERIALS INFORMATICS FOR PERMANENT MAGNET DESIGN

[1]T. Schrefl, [1]A. Kovacs, [1]C Wager, [1]Q. Ali, [1]J. Fischbacher, [1]D. Böhm, [1]L. Breth
[2]M. Yano, [2]N. Sakuma, [2]A. Kinoshita, [2]T. Shoji, [2]A. Kato

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Abstract

In materials science, it is difficult to establish reliable machine predictions due to the limited available data. Accurate physics simulations based on electronic structure and micromagnetic theory are time-consuming even on modern hardware. Similarly, gathering experimental data that relates to the structure and property of magnetic materials is cumbersome. In this talk, I will propose strategies to address these problems. I will discuss several approaches for data generation and data analysis which may form building blocks for artificial intelligent assisted magnet design.

I. INTRODUCTION

Classical artificial intelligence algorithms, such as genetic optimization[1], facilitate the inverse design of materials. This process begins with the desired target properties, and then alterations are made to the chemical composition and microstructural features to achieve optimal design points. A crucial requirement for this process is the rapid evaluation of the objective function. This typically necessitates the substitution of experimental measurements and physics simulations with surrogate models, which can quickly provide estimates of the desired properties. To construct reliable models, data must be collected from a variety of sources.

II. COMBINING DATA

A strategy for constructing data-driven predictors involves the integration of data from diverse sources. I will present the use of partial least square regression for estimating the intrinsic magnetic properties, which combines data from both ab-initio simulations and experimental measurements.[2] The method utilizes projection to latent space for reducing dimensionality. It is a traditional machine learning method in the field of materials informatics.[3] When this technique is paired with a predictor for the hysteresis properties of a core-shell grain, it enables us to optimize both the chemical composition, $(Nd,La,Ce)_2(Fe,Co)_{14}B$, and the core-shell geometry for hot-deformed magnets. Fig. 1. shows a scenario where the goal is to achieve the highest possible coercivity while simultaneously minimizing costs. This is relevant in cases where certain defects are inevitable. For example, a defect shell (Fe-containing grain boundary phase) of a fixed thickness might surround the grains.

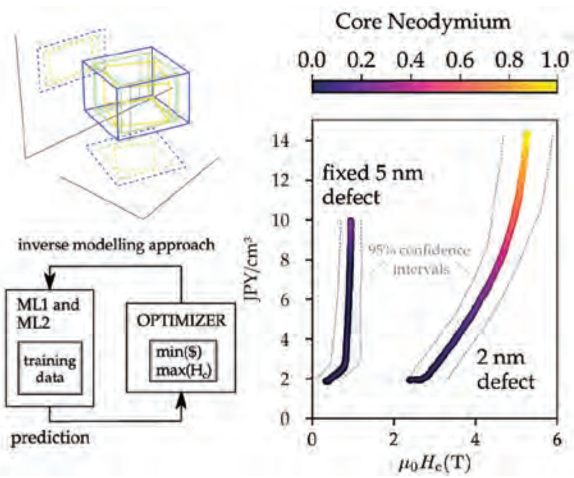

Fig. 1 Minimizing materials costs and maximizing coercive field by multi-objective optimization using machine learning models (ML) as surrogate. ML1 predicts the intrinsic magnetic properties from the chemical composition; ML2 predicts the coercive field from the intrinsic properties and the geometry. The right part shows the Pareto fronts for a fixed soft magnetic defect thickness of 2 nm or 5 nm. The results show the Nd-content of the core can be reduced significantly.

III. STATISTICAL MICROSTUCTURE MODELS

Reliable predictions of magnetic properties require computational models that accurately represent the granular structure of a magnet. I will present a method that extracts statistical features from Scanning Electron Microscopy (SEM) images and tunes the parameters for synthetic microstructure generation to statistically match the experimental images. The process includes image segmentation using U-net neural networks[4] to identify grains, grain boundaries, and secondary phases. A Bayesian optimizer is then used to minimize the Euclidean norm between the power spectra derived from the SEM image and the model.

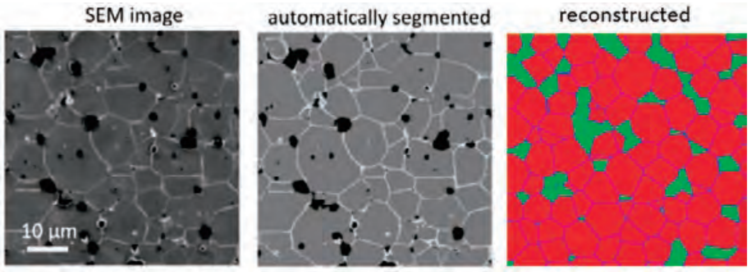

Fig. 2 Synthetic microstructure generation based on SEM images.

IV. INFORMATION RETRIEVAL WITH LARGE-LANGUAGE MODELS

Valuable data is hidden in documents including scientific papers, internal reports, and datasets from experiments and simulations. These documents are mostly unstructured which make it difficult to automatically search and extract material properties. I will show how open-source language models combined with semantic search allow users to extract relevant data from unstructured documents. Fine-tuned prompts[5] for chain-of-thought retrieval help to find correct values of material properties and avoid hallucination.

V. ACKNOWLEDGEMENT

The financial support by the Austrian Federal Ministry for Digital and Economic Affairs, the National Foundation for Research, Technology and Development, Austria and the Christian Doppler Research Association, Austria is gratefully acknowledged. Data of first-principles computations was computed using the facilities of the Supercomputer Center of the Institute for Solid State Physics at the University of Tokyo, and computational resources of supercomputer Fugaku provided by the RIKEN Center for Computational Science (Project ID: hp220175).

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[3] R. Krishna, *Materials Today* 8.10 (2005), pp. 38-45.
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[5] M. P. Polak and D. Morgan, arXiv:2303.05352 (2023).

Thomas Schrefl, Christian Doppler Laboratory for magnet design through physics informed machine learning, University for Continuing Education, Krems, Austria

Thomas Schrefl is the head of the Center for Modelling and Simulation at the University for Continuing Education in Krems, Austria. He received his PhD from TU-Wien in 1993 and habilitated in “Computational Physics” in 1999. He has worked at IMB Research on parallel solvers for micromagnetic problems and served as a Professor of Functional Materials at the University of Sheffield. He has applied numerical micromagnetic simulations to address design questions in magnetic recording, magnetic sensors, and permanent magnets. His current research interests include the use of machine learning in materials science.

Session 2

Collaboration of DxMT and ARIM

DxMT、ARIM の融合

“Materials research DX activities in the Digital Transformation Initiative Centerfor Magnetic Materials”

「データ創出・活用型磁性材料研究拠点における材料研究 DX の取り組み」

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Yoshio Mita (The University of Tokyo)

三田 吉郎（東京大学）

データ創出・活用型磁性材料研究拠点における材料研究 DX の取り組み
Materials research DX activities in the Digital Transformation Initiative Center for Magnetic Materials

K. Sodeyama

National Institutes for Materials Science,
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Abstract

As the activities of the Digital Transformation Initiative Center for Magnetic Materials (DXMag) in the Data generation and utilization materials Research and development projects (DxMT), experimental and computational data are accumulated in the RDE system developed by NIMS. In order to use these data from different researchers, it should be integrated for the materials informatics analysis. To integrate the data, we create common vocabulary lists of magnetic materials and sets up measurement rules. In this presentation, such activities will be introduced.

For the new materials search through big materials data, DXMag is accumulating experimental data, mainly from XRD, VSM and SEM, to the RDE system. To accumulate data in the RDE, the data structure is determined in advance for each measurement. Especially for the table data, it is necessary to perform format conversion in advance and we have prepared the scripts for the usage.

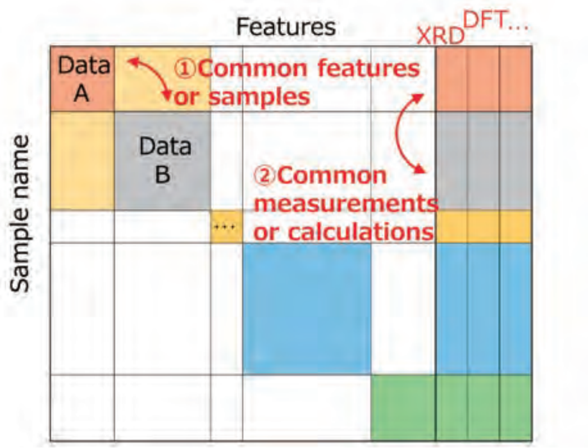

Fig. 1 Big table integrated by different researchers materials data

The accumulated data itself can be immediately used for MI analysis without uploading process for the RDE. In order to proceed with the material DX, the data from different researchers are neeed to be integrated. Specifically, the constructing large table data, as shown in Fig. 1, should be carried out. At this point, if the data held by researchers A and B are completely independent, it is difficult to integrate the data, and the non-diagonal components of the big table will contain only blanks. However, even if the data are from different researchers but using the same features obtained by the same measurements or the same samples, it is possible to extend the searching space.

Here, when different researchers use different vocabularies for the same physical phenomenon, it is difficult to integrate the data items correctly for making the big table. To overcome this difficulty, DXMag is making a vocabulary list for magnetic materials. All the vocabulary used by each researcher is listed, and the information about the relationship between the vocabularies which have similar meaning is stored. Furthermore, the MatVoc system, which is developed by the NIMS data platform center, is used for the integration of the data obtained in the whole centers in DxMT. A unique ID is assigned to each vocabulary and the relationships between vocabulary words are stored together with their descriptions and thesauri.

Another difficulty in data integration is the difference in experimental conditions of the measurement data. For example, if the measurement range of the spectrum measured by researcher A is different from that of researcher B, it is difficult to use them together; DXMag has determined recommended values for the measurement ranges of XRD and SEM. Regarding this measurement rules, we will refer the ARIM’s treatment.

- - - - - <Keitaro Sodeyama>, <National Institute for Materials Science>

<CV>
Keitaro Sodeyama is the field director of Data-driven Materials Research Field, Center for Basic research on Materials, National Institute for Materials Science, Japan.
Keitaro Sodeyama received PhD in Waseda University

Toward DX
～ Common measurement condition for Material map ～
DXに向けて
～計測の標準条件とマテリアルマップ構築に向けて～

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[1]Toyota Motor Corporation, Advanced Data Science Management Div. Otemachi Bldg. 6F, 1-6-1 Otemachi, Chiyoda-ku, Tokyo, Japan

[2]DXMag PI,

Abstract

Recent rapid evolution of computational power and generalization of AI technology make us easier to access data analytics for material science. Using dimensionality reduction properly, one can project high dimensional spectrum data into lower dimensional space. When one create this like space by material structural data, e.g. XRD, one can draw Material Map as common latent space for gathering data. In order to do so, one has to recognize range and dimension of data records. In this talk, I will introduce data management activities in DXMag to establish Material Map for magnetic materials.

I. Introduction

Recent rapid evolution of computational power and generalization of AI technology enables information extraction from variety types of data. Commonly, material researchers and engineers tend to recognize AI technology as tools for machine learning for table data in their material R&D scene. But most important point of material informatics is how to access meaningful descriptor buried in high dimensional material measurement data which is difficult to quantify. Moreover, material data have multi-scale and multi-modal problem. This fact makes data utilization more difficult. In order to get over this situation, we focused on wave number “q-space” expression for handling multi scale structural data, as shown in Figure 1. Using q-space expression, we can connect from atomistic diffraction information to structural scattering information based on principle of diffraction and scattering. In low q range, we can use power spectrum of microscope image instead of low-q scattering measurement. Based on this fact, we can recognize that we can express multi-scale structural information in one curve which is consist of scattering, or power spectrum, and diffraction[1]. To extract information from multiscale dataset, we utilize dimensionality reduction technique for high dimensional multiscale data.

