# マテリアル戦略総合シンポジウム 2025

Materials Innovation Strategy Symposium 2025

# Proceedings

## Date

January 31st (Fri), 2025

## Venue

Tokyo Big Sight, Conference Tower 1F, Reception Hall (Tokyo)
※ Online

## Organized by

MEXT Advanced Research Infrastructure for Materials and Nanotechnology (ARIM)
MEXT Data creation and utilization-type MaTerial R&D project (DxMT)
NIMS Materials Data Platform (MDPF)

## Supported by

Cabinet Office

## Participating Institutions

MEXT 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, National Institute of Advanced Industrial Science and Technology, Waseda University, Institute of Science Tokyo, The University of Electro-Communications, Japan Advanced Institute of Science and Technology, Shinshu University, Nagoya Institute of Technology, Toyota Technological Institute, National Institutes of Natural Sciences Institute for Molecular Science, Osaka University, Japan Atomic Energy Agency, National Institutes for Quantum Science and Technology, Nara Institute of Science and Technology, Hiroshima University, Kagawa University

MEXT Data creation and utilization-type MaTerial R&D project (DxMT):
Tohoku University, National Institute for Materials Science, The University of Tokyo, Institute of Science Tokyo, Kyoto University

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Materials Innovation Strategy Symposium 2025

# マテリアル戦略総合シンポジウム2025

## 予稿集

**開催日**

2025年1月31日(金)
※オンライン併用開催 LIVE

**会場**

東京ビッグサイト　会議棟1階　レセプションホール（東京都江東区有明）

**共催**

文部科学省 マテリアル先端リサーチインフラ（ARIM）、
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）、
NIMS　データ中核拠点事業（MDPF）

**後援**

内閣府

**参画機関**

文部科学省マテリアル先端リサーチインフラ（ARIM）：
NIMS、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、東京科学大学、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
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、NIMS、東京大学、東京科学大学、京都大学

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ARIM Japan　DxMT　NIMS MDPF

## January 31st (Fri), 2025, Tokyo Big Sight
## 2025 年 1 月 31 日 ( 金 ) 東京ビッグサイト（会議棟 1 階 レセプションホール）

### 10:00-10:10 Opening Remarks / 開会挨拶

1）10:00-10:05

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

2）10:05-10:10

**Kazuhiro Hono** (President, National Institute for Materials Science)
**宝野 和博**（NIMS 理事長）

### 10:10-11:40 Plenary Lecture 1 / 基調講演 1

**Hiroko Takuma** (Director, Material Science and Nanotechnology Division, Research Promotion Bureau, Ministry of Education, Culture, Sports, Science andTechnology (MEXT) Director, Materials Section, Secretariat of Science, Technology and Innovation Policy, Cabinet Office (CAO))

**宅間 裕子**（文部科学省研究振興局 参事官、内閣府科学技術・イノベーション推進事務局参事官）
“Government Initiatives under the "Materials Innovation Strategy"”
「マテリアル革新力強化戦略に基づく政府の取組について」

### 10:40-11:15 Plenary Lecture 2 / 基調講演 2

**Ryo Yoshida** (Director, Research Center for Materials Informatics, The Institute of Statistical Mathematics)
**吉田 亮**（統計数理研究所 マテリアルズインフォマティクス研究推進センター長）
“The Role of Data Infrastructure in Data-Driven Materials Research: Perspectives on AI Utilization”
「データ駆動型材料研究におけるデータ基盤の在り方：AI 活用の視点から」

### 11:15-11:50 Special Lecture / 特別講演

**John A. Schlueter** (Program Director, DMREF, NSF)
“The Designing Materials to Revolutionize and Engineer Our Future (DMREF) Program at the National Science Foundation (NSF)”

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11:50-13:10 【 Lunch / 昼食 】

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### Session 1 13:10-14:50 Progress in Materials DX Platform Initiatives / マテリアル DX プラットフォーム構想の進展

1）13:10-13:30

**Kentaro Totsu** (Tohoku University)
**戸津 健太郎**（東北大学）
“DX of Fabrication Processes Accelerating Development of Diverse Devices”
「多様なデバイス開発を加速させる加工プロセスデータ収集・利活用の取り組み」

2）13:30-13:50

**Yoshinobu Baba** (Nagoya University)
**馬場 嘉信**（名古屋大学）
“Nagoya University ARIM Hub for Accelerated Data-Driven R&D of Biomaterials and Biodevices”
「名古屋大学 ARIM ハブ拠点におけるバイオマテリアル・バイオデバイスのデータ駆動型研究開発支援」