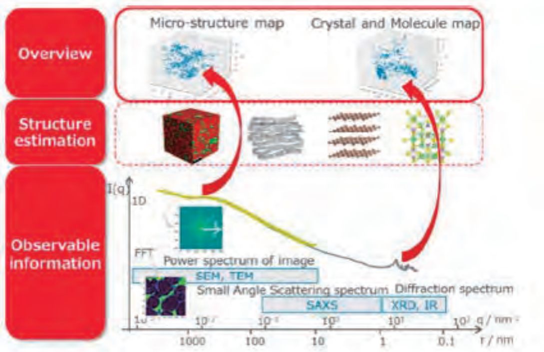

Figure 1 q-space expression of multiscale expression and corresponding measurement.

II. Dimensionality Reduction

For example, we start with 35 different composition and nanostructure Light Rare Earth alloyed nano structured $Nd_2Fe_{14}B$ rare-earth magnet samples and measure X-ray diffraction (XRD)[2]. One XRD data consists of 3500 dimensions. Commonly known that XRD spectrum consist of diffraction information from atomistic configuration and small angle scattering information from nano and microstructure. To extract feature from these 35 XRD data, we use PCA, principal component analysis, to decompose 10 independent vectors as shown in Figure 2. In this case cumulative contribution ratio is more than

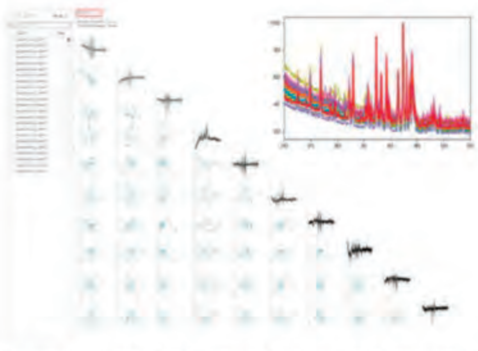

Figure 2 35 XRD data of Nd reduced rare earth magnet and 10 decomposed vectors by PCA analysis

0.95 with these 10 vectors. Looking at decomposed vector with knowledge of diffraction and small angle scattering, one can understand meaning of each vector. In this case, 1st principal component (PC) corresponds to difference of scattering by nanostructure and part of peak shape change and 2nd PC corresponds to peak shift of $RE_2Fe_{14}B$ phase, this means that change of lattice parameter by alloying Light Rare Earth element in $Nd_2Fe_{14}B$ phase. 3rd PC represent change of peak width. Then we use coefficient of each PC as descriptor for magnetic performance machine learning model. Coefficient of PC seems to works well as good descriptor shown in Figure 3.

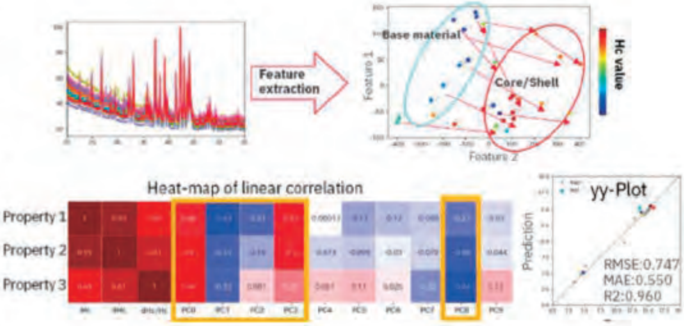

Figure 3 Correlation of properties and PC coefficient.

From our attempt, one can recognize dimensionality reduction is good tool to extract features from high dimensional data set.

III. Material Map

One more way to use dimensionality reduction is drawing Material Map. If one chooses dimensionality reduction technique like UMAP or t-SNE, or defining more complicated embedding space, one can define common latent space in relatively secure manner. Using this space for projecting material structural data like XRD, we, or member of DXMag call this latent space as Material Map. To draw Material Map, data management activities are very important. Currently, we trying to set common rule for measurement and calculation conditions. Also, we are trying to define DX routine as standard workflow to accumulate data. During carrying out brush up data management activity, our understanding of material data become deeper. For example, “accuracy” and “precision” for first principle calculation, difference of pixel resolution of microscope images, scattering and diffraction information included in XRD, etc. We are now trying to understand what we have to take into consideration for data acquisition and data utilization and integration among DXMag members. Hopefully, our activity become one of the solutions for next generation data utilization R&D activity.

Acknowledgement

This work was partially carried out in MEXT Program: Data Creation and Utilization Type Material Research and Development Project（Digital Transformation Initiative Center for Magnetic Materials） Grant Number JPMXP1122715503.

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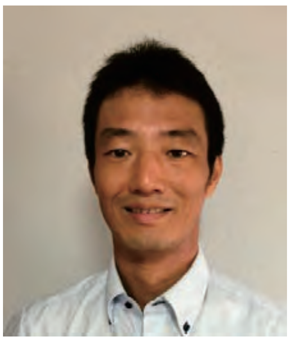

Tetsuya Shoji, Advanced Data Science Management Div. Toyota Motor Corporation

Tetsuya Shoji is Project Head of WAVEBASE project, supporting service of Material informatics and Digital transformation of corporation R&D from 2022. He received his PhD from Hokkaido-University in 2003. He started his carrier at Toyota Motor corporation from 2003. He involved in permanent magnet research from 2004 and establish low melting point NdCu alloy infiltration to hot deformed magnet in 2010 (patent filed). During 2014 to 2015 fiscal year, he spent his carrier at MEXT. After back to TMC, he developed Nd reduced magnet, Gallium Oxide power semiconductor and MI platform WAVEBASE as Chief Professional Engineer from 2019.

New Energy Materials and Devices Research with 1000 comrades in UTokyo
東大ARIM拠点1000名の仲間と拓く新規エネルギーマテリアル・デバイス研究の新展開

Yoshio Mita[1,2,3]

[1]Dept. of Elec. Eng. and Info. Sys., [2]Systems Design Lab. Platform Device Research Division, [3]Nanosystem Integration Center Device Research and Development Division, Graduate School of Engineering, The University of Tokyo. 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656 Japan

Abstract
Among the Sustainable Development Goals, energy is of the highest priority in order to share advanced information technology with billions of humans. Towards the challenge, three independent groups in the University of Tokyo, specialized in Nanofabrication, Nanoanalyses, and Information Technology form the ARIM “Energy Five Star” one team, in collaboration with Hiroshima University and JAEA spokes. The speaker is leading Nanofabrication since 2003 in Takeda Sentanchi Supercleanroom. In the talk, the new vision of UTokyo ARIM NanoHub center on the Energy Materials and Devices Research with his 1000 comrades will be discussed.

I. INTRODUCTION
When talking about “Energy Device”, one can intuitively imagine (1) electricity generators such as photovoltaic cells, Seebeck electricity generator, and MEMS energy harvesters. Another one may imagine (2) electricity storages such as battery, supercapacitors, and flywheels. Of course these are all important devices; however, these points of views are only highlighting a limited aspect of energy. In an electro information system, in fact, both *increasing* the *energy providing capability* and *decreasing* the *energy loss and consumption* works equally. The UTokyo ARIM group is aware of the principle and have identified three other domains under “Energy” umbrella: (3) Transporting devices such as inverter-converters and matching circuitry and devices, (4) Using devices such as sensors, processors, and actuators with reduced energy consumption. By naturally extending the consideration, one can reach the conclusion that the real goal to share advanced information technology with billions of humans is to (5) *increase* the *amount of functionality* with the available energy. We call it Energy Five Stars (Fig.1). In the talk, a couple of supporting examples composing the energy five stars, will be presented such as monolithic series-connected photovoltaic cells[1] and high-sensitivity integrated Piezoelectric MEMS Ultrasound Transducer (PMUT)[2], all developed in the UTokyo Takeda Supercleanroom by using CMOS-MEMS scheme[3].

II. Methods for sustainable development in the University’s open platform
In Dec. 2003, Takeda Sentanchi Supercleanroom was open to UTokyo researchers. Since 2007, MEXT has been sponsoring Takeda SCR to open it to external users. In 2022, 186 independent research groups worked actively. They are composed of UTokyo School of Engineering, Other Faculties of UTokyo, Other Universities and Public Research Institutes, and companies. The potion is approximately 1:1:1:1, thereby underlines the unique value of Takeda: A Real Open Platform. The number of comrades (not “clients”, and more than “users”, because they accept the “common value” of open platform) is around 1000. To handle such a big number of projects, the only way is “to be successful in the minimum trials”. For that purpose, “DX” has become one of our core interests. The UTokyo NanoFab hub site tries to realize “minimum trial” by three steps, as shown in Fig.2: (1) *provide as-is* available process data, (2) receive the *feedback* of individual process, then (3) *improve* the process data by ARIM engineers. In the talk, some initial attempts as well as similar attempts in worldwide open platforms will be presented.

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[2] K. Suzuki *et al.*, *in Proc. of IEEE IUS* (2020). doi: 10.1109/ius46767.2020.9251511
[3] Y. Mita *et al.*, *Jpn. J. of Appl. Phys.*, **56** (2017), pp.06GA03. doi: 10.7567/JJAP.56.06GA03

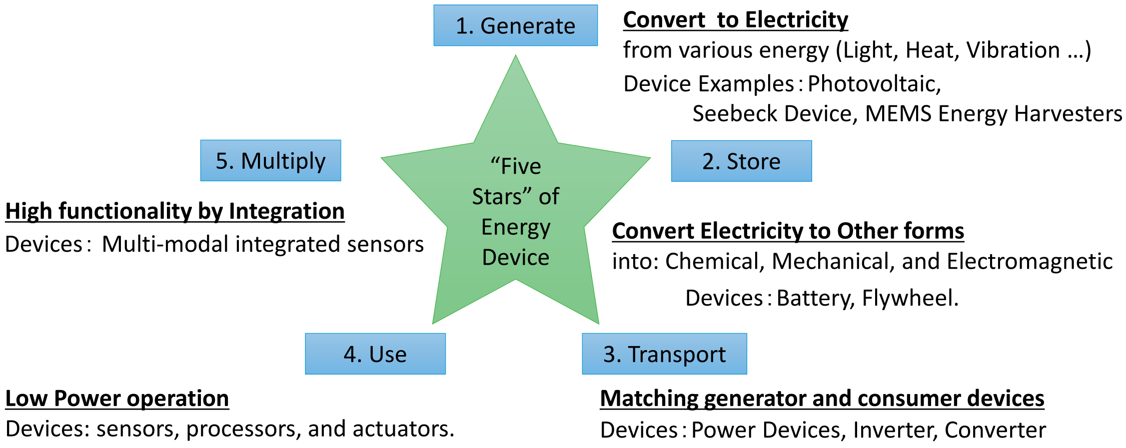

Fig. 1
"Energy Five Stars" concept. Not only generating and storing but also matched transport and use can contribute.

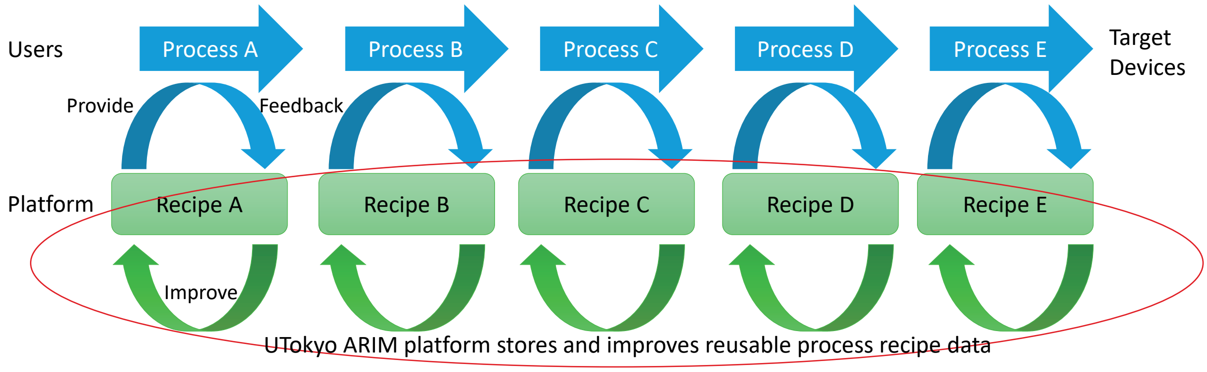

Fig. 2
"Provide, feedback, and improvement" can store excellent process recipes and will lead 1000 users' success with minimum trials.

Yoshio Mita, Dpt. of Electrical Engineering and Information Systems, the University of Tokyo, Japan

Yoshio Mita is a professor of Department of Electrical Engineering and Information Systems, The University of Tokyo, Japan. He obtained his BE (1995), ME (1997), and PhD (2000), from Departments of Electrical and Electronic Engineering, UTokyo. He served as an assistant professor of VLSI Design and Education Center (VDEC), UTokyo, and was promoted to Lecturer in 2001, to Associate Professor in 2005, and Professor in 2022, all at the Department of Electrical Engineering and Information Systems. He has been a co-principal investigator (PI) of Intelligent Semiconductor Microdevices Laboratory (SML) since 2002, and a single PI since 2013, as well as serving as a leader of UTokyo's open nanotechnology platform federal class1 supercleanroom (Takeda SCR). His research interest includes CMOS and MEMS integration technology. Until now, he has been co-(and first-) authored 75 journal papers and 152 International Conferences, including 4 keynote talk and 13 invited talks. In 2021, Pr. Mita has been awarded as senior member both from IEEE and IEE of Japan.

Session 3

Expectations for DPF infrastructure development for ARIM-DxMT collaboration

ARIM-DxMT 融合に向けた DPF インフラ発展への期待

Expectations for DPF infrastructure development for ARIM-DxMT collaboration
ARIM-DxMT 融合に向けた DPF インフラ発展への期待

14:30-14:35　Introduction of panelists and explanation of purpose / パネラー紹介・趣旨説明
Facilitator / ファシリテーター:
Takuya Kadohira (NIMS) / 門平 卓也(物質・材料研究機構)

14:35-15:10　Topic (1): Data from experimental equipment - advanced and general purpose /
トピック(1)：実験装置からのデータ　-先端と汎用-

Why accumulate data? Beyond that, there are two main objectives. High-generality and quality data required by data science methods. Data to achieve the focused objectives of cutting-edge research at the world level. Can general-purpose and cutting-edge be compatible? Can they be integrated for the future?

なぜデータを蓄積するのか。この問いの先には、大きく分けてふたつの目的がある。データ科学手法が要求する汎用的でかつ高品質なデータ。世界レベル最先端研究の絞り込まれた目的に向かうためのデータ。汎用と先端は両立できるのか?将来に向けて統合はできるのか?

Topic Provider / 話題提供:
- Yu Hoshino (Kyushu University) / 星野 友(九州大学)
- Shoichi Matsuda (NIMS) / 松田 翔一(物質・材料研究機構)
- Taro Takemura (NIMS) / 竹村 太郎(物質・材料研究機構)
- Koichiro Kato (Kyushu University) / 加藤 幸一郎(九州大学)
- Toshiyuki Tsuchiya (Kyoto University) / 土屋 智由(京都大学)

15:10-15:45　Topic (1): Data from experimental equipment - advanced and general purpose /
トピック(2):ツールを使いこなす人材 -現状と未来-

The platform function is supported by the development of ICT technology. Not only the evolution of the tool ecosystem surrounding data-driven research but also the human resources to use it are extremely important. What is the state of the art now and how will it change in the future? What precedents should we refer to, and what should the DPF's position be?

プラットフォーム機能は、ICT 技術の発展に支えられている。データ駆動型研究を取り巻くツールエコシステムの進化はもちろんのこと、それを利用する人材の充実も極めて重要。今どのような状態にあり、未来に向かってどう変化していくのか?参考にすべき先行例は? DPF の立ち位置はどうあるべきなのか?

Topic Provider / 話題提供:
- Tetsuya Shoji (TOYOTA) / 庄司 哲也(トヨタ自動車株式会社)
- Katsufumi Ohsumi (Nagoya University) / 大住 克史(名古屋大学)
- Mitsuaki Kawamura (The University of Tokyo) / 河村 光晶(東京大学)
- Tadashi Furuhara (Tohoku University) / 古原 忠(東北大学)
- Toshio Kamiya (Tokyo Institute of Technology) / 神谷 利夫(東京工業大学)

15:45-15:50　Closing / クロージング

Session 4

Poster Session

ポスターセッション

World-Class Materials Database provided by NIMS

I. Kuwajima, T. Itoh, A. Matsuda, M. Ishii, Y. Xu, Y. Ono, K. Sawada and M. Demura

Materials Data Platform, Research Network and Facility Service Division
National Institutes for Materials Science (NIMS),
1-1 Namiki, Tsukuba, Ibaraki, 305-0054, Japan

Abstract

NIMS serves as a core data center in an initiative to establish materials DX platforms across Japan led by the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). The materials data platform, DICE[1)], plays a pivotal role in the imitative. As one of the DICE services, we offer the NIMS Materials Database (MatNavi)[2)] available via the internet to contribute to the development of new materials and material selection.

The MatNavi is an integrated database system comprising 8 materials databases. As shown in Table 1, MatNavi is the world's largest and can be regarded as the one and only materials database. The Polymer DB, PoLyInfo, provides the information curated from academic papers such as the chemical structures of monomers and polymers, the physical properties, the polymerization conditions together with additional characterization data obtained by our own experiments. We offer two types of inorganic materials databases: AtomWork (free version) and AtomWork-Adv[3)] (paid version). The AtomWork-Adv have much more data than AtomWork as well as various viewing features and data download capabilities, which are not available in AtomWork. Both the Inorganic Material DBs includes crystal structures, phase diagrams, physical properties curated from academic papers. The Metallic Material DB, Kinzoku, provides the reliability information of commercially used metallic materials such as the creep and fatigue properties as well as the fundamental mechanical properties. These data are provided in the form of datasheet as the NIMS Structural Materials Data Sheets (4 types: creep, fatigue, corrosion, space use materials). Note that these data on metallic structural materials are obtained by our own experimental testing lasting over 40 years.

In addition to the conventional use of searching and browsing material data and referring to the results, in recent years, data-driven research has attracted attention as a dataset for use in machine learning and other applications. To respond to these requests, we are considering and providing rules for the use of data as a single dataset.

Table 1. Data sources, number of data and characteristics of representative databases (As of 28 October 2023.)

Database name	Data source	Number of data	Characteristic
Polymer Database (PoLyInfo)	From academic papers	Polymer structures: 29,004 Polymer samples: 150,351 Properties data points: 494,837	World-class polymer data with no comparison
Inorganic Material Database (AtomWork-Adv)	From academic papers	Crystal structures: 364,668 X-ray diffraction: 659,240 Phase diagrams: 46,607 Properties data points: 459,238	Integrated handling of world-class data
Metallic Materials Database (Kinzoku)	NIMS original experimental data	Materials: 500 Different condition samples: 3,500 Properties data points: 82,700	Systematic experimental data using a standardized test method
NIMS Structural Materials Data Sheets	NIMS original experimental data	Creep DS: 61 books Fatigue DS: 134 books Corrosion DS: 7 books Space Use Materials DS: 32 books	

References

[1] DICE: https://dice.nims.go.jp/
[2] MatNavi: https://mits.nims.go.jp/
[3] AtomWork-Adv: https://atomwork-adv.nims.go.jp/

Research activities at Digital Transformation Initiative for Green Energy Materials

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Abstract

In order to achieve carbon neutrality in 2050, it is essential to introduce large amounts of renewable energy power generation and replace fossil fuels with hydrogen. To achieve this, it is necessary to develop ultra-large capacity, low-cost storage batteries and water electrolyzers at low cost without using rare metals. It is required that this be realized using suitable materials. In DX-GEM, the University of Tokyo and 11 research partner institutions will collaborate to develop data-driven advanced research methods that incorporate data science techniques and efficiently create these innovative materials.

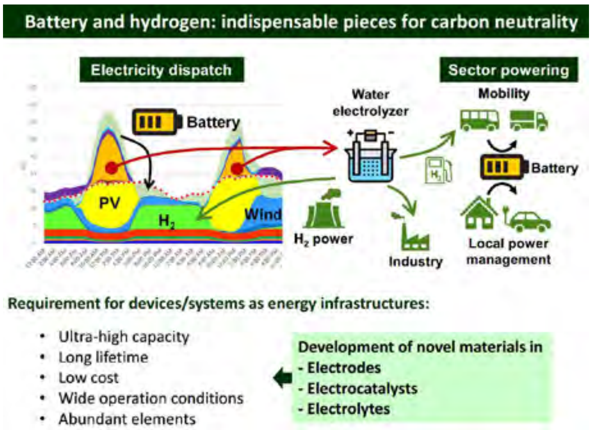

Fig. 1
Battery and hydrogen: indispensable pieces for carbon neutrality

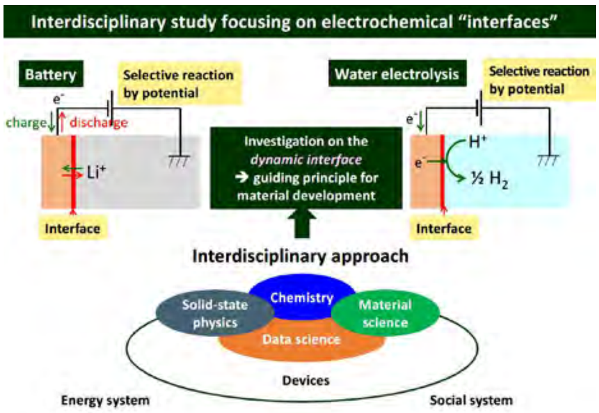

Fig. 2
Interdisciplinary study focusing on electrochemical “interfaces”

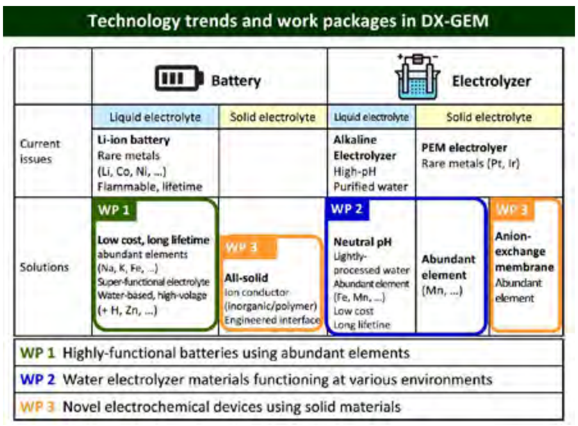

Fig. 3
Technology trends and work packages in DX-GEM

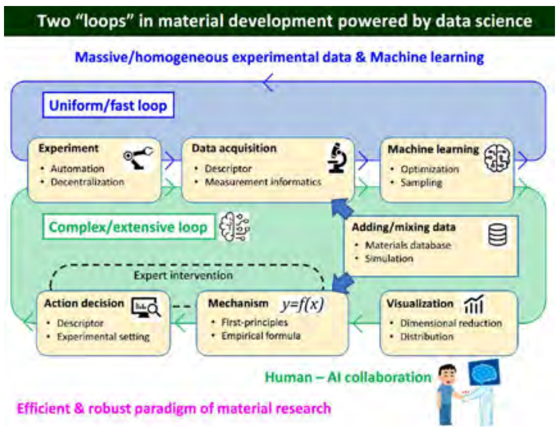

Fig. 4
Two “loops” in material development powered by data science

Cloud data storage and sharing system with worklows to structure materials research data for MI

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I. INTRODUCTION

The Materials DX Platform concept by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) promotes the strategic collection, accumulation, distribution, and use of structured materials research data with their schema. The Research Data Express (RDE) cloud data storage and sharing system, which allows materials research data to be registered online, structured and shared [1]. Figure 1 shows a conceptual diagram of the workflow in the RDE.