3）13:50-14:10

**Satoshi Minamoto** (National Institute for Materials Science)
**源 聡**（NIMS）
“The Future of Data-Driven Materials Research Enabled by Materials DX Platform Integration”
「マテリアル DX プラットフォーム連携が切り拓くデータ駆動型材料研究の未来」

4）14:10-14:30

**Taro Hitosugi** (The University of Tokyo)
**一杉 太郎**（東京大学）
“Global Trends and Future Prospects for Data- and Robot-Driven Materials Science”
「データ・ロボット駆動材料科学の世界的動向と将来展望」

5）14:30-14:50

**Kyosuke Yoshimi** (Tohoku University)
**吉見 享祐**（東北大学）
“DX Approaches for Structural Materials Research Incorporating Microstructures”
「材料ミクロ組織を取り入れた構造材料研究のための DX アプローチ」

14:50-15:20　【 Coffee Break / 休憩 】

## Session 2 15:20-16:00 Promoting R&D via Materials DX Platform / マテリアル DX プラットフォームを活用した研究開発の推進

1）15:20-15:40

**Shingo Akao** (Ball Wave Inc.)
**赤尾 慎吾**（ボールウェーブ株式会社）
“Social Implementation of Ball SAW Sensors, a Palm Sized Gas Chromatograph”
「ボール SAW センサの社会実装、超小型可搬ガスクロマトグラフ」

2）15:40-16:00

**Yuichi Ikuhara** (The University of Tokyo)
**幾原 雄一**（東京大学）
“New Characterization Technology and Methods from ARIM- University of Tokyo”
「ARIM 東京大学発の新しい評価技術と手法」

16:00-16:10　【 Break / 休憩 】

## Session 3 16:10-17:10 Material Innovation Accelerated by Data Driven Approaches / データ駆動で加速するマテリアルイノベーション

1）16:10-16:30

**Yoshishige Okuno** (Resonac Corporation)
**奥野 好成**（株式会社レゾナック）
“Resonac's Data-Driven Materials Development DX Initiative and Expectations for the Materials DX Platform”
「レゾナックでのデータ駆動型材料開発 DX の取組み紹介とマテリアル DX プラットフォームへの期待」

2）16:30-16:50

**Toru Ujihara** (UJ-Crystal Inc., Nagoya University)
**宇治原 徹**（株式会社 UJ-Crystal, 名古屋大学）
“Machine Learning Technology in SiC Solution Growth Method”
「SiC 溶液成長法における機械学習技術とその応用」

3）16:50-17:10

**Mikiya Fujii** (Nara Institute of Science and Technology)
**藤井 幹也**（奈良先端科学技術大学院大学）
“Materials Design and Drocess Development using Closed-Loop Digital Technology”
「デジタル技術によるクローズドループを用いた材料設計とプロセス開発」

## 17:10-17:15 Closing Remarks / 閉会挨拶

**Kazue Kurihara** (Program Director, DxMT)
**栗原 和枝**（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 プログラムディレクター）

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## Session 2 Promoting R&D via Materials DX Platform / マテリアル DX プラットフォームを活用した研究開発の推進



## Session 3 Material Innovation Accelerated by Data Driven Approaches / データ駆動で加速するマテリアルイノベーション

# Plenary Lecture

## 基調講演

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# 【Plenary Lecture1 / 基調講演 1】

# “Government Initiatives under the "Materials Innovation Strategy"”

「マテリアル革新力強化戦略に基づく政府の取組について」

**Hiroko Takuma**
**(Director, Material Science and Nanotechnology Division,**
**Research Promotion Bureau, Ministry of Education, Culture, Sports,**
**Science and Technology (MEXT)**
**Director, Materials Section,**
**Secretariat of Science, Technology and Innovation Policy,**
**Cabinet Office (CAO))**

宅間 裕子
（文部科学省研究振興局 参事官、内閣府科学技術・イノベーション推進事務局参事官）

# Government Initiatives under the “Materials Innovation Strategy”

マテリアル革新力強化戦略に基づく政府の取組について

**[1]H. Takuma**

[1] Director, Material Science and Nanotechnology Division,
Research Promotion Bureau,
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3-2-2, Kasumigaseki, Chiyoda-ku, Tokyo, Japan