II. WORKFLOW AND DATA ACCUMULATION

The RDE has a workflow for automatically extracting, visualizing and registering metadata and features, used for Materials Informatics (MI), from the data files produced by the experimental equipment. The RDE then structurizes the materials research data in an MI-ready form, making it easy to perform data-driven materials research on the registered data. The RDE is responsible for automating routine pre-processing and efficiently storing data until it can be linked to advanced uses such as machine learning. This functionality can be shared among users as workflow templates.

III. SHARING

The data recorded in the RDE is stored in a common schema for each record, which is a unit for storing a group of structured data. Since the schema definition file is registered together with the data, the structure of the registered data is also explicitly shared. The RDE also has the ability to set the shared range of the dataset flexibly. The accumulated datasets can therefore be used in areas dedicated to the research group or shared with other research groups. With these features, RDE supports the digital transformation of materials research and development.

References

[1] Research Data Express (RDE), https://dice.nims.go.jp/services/RDE/

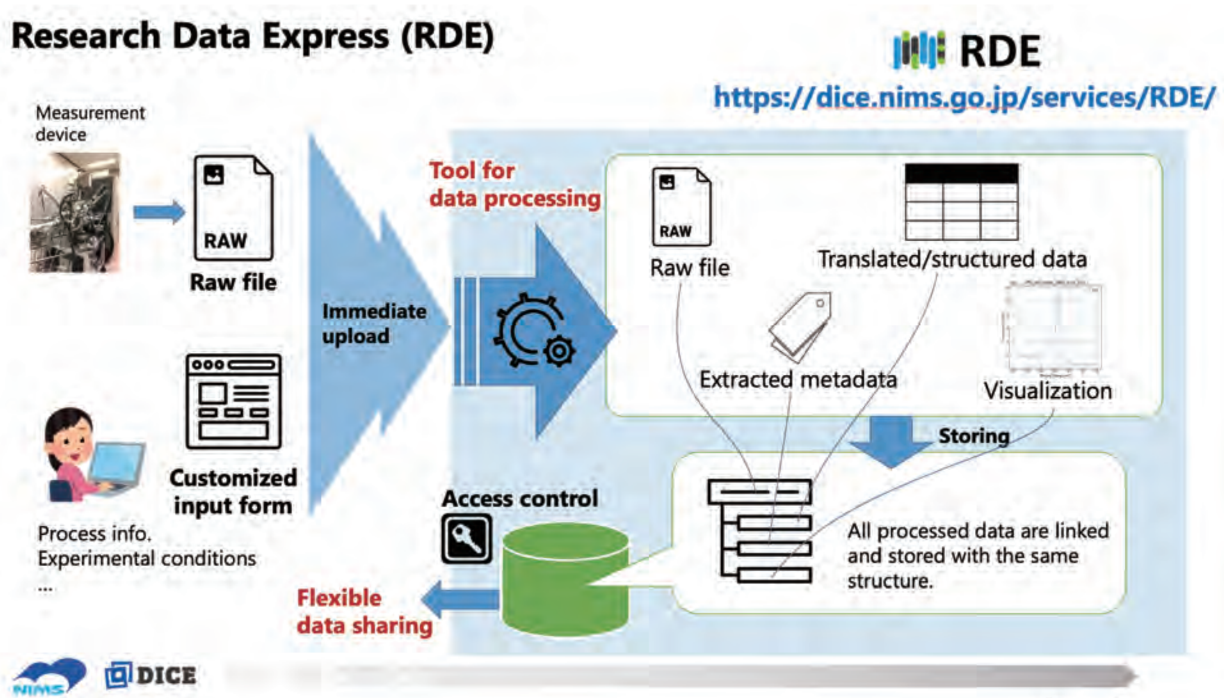

Fig1. Conceptual diagram of the workflow in the Research Data Express (RDE).

MInt and pinax: Systems for Data-Driven Research and Development for Materials Science

Yasuhiro FUJIWARA[1], Jun FUJIMA[1] and Satoshi MINAMOTO[1]

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Abstract

The materials data platform DICE [1] operated by National Institutes for Materials Science (NIMS) has become a system that supports a wide range of research data accumulation and application, including MatNavi [2], one of the world's leading materials databases. As a system for data accumulation and structuring, RDE [3] collects data from measurement devices nationwide and experimental data from researchers. As a system for data application, prediction models based on materials engineering theory or experiments are equipped in MInt [4]. In this report, we introduce MInt, a main data applicattion system, and pinax [5], a new system for developing machine learning models using DICE data.

I. Overview of MInt and pinax systems

Materials research and development reveals the linkage between the process of experimental work, the structure of the material, its intrinsic properties, and its environment-dependent performance. MInt, a data-driven materials development system, flexibly connects various predictive calculation tools, called modules, to predict from process (P), through structure (S) and properties (P), to performance (P) on the same environment. Conversely, the process conditions can be optimized from the desired performance as an inverse problem to facilitate research and development.

The pinax system was newly developed to provide a place for developing explainable machine learning models for materials research. It has an ability to record histories of model creation, including the sources of data used by the data scientist to develop a model and relationships between data, as well as an ability to share prediction models developed among specific researchers or with researchers across Japan.

II. Linkage image between MInt and pinax in DICE system

An example of the linkage image between MInt and pinax in a DICE system is shown in Fig. 1. In this example, MInt is used as iterative computational resources to optimize prediction models [6].

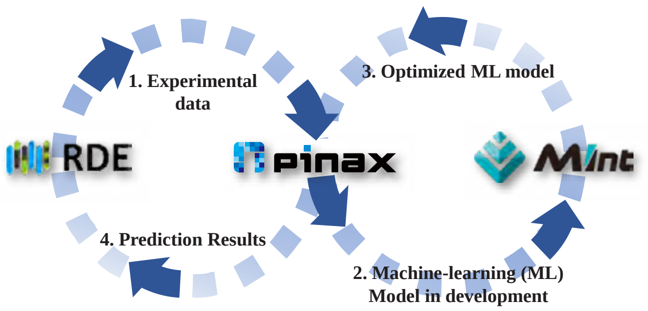

Fig. 1. Schematic of a linkage between MInt, pinax and RDE

2. Experimental data are structured by RDE to produce data on the structure of the material in the PSPP linkage. Those structured data are then sent to pinax.
3. In the pinax, machine learning model is developed to predict the property data from the structural data of materials.
4. The developed model is brought to MInt, which performs optimization calculations to maximize the performance of the prediction model. The optimized model is then brought back to pinax for more accurate predictions. By returning these predictions to user, the system can provide better insight and suggest next actions to the researcher.

We consider that the above-mentioned data utilization and improving accuracy of analysis are essential for the development of materials.

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[6] S. Minamoto, K. Daimaru, and M. Demura, *STAM-M*, 3 (2023) 1.

極限環境対応構造材料研究拠点　概要紹介
Overview of Research Initiative of Structural Materials for Extreme Environment（RISME）

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[1]拠点長，東北大学大学院工学研究科，宮城県仙台市青葉区荒巻字青葉6-6-02
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本拠点は，超耐熱性，耐水素性，耐疲労性，耐摩耗性など，多様な極限環境下で長期使用に耐え得る機能（「極限機能」）を備えた構造材料とその利用技術のデータ駆動型開発を、産官学のオールジャパン体制で推進します。そして，構造材料の長寿命化や新しい構造システムの高効率化に向けた、データ駆動型マテリアルの科学と工学の構築を目指します。我が国の構造材料研究の拠点として，デジタル・トランスフォーメーション（DX）の可能性を無限に拡げながら、世界の構造材料分野をリードしていきます。そのために，高強度耐水素材料（P1），耐疲労表面硬化材料（P2），超耐熱材料（P3）の３つの課題プロジェクトを設定し，各課題に対して，材料創製（G1），計測評価（G2），理論計算（G3），データ活用促進（G4）の４グループがシンクロしシナジー効果を発揮するよう，グループとプロジェクトの縦串・横串研究を紡いでいきます.

1. パブリック構造材料データベースの構築
2. 複雑な階層ミクロ構造の特徴量の最先端データサイエンスでの抽出
3. 順問題・逆問題解析を通した材料性能予測
4. ３次元＋時間軸の４次元の精密計測技術
5. ハイスループット計測技術
6. 計算材料科学による大規模計算技術

により、学界と産業界がデータ共有の新しい関係を構築し，“使える”構造材料データでブレイクスルーを創出します．10 機関が連携し先駆的なデータ駆動型研究手法を生み出し，参画企業や関連協議会との緊密な連携の下で，未来を見据えた極限環境対応構造材料の研究開発，新領域の創生，マテリアル×デジタル人材育成を推進しています（図 1）.

図 1．極限対応構造材料研究拠点　概要図

連携機関・企業： JAXA，鉄鋼メーカー，特殊鋼メーカー，重工メーカー， 材料プロセスメーカー，分析機器メーカー	人材育成連携： 東北大学グリーン×デジタル人材育成産学共創大学院プログラム 計算物質科学人材育成コンソーシアム

データ創出・活用型磁性材料研究拠点

Digital Transformation Initiative Center for Magnetic Materials (DXMag)

研究担当

大久保　忠勝　データ創出・活用型磁性材料研究拠点　代表研究者　OHKUBO.Tadakatsu@nims.go.jp

加藤　晃　データ創出・活用型磁性材料研究拠点　企画マネージャー　KATO.Akira@nims.go.jp


Keywords Data-driven materials design, Permanent magnets, Soft magnetic materials, Functional magnetic materials

研究の狙い

データサイエンス的手法を用いたデータ駆動型の先進的新奇材料創製技術により、10年先の社会像に重要な役割を果たす、革新的な機能、従来を上回る性能強調を発現する、永久磁石、軟磁性材料、機能性磁性物質等の多種多様なエネルギー変換マテリアルを効率的に創出する。

研究の要点

データ創出・活用型磁性材料研究において、①.データ創出から、②.データ統合・管理、③.データ利活用まで、一気通貫した材料研究のDXを推進し、世界を先導する価値創造の核となる｢材料研究DXプラットフォーム(PF)｣を構築、その材料DX・PFを通じて革新的な磁性材料を創製する。

DXMagビジョン

①データ蓄積の推進

マテリアルDXプラットフォーム構築に向けて、広範囲のデータを、実験、計算、文献データ等から効率的に収集する手法を確立し、データ蓄積を進めていきます

②データ活用手法の確立

人のドメイン知識によらないデータ科学を活用する手法を確立し、蓄積したデータから、材料開発の指針を獲得、活用していきます

③社会に貢献できる材料開発

材料研究者は対象とする分野においてそれぞれ最先端の研究を実施し、社会に貢献できる材料、デバイスの開発を目指します

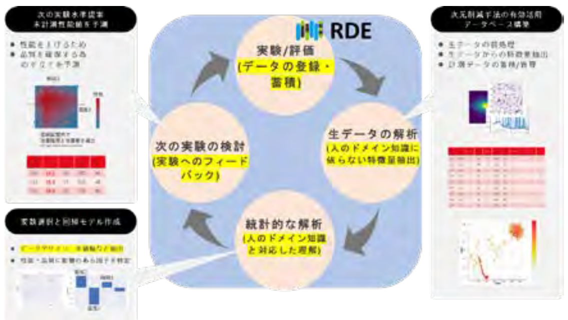
④マテリアル×デジタル人材育成

デジタルデータ活用の未経験材料研究者が、データ科学専門家のサポートで、デジタル手法によるデータ活用を体験し、その有効性を理解することで、材料とデータ科学の両輪で研究推進できる人材を育成します

⑤異分野連携の推進

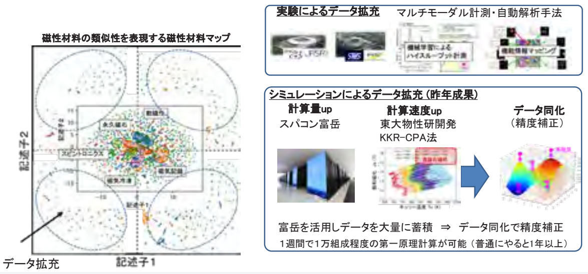
マテリアルDXプラットフォーム構築・拡張のため、拠点内の異分野材料のデータ連携から開始し、多拠点との連携、DxMT外機関との連携を目指していきます

データ蓄積・活用(DXルーティーン)



各実験Grでのデータ取得から機械学習的に特徴を取出し、構造・特性相関理解回帰モデルの重要度から物理現象理解に繋げるサイクルを回すのをルーティーンに

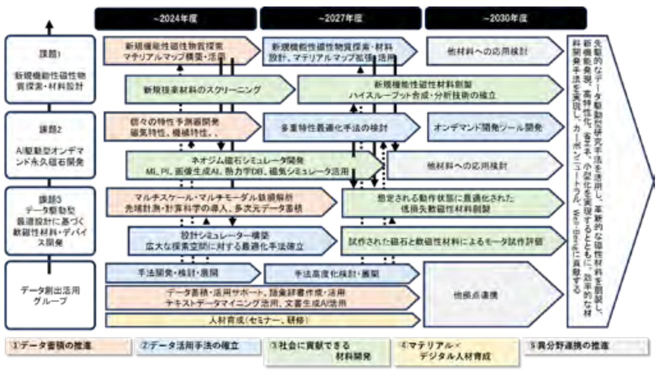
探索範囲を未探索領域に拡張し、高機能、高性能を有する未知の物質・材料をも見つけ出すための具体的な方策



磁性材料マップを拡張することで新たなデータ空間が創出され、拡張した領域での内挿により新規磁性材料創出につなげる

DXMag 研究体制 および ロードマップ

｢データ利用促進G｣を中心に｢材料創製G｣、｢計測評価G｣、｢理論計算G｣が一体となり、大規模先端施設、NIMSに設置されるデータ中核拠点、マテリアルリサーチインフラ事業、磁石MOP、産業界と連携



課題1｢新規機能性磁性物質探索・材料研究｣における、磁性材料をモデルとした他材料へも広く応用展開可能な、材料DX・PFの構築を通じたハイスループット物質探索等により、従来を上回る高性能な課題2｢永久磁石｣、課題3｢軟磁性材料｣の候補物質を見出し、それぞれの応用分野で産業競争力の高い新材料を創製し、社会実装することで、10年先の社会像・産業像を実現する。

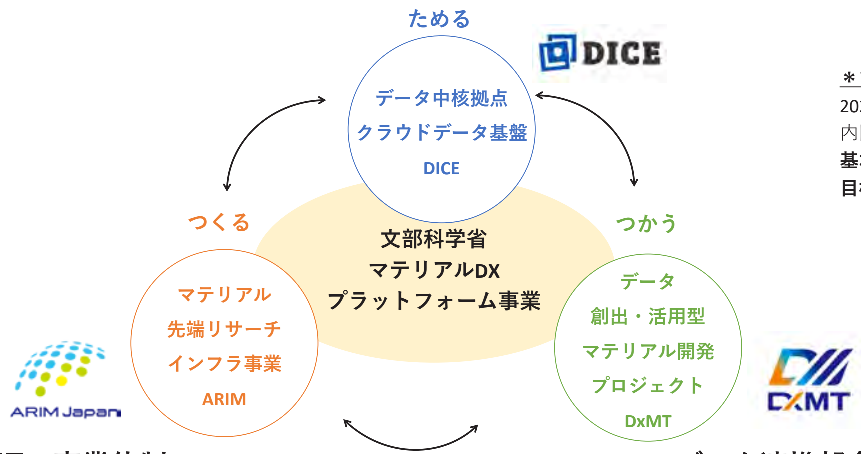
課題

- 磁石、軟磁性材の領域を越えた磁性材料マップの構築
- 広大な材料空間を効率よく調べる材料設計手法
- データの蓄積と相互利用の考え方、協調と競争、データ連携を進める上でのルール作り

文部科学省データ創出・活用型
マテリアル研究開発プロジェクト（DxMT）
データ連携部会中核機関

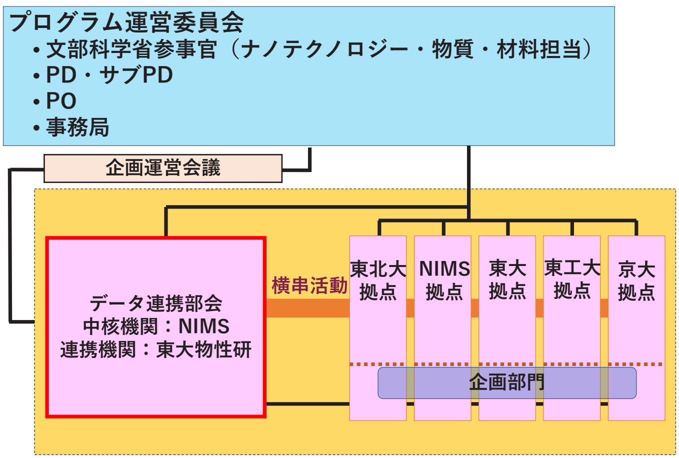
石　一智、吉川　英樹、源　聡、木野　日織、出村　雅彦（物質・材料研究機構(NIMS)）
三澤　貴宏、古宇田　光、吉見　一慶、尾崎　泰助　（東京大学物性研）

日本全国をDX化して、マテリアル革新力強化＊へ



＊マテリアル革新力強化戦略
2021年4月27日
内閣府統合イノベーション戦略推進会議決定
基本方針2：データ駆動型研究開発基盤の整備
目標「マテリアルDXプラットフォーム」整備

DxMTの事業体制

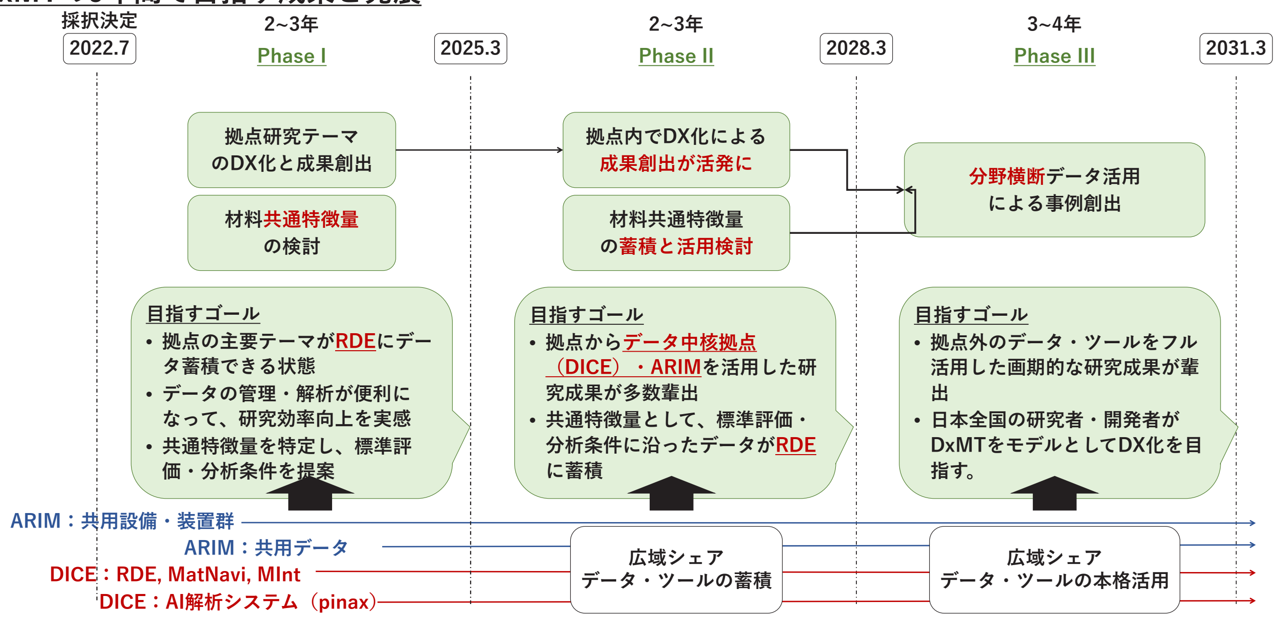


データ連携部会の活動内容

5拠点と連携した以下の活動
➤データ連携部会の運営：プログラム運営委員会の方針に従った運営
➤共通課題に対する技術開発・支援：「研究DX推進WG」と「データ駆動・計算基盤WG」の活動を通して下記に取り組み、日本の研究力向上に貢献
- ✓ 共通技術課題の抽出
- ✓ データ駆動型材料研究に必要な技術の開発
- ✓ 開発した技術は拠点間に横展開の後、広く共用化

➤データ駆動人材育成：セミナーや講習会の実施
➤事業広報：事業ポータルサイトを通じてデータ駆動型材料研究の有効性をアピール
➤関連事業連携：データ中核拠点、ARIM、HPC・大型設備等との連携促進
※事業広報と関連事業連携の一部は連携機関（東大物性研）に再委託

DxMTの9年間で目指す成果と発展



Bayesian optimization and evolutional algorithm for new structure search

T. Tada

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International Research Frontiers initiative MDX Research Center for Element Strategy, Tokyo Inst. of Tech.,
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Abstract
To extend the target area in computational materials designing, we adopted Bayesian optimization and an evolutional algorithm (EA) for the search of stable ionic configurations in binary compounds including dopants. We present a trial result on defect configuration/structure search in dielectric materials composed of Al and N.

I. INTRODUCTION
Developments of first principles methods have accelerated the theoretical research on stable, reactive, and functional materials in the atomistic point of view. The high precision of the first principles method is a theoretical foundation for detailed materials designing, although the relatively large computational costs of the first principles method sometimes limit the scope of theoretical research. To extend the theoretical targets for materials explorations, further theoretical developments combined with data science and artificial intelligence are required.

II. METHODS
In our group, we have developed a computational method for large-scale and long-term dynamics simulations; over micro-sec dynamics for one-million atoms that are atomistically modeled for batteries and catalysts are now aveilable[1]. However, to execute such a dynamical simulation, we firstly need precise structural information of target materials; e.g., ionic configurations, defect structures, interfacial structures, and so on. Structural investigation so far has been conducted mainly based on knowledge and intuition of researchers, but there are limits in such a strategy. Thus, we have adopted Bayesian optimization for searching stable ionic configurations, and an evolutional algorithm (EA) for new (unexpected) structure generation[1]. In this presentation, we present a trial result on defect configuration/structure search in dielectric materials. Since all the electronic structure calculations in the structure search were done with first principles method, an acceleration on computational time is required to execute the structural exploration in wider configurational space. Thus, we also introduce a promising framework (Fig. 1) including the atom-centered neural-network potential approach invented by Behler and Parrinello.

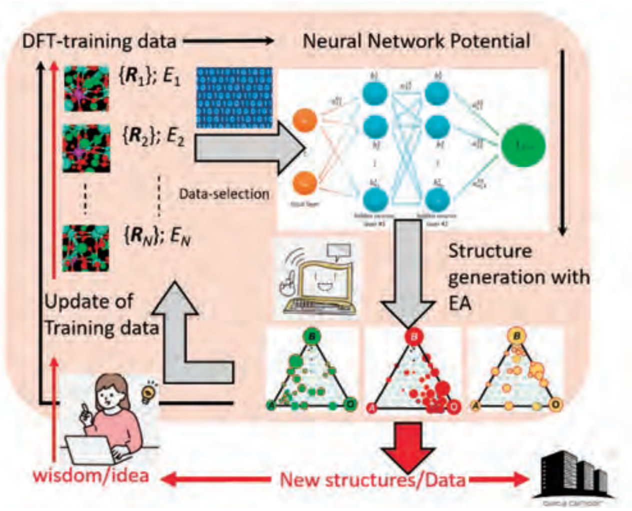


Fig. 1 Schematic of the workflow for Bayesian optimization, evolutional algorithm (EA), and neural-network potential method for big data generation and inspiration.

References
[1] H. Nakata and T.T., et al., *Sci. Technol. Adv. Mater.:Methods,* 1 (2021), pp. 109-122.

文部科学省データ創出・活用型マテリアル研究開発プロジェクト（DxMT）

京都大学
バイオ・高分子ビッグデータ駆動による完全循環型バイオアダプティブ材料の創出拠点

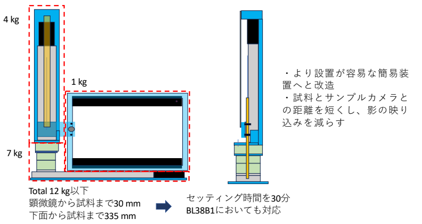
拠点概要

Society 5.0 の実現には、サイバー空間を担うデジタル技術だけでなく、最適な実空間を支えるマテリアル技術が、カーボンニュートラルの実現には二酸化炭素を回収する機能材料が、Well-Being社会にはQOLを向上させるバイオマテリアルが必要不可欠である。また、高分子材料は多様な自然環境・生体環境・工業プロセスで利用されており、日本における基幹材料の一つである。本拠点研究では、日本固有のビッグデータと大型研究施設を基軸としたマテリアル研究開発のプラットフォームを京都大学で拠点化する。重要な実装領域である、高タフネス・環境低負荷高分子、高度循環型高分子、QOLバイオマテリアル、および二酸化炭素分離回収材料を含む機能性や自己修復能を付帯するバイオアダプティブ材料の開発を目指す。

大型研究施設・計測評価

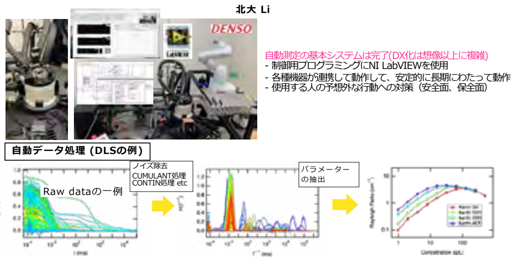
SPring-8における自動散乱測定システムの構築

増永啓康 BL03XU & 05XU JASRI



光散乱の自動測定と自動データ処理

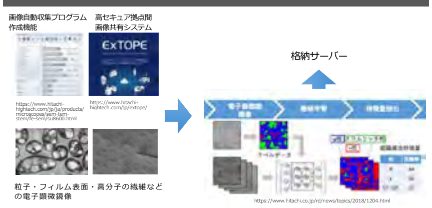
李响 北海道大学



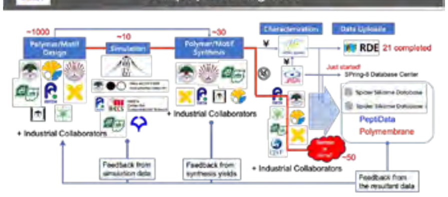
名古屋大学　鳴瀧彩絵

電顕自動化測定による高分子試料撮像から特徴量抽出およびデータ格納

豊岡公德 理化学研究所



Sample/Data Logistics



ARIM連携

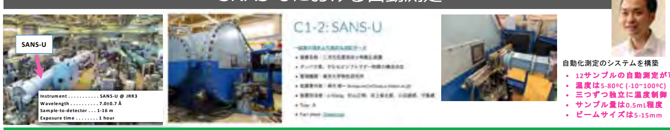
九大 藤ヶ谷 教授, 名大 馬場 教授

九大ARIM：分光装置を中心に３６機種を配置
名大ARIM：次世代バイオマテリアル領域ハブ拠点としてPr2関連装置（主にプロテオミクス関連）を配置

ARIM＝メタデータ付与と収集の仕組みを共用装置で実践

DxMTでも参照し、学びを活かす。

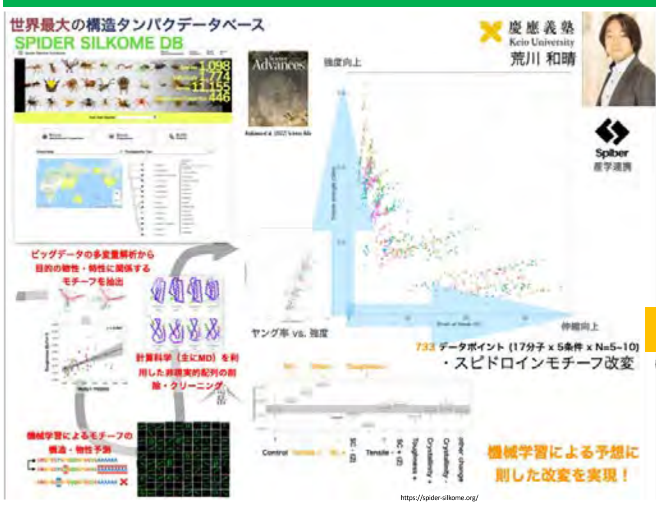
SNAS-Uにおける自動測定



分子動力学ソフトウェアGENESISによる「富岳」の効率的な利用

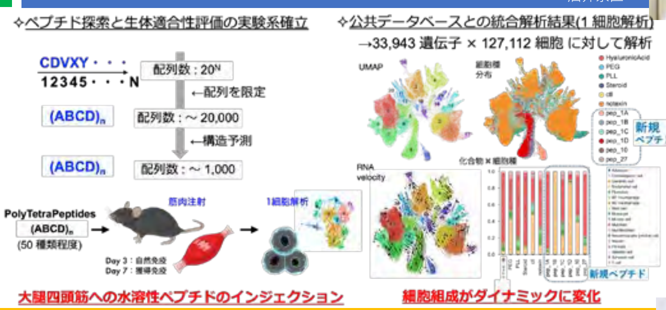
プロジェクト1:高度循環型・高タフネス高分子材料
拠点全体の基礎物性データ系の確立とSilkomeを利用したin-silico高分子設計

慶應義塾 Keio University　荒川 和晴



プロジェクト2: 生体反応性を制御した高分子
水溶性ペプチドの探索と1 細胞解析を用いた生体適合性評価

東京大学　酒井崇匡



プロジェクト3：バイオ・高分子ビッグデータ駆動による完全炭素循環を実現するバイオアダプティブ材料の創出

九州大学　星野友

文部科学省
マテリアル先端リサーチインフラ(ARIM)

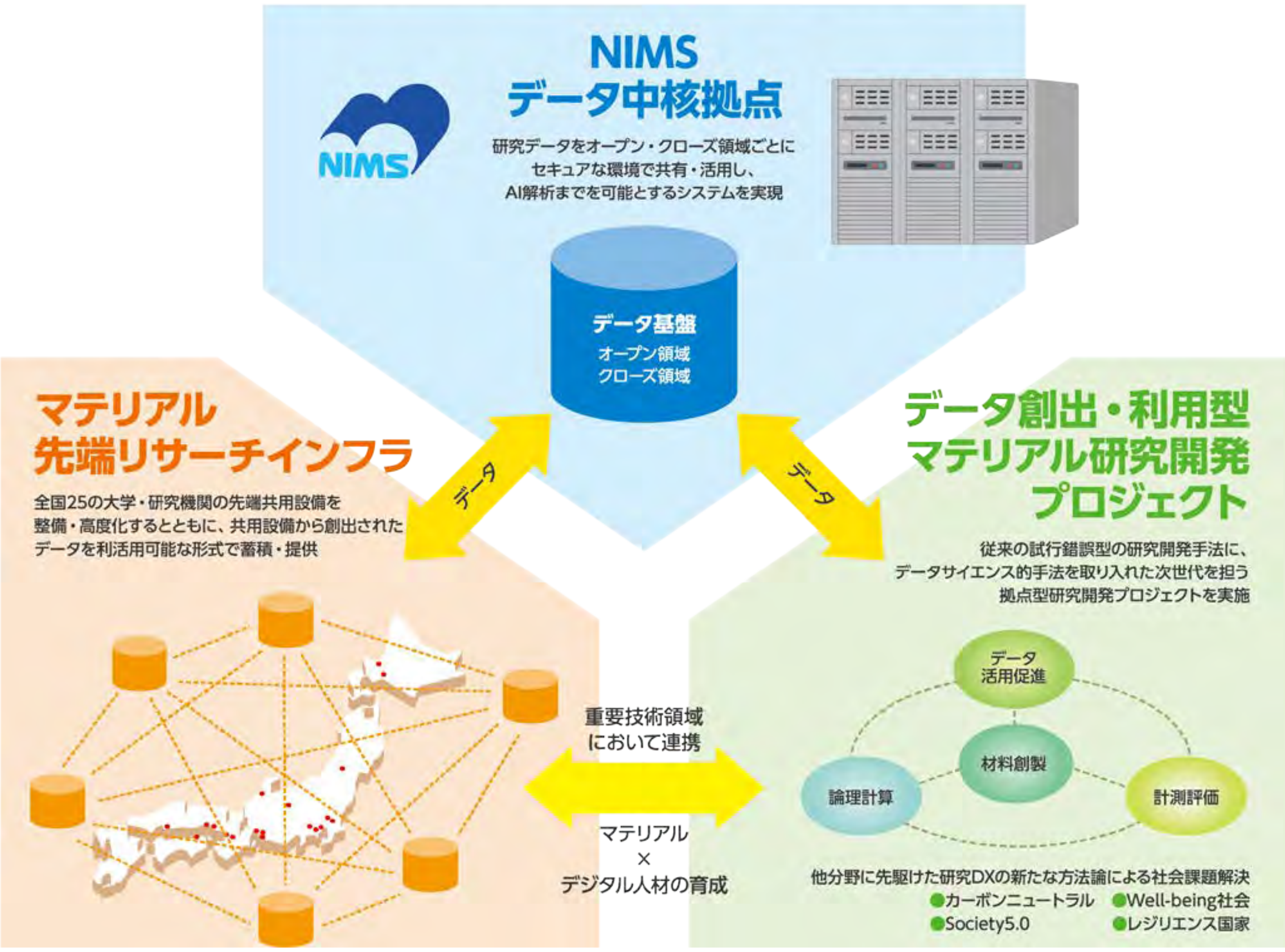
Advanced Research Infrastructure for Materials and Nanotechnology in Japan, MEXT

ナノテクノロジープラットフォームのレガシーを活かし、設備共用ネットワークに加え、データ収集・利活用の新しい境地へ挑戦

概 要 | Overview

最先端装置の共用・高度専門技術者による技術支援に加え、装置利用に伴い創出されるマテリアルデータを利活用しやすくした上で提供します。また、物質・材料研究機構(NIMS)が構築するデータ中核拠点を通じて、データを全国で利活用できる環境を整備します(2023年度全国提供開始予定)。さらに、文部科学省の「データ創出・活用型マテリアル研究開発プロジェクト」とも連携して「マテリアルDXプラットフォーム」を構築することで、我が国のマテリアル革新力の一層の強化に貢献して行きます。

マテリアルDXプラットフォームの全体イメージ



CONTACT
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〒305-0047 茨城県つくば市千現1-2-1
国立研究開発法人 物質・材料研究機構 技術開発・共用部門
https://nanonet.mext.go.jp/

ARIM Japan

ARIMの推進体制

Project Organization

ハブ・スポークの推進体制（全25法人）
Hub-spoke network（25 universities and institutes）

全国を網羅する装置共用ネットワーク

実施体制図
Project organization

CONTACT

マテリアル先端リサーチインフラセンターハブ 運営室
〒305-0047 茨城県つくば市千現1-2-1
国立研究開発法人 物質・材料研究機構 技術開発・共用部門
https://nanonet.mext.go.jp/

ARIM Japan

7つの重要技術領域

7 Key Fields of Science and Technology

マテリアル・イノベーションが大きなバリューをもたらす社会実装領域と、我が国が真に伸ばすべき重要技術領域として次の7つの領域を強化の対象として設定
担当のハブ機関がリーダーシップを取って機関間・領域間で 積極的な 連携を取りながらデータ収集、蓄積、構造化を図り、データの利活用により成果創出に貢献

高度なデバイス機能の発現を可能とするマテリアル　＜東北大学＞

多種多様な材料・構造・プロセスから成る高度なデバイスは、例えばIoT普及のために必須であり、新しい価値と産業の創出につながります。各スポーク機関の特徴を有機的に結び付けて、機能材料を含む幅広いマテリアルに対応する共用設備群に発展させるとともに、最適な材料・構造・プロセスの組合せ検討に役立つマテリアルデータを収集し利活用できる環境を構築し、最先端のMEMSやパワーエレクトロニクスなど、高度なデバイスの社会実装に貢献します。

東北大学

革新的なエネルギー変換を可能とするマテリアル　＜東京大学＞

高効率・高機能なエネルギー材料の開発は、環境問題や希少資源問題の克服、カーボンニュートラルの実現などに直結しています。ハブ・スポーク機関が連携して、これら課題に取り組むべく、高度な微細構造解析および微細加工技術に加えて、mdx（データ活用型社会創成プラットフォーム）を融合した新しい研究体制をとります。これより、高度解析・加工技術による支援、データの収集、蓄積、構造化、利活用などを行う環境を構築し、太陽電池、熱電素子など革新的なエネルギー変換を可能とするマテリアルの開発に貢献します。

東京大学
THE UNIVERSITY OF TOKYO

量子・電子制御により革新的な機能を発現するマテリアル　＜物質・材料研究機構＞

量子・電子技術は、Society 5.0の実現に向け重要な鍵となる最先端基盤技術の1つであり、今後の経済・社会の飛躍的な発展を遂げるために必要不可欠な革新的技術です。本領域では、ハブ・スポーク機関が有する、特徴的な解析装置と高度な微細加工技術の共用およびマテリアルデータの収集・蓄積・構造化を強力に推進し、量子センサ、フォトニクスデバイスなど革新的機能を持つ量子・電子材料の戦略的開発に貢献します。

NIMS
国立研究開発法人
物質・材料研究機構

マテリアルの高度循環のための技術　＜物質・材料研究機構＞

持続的発展可能な社会の実現には、マテリアルの使用量低減・代替・再利用や未使用資源の有効利用など、マテリアル循環のための技術が欠かせません。本領域では、代替材料や再生材料由来の物質合成、材料削減に資する触媒反応の可視化等、種々の先端機器共用を通じてマテリアル循環に関わる全国の研究者を支援するとともに、創出されたデータを効率よく収集・蓄積・構造化しその利活用を図ることで、サステイナブルなマテリアルの革新力強化に貢献します。

NIMS
国立研究開発法人
物質・材料研究機構

次世代バイオマテリアル　＜名古屋大学＞

バイオマテリアルは、持続可能で一人ひとりの多様な幸せが実現できる社会を構築するために必要不可欠な最先端基盤材料の一つであり、その研究開発はホワイトバイオからレッドバイオまで非常に幅広い分野において加速しています。本領域は、各機関が有する合成、加工、構造解析の世界有数の先端設備群に加えて、生体適合性検証支援のためにin vivo実験環境の実現、高品質データ創出・収集・蓄積・構造化、データ利活用環境の整備を図ることで、データ駆動型のバイオマテリアル研究開発に貢献します。

名古屋大学
NAGOYA UNIVERSITY

次世代ナノスケールマテリアル　＜九州大学＞

SDG'sの具現化、Society 5.0の実現に必要な材料の宝庫である、ナノスケールマテリアル、ナノ構造材料に高い実績を持つハブ・スポーク機関が協働して支援します。これまでに培った合成、解析、材料機能開発の支援基盤に加えて、放射光を含めた多面的なデータ収集や、情報科学と先端計測の融合に基づくデータ解析の高度化など、新たな支援機能を整備展開します。研究支援を通して材料の構造・特性・プロセスが紐付けされた高価値なデータを創出し、ナノマテリアル領域におけるデータ駆動型の研究推進に貢献します。

九州大学
KYUSHU UNIVERSITY

マルチマテリアル化技術・次世代高分子マテリアル　＜京都大学＞

SDGsに示された様々な社会課題の解決のため、各種材料を接合・積層・複合化して飛躍的な特性を発現するマルチマテリアル化技術の重要性が高まっています。本領域では、マテリアル・イノベーションの鍵となる高強度・生分解性・生体親和性・自己修復性などの固有な特性を示す次世代高分子マテリアルを中心にハブ・スポーク機関が特徴を有する加工・分析・構造解析設備の機器利用・技術代行等の共用を通じてマテリアルデータを創出し、その利活用による回路集積化学分析デバイスや生体機能チップなどの実現に貢献します。

KYOTO UNIVERSITY
FOUNDED 1897

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https://nanonet.mext.go.jp/

ARIM Japan

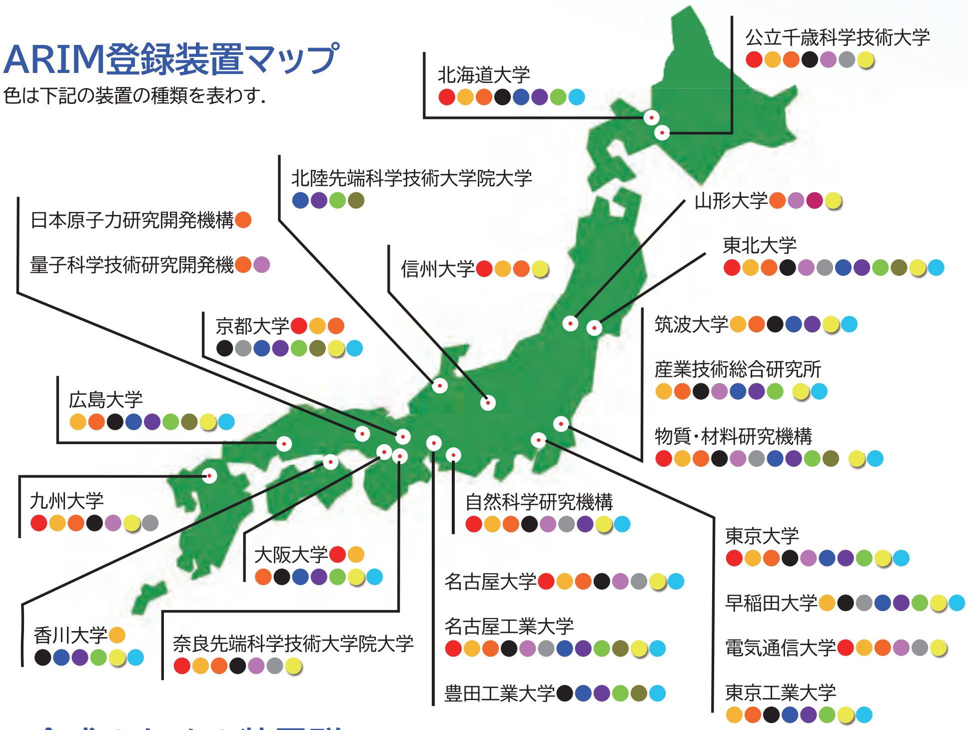
材料開発のための計測/加工/合成 装置群

Facilities of Microstructural Characterization/
Nanofabrication/Molecule & Material Synthesis for Material Research & Development

ナノテクノロジープラットフォーム(ナノプラ)で培われた装置共用の文化を発展、計測・加工・合成に関係する1100台以上の装置・設備による装置共用に加えて、データ収集・共用をサポートし、データ駆動型研究開発に貢献します。

ARIM登録装置マップ

色は下記の装置の種類を表わす.

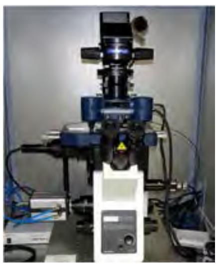


主要な計測・加工・合成のための装置群

●透過電子解析
・TEM/STEM
・EDS, EELS, tomography

●走査電子/イオン解析
・SEM/FIB/SIMS
・Auger, EBSD, CL

●X線回折
・XRD/SC-XRD
・CT, tomography



●走査プローブ解析
・AFM, KFM, PRM, EFM
・段差計

●共鳴分光
・NMR, MRI
・ESR, Mössbauer

●質量分析
・Chromatography
・ICP

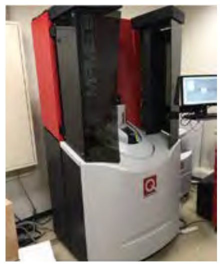
●成膜
・スパッタ
・CVD
・蒸着装置
・原子層堆積装置

●リソグラフィ
・電子線露光装置
・マスクレス露光装置
・レーザー直描装置
・線ステッパ
・ナノインプリント

●エッチング
・プラズマエッチング
・ウェットエッチング
・スエッチング
・レーザー加工

●熱処理・ドーピング
・酸化炉
・ランプアニール
・イオン注入

●樹脂成型



●機能評価
・DSC, TGA, TG-DTA
・PPMS, MPMS
・デバイスシミュレータ
・プローバ, マニピュレータ

●光分光・顕微鏡
・FT-IR, UV, Raman
・XPS, XRF, XAFS
・レーザー顕微鏡
・膜厚計, 粒度計

CONTACT

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ARIM Japan

データ構造化とデータ共用の流れ

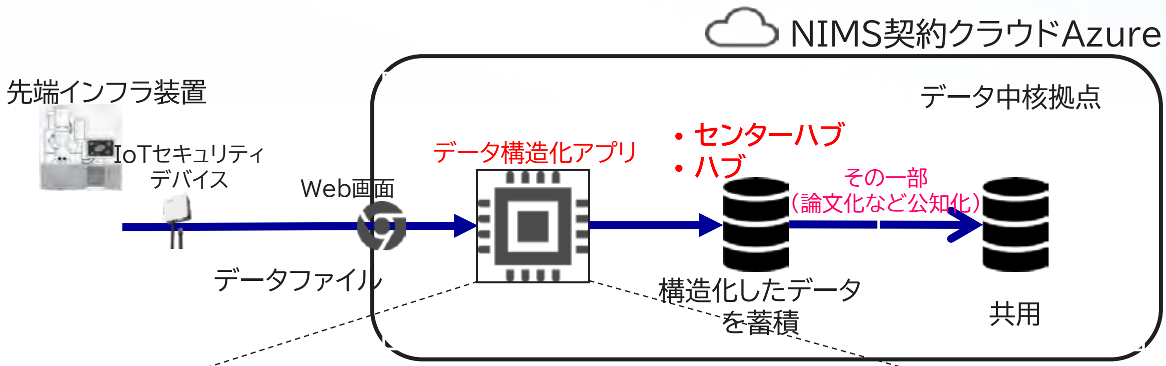
Structuring and Handling of Materials Data

材料データの構造化
Structuring of materials data

データを利活用しやすくするマテリアルデータの構造化

ARIMにおけるデータ構造化戦略

■　データ構造化はできる限り「人が介さず」に実行できる環境を整える.



- 自動化項目：装置メタデータ, 数値化, 可視化　⇒ 自動翻訳ツール（python）
- 手入力項目：ユーザー入力による試料メタデータ等　⇒ テンプレート（WEB入力, HTML）

✓　データ構造化にかかるツールを整備する
✓　データ構造化の作業をできる限り自動化・省人化する

データの流れ
Handling of materials data

ARIM事業

非共用

●データを取得した研究チーム内に閉じて利用(※)

●他の研究チームからは、データセットの存在は見えない

※データを取得した研究チームが承認した他の研究チームに限ってデータセットを共用することは可能

アクセス権

データを取得した研究チーム

最大2年(※1)

エンバーゴ後

事業内共用(広域シェア)

●非共有期間後は事業内へ共用

●事業内データ利用者であれば閲覧や検索が可能。

●データ提供は、原則、有償

アクセス権

- ARIM事業者
- ARIMデータ利用者のアカウントをもつ者

主となるデータの論文等での公知化など

データ中核拠点共用

● データ中核拠点(NIMS)のアクセス権を持つ者で利用可

アクセス権

- データ中核拠点アカウントを持つ者(※2)

(※1)事業の定める申請書を受理した日の翌日からデータ登録終了となる年度の年度末の翌日(4月1日)から起算して最大2年までの間

(※2)ARIMのデータ利用者と同じく、国内の産官学の機関が保証する(外為法の規制対象外の)研究者・技術者

CONTACT

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https://nanonet.mext.go.jp/

ARIM Japan

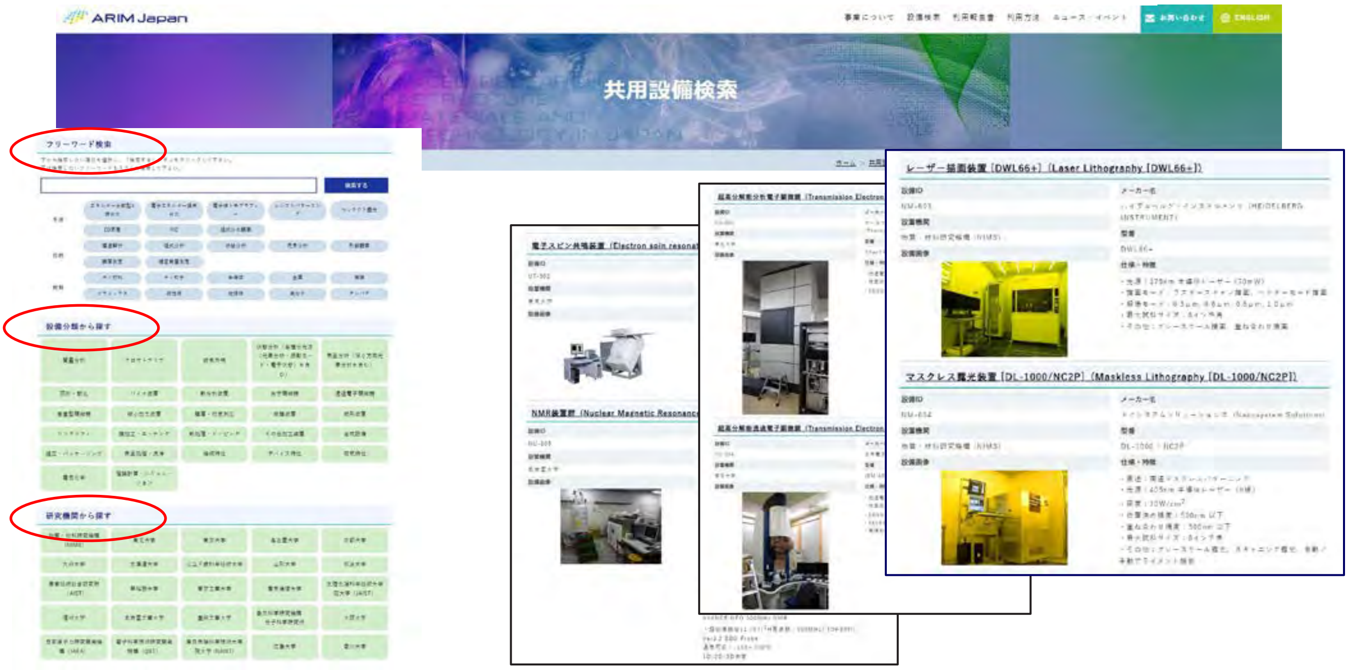
装置検索とサポート内容

Facilities Search and a Variety of Services in ARIM

装置検索
Facilities search

ナノプラット事業から引き続き提供されている装置を含め、1100台以上の最先端研究設備をインターネットを介して一元的に運用・情報共有

共用設備検索サイトより使いたい装置が探せます
https://nanonet.mext.go.jp/facility.php



フリーキーワード、設備分類、支援機関による検索

サポート内容
A variety of services in ARIM

技術相談 | 専門技術でアドバイス

技術的な問題解決に向けて、各ハブ・スポーク機関の技術スタッフが様々な問題に応じます。

機器利用 | 利用者自身で操作

機器は利用者自身が操作し、実験します。データ解析や考察も利用者が行います。

技術補助 | 補助スタッフが補助

利用者は操作方法などについて、技術スタッフの補助を受けながら機器を使用します。

技術代行 | 利用者に代わり操作

依頼に基づきハブ・スポーク機関の技術スタッフが実験・測定・評価・解析を行います。

共同研究 | 利用者とハブ・スポーク機関が共同で実施

データの解析や学術的な議論を含めて、利用者とハブ・スポーク機関とが共同で行います。

データ利用 | 蓄積したデータの利活用

蓄積したデータはデータベースとして用いる他、新たな情報を導き出す利活用が可能です。

CONTACT

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https://nanonet.mext.go.jp/

ARIM Japan

利用事例とご利用の流れ

Use case Search and a Step of Usage in ARIM

利用事例検索
Use case search

年間2000件以上の利用報告書をWEBページから閲覧でき、過去の利用事例を調べることができます

利用報告書をホームページで無料公開しています
https://nanonet.mext.go.jp/user_report.php

フリーキーワード、技術分類、支援機関による検索

利用の流れ
Flow of usage

1 利用相談
希望する試料が実験・測定可能かどうか、技術スタッフにお問い合わせください。

2 申 請
申請書を各ハブ・スポーク機関の窓口にご提出いただければ、審査の結果をお知らせします。

3 予 約
ご希望のスケジュールに合わせて予約してください。

4 設備利用
申請内容に基づいて設備・機器を利用します。

5 報 告
終了後、利用報告書を提出していただきます。

6 利用料支払
ご利用に応じて利用料をお支払いいただきます。

CONTACT

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https://nanonet.mext.go.jp/

ARIM Japan

プログラム委員会/Program Committee

柴田 直哉（委員長）	Naoya Shibata (Chair)	東京大学/The University of Tokyo
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横川 隆司	Ryuji Yokokawa	京都大学/Kyoto University
横山 利彦	Toshihiko Yokoyama	自然科学研究機構分子科学研究所/Institute for Molecular Science

協　　賛/Cooperating Organizations

IEEE Japan Council	IEEE Japan Council
応用物理学会	The Japan Society of Applied Physics
計算物質科学協議会	Computational Materials Science Forum, Japan
総合科学研究機構	Comprehensive Research Organization for Science and Society, Japan
高輝度光科学研究センター	Japan Synchrotron Radiation Research Institute
高度情報科学技術研究機構	Research Organization for Information Science and Technology
高分子学会	The Society of Polymer Science, Japan
電気学会	The Institute of Electrical Engineers of Japan
電子情報通信学会	The Institute of Electronics, Information and Communication Engineers
ナノ学会	The Society of Nano Science and Technology
ナノテクノロジービジネス推進協議会	Nanotechnology Business Creation Initiative
NanoTerasu 利用推進協議会	Nano Terasu Utilization Promotion Council
日刊工業新聞社	The Nikkan Kogyo Shimbun
日本ＭＲＳ	The Materials Research Society of Japan
日本化学会	The Chemical Society of Japan
日本金属学会	The Japan Institute of Metals and Materials
日本顕微鏡学会	The Japanese Society of Microscopy
日本再生医療学会	The Japanese Society for Regenerative Medicine
日本材料学会	The Society of Materials Science, Japan
日本人工臓器学会	Japanese Society for Artificial Organs
日本セラミックス協会	The Ceramic Society of Japan
日本 DDS 学会	The Japan Society of Drug Delivery System
日本バイオマテリアル学会	The Japanese Society for Biomaterials
日本表面真空学会	The Japan Society of Vacuum and Surface Science
日本物理学会	The Physical Society of Japan
光科学イノベーションセンター	Photon Science Innovation Center
ファインセラミックスセンター	Japan Fine Ceramics Center
マイクロマシンセンター	Micromachine Center
モノづくり日本会議	MONODZUKURI Nippon Conference
量子科学技術研究開発機構	National Institutes for Quantum Science and Technology

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Materials Innovation Strategy Symposium 2023

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文部科学省マテリアル戦略総合シンポジウム 2023　予稿集