Director, Materials Section, Secretariat of Science, Technology and Innovation Policy,
Cabinet Office (CAO)
1-6-1, Nagata-cho, Chiyoda-ku, Tokyo, Japan

## Abstract

Materials science is an important fundamental technology that will contribute to the realization of Society 5.0 and the transition to a sustainable society that achieves both economic development and the resolution of social issues. The Japanese government formulated the "Materials Innovation Strategy" in April 2021 to strengthen Japan’s R&D capabilities in this field. An important pillar of this strategy is the promotion of data-driven R&D that will lead to the dramatic improvement of the speed, quality, and quantity of research and development. Along with Based on this strategy, The Ministry of Education, Culture, Sports, Science and Technology (MEXT) is implementing our ‘Material DX Platform’, a national initiative to promote the digital transformation of research and development in this field. We are building nationwide networks to collect materials data from universities and research institutes. These networks will enable researchers around the country to utilize the data for their research. We are also conducting research projects addressing global challenges by the creation of innovative materials through data-driven R&D. This presentation will introduce the government's initiatives under "Materials Innovation Strategy" focusing on MEXT’s ‘Material DX Platform’.

Hiroko Takuma,
Director, Material Science and Nanotechnology Division,
Research Promotion Bureau, Ministry of Education, Culture, Sports, Science and Technology (MEXT)

Director, Materials Section,
Secretariat of Science, Technology and Innovation Policy,
Cabinet Office (CAO)

<CV>
Hiroko Takuma is working for the MEXT since 2001, where she has held several managerial positions related to the promotion of Research and Development. Policy. She is now in charge of the promotion of Material Science and Nanotechnology at MEXT. She also holds the position at the CAO, where she is responsible for promoting the Materials Innovation Strategy.

## 【Plenary Lecture2 / 基調講演 2】

# “The Role of Data Infrastructure in Data-Driven Materials Research: Perspectives on AI Utilization”

「データ駆動型材料研究におけるデータ基盤の在り方：AI 活用の視点から」

**Ryo Yoshida**
**(Director, Research Center for Materials Informatics, The Institute of Statistical Mathematics)**

吉田 亮
（統計数理研究所 マテリアルズインフォマティクス研究推進センター長）

# The Role of Data Infrastructure in Data-Driven Materials Research: Perspectives on AI Utilization
# データ駆動型材料研究におけるデータ基盤の在り方：AI活用の視点から

**[1,2]R. Yoshida**

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Research Organization of Information and Systems,
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[2]National Institutes for Materials Science,
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## Abstract

The major obstacle in data-driven materials research, the lack of data resources, remains unresolved. High experimental costs and the cultural barrier of researchers to disclose their laboratory data contribute to this issue. In this lecture, I will introduce our efforts in polymer material research and discuss strategies to overcome the challenge of insufficient data resources.

### Transferability and Scalability of Materials Database

Our research group is advancing the development of RadonPy, a software designed to fully automate computer experiments for polymer systems using molecular dynamics and first-principles calculations, to address the challenge of data scarcity in polymer materials research [1]. The latest version of RadonPy supports automated computer experiments for 34 distinct properties. It can handle a wide range of polymer systems, including amorphous, stretched, crystalline structures, as well as homopolymers, copolymers, crosslinked polymers, and blends. Currently, an industry-academia consortium comprising approximately 240 participants from two national research institutes, nine universities, and 37 companies is collaboratively advancing the open-source development of RadonPy. Leveraging supercomputer Fugaku, the consortium is building the world's largest polymer property database, encompassing $10^5$ or more polymer materials.

A key feature of the RadonPy database is its ability to bridge the gap between computational and real-world systems using Sim2Real transfer learning. In transfer learning, a foundational model trained on extensive computational data is fine-tuned with a limited set of experimental data to create a highly generalizable predictor for real-world systems [2-3]. A crucial concept here is the scaling law of Sim2Real transfer learning: the generalization performance of a Sim2Real transfer model for real-world systems improves monotonically according to a power law as the size of the computational database increases. Indeed, predictors fine-tuned from RadonPy foundational models have shown exceptional scalability in predicting various experimental properties such as polymer miscibility, specific heat, refractive index, and thermal conductivity [4]

The goal of data-driven materials research is to establish scalable and transferable data generation protocols and analytical workflows. In many target domains, accumulating sufficient data for data-driven research is challenging, especially in cutting-edge research areas. This highlights the importance of defining a source domain capable of producing large datasets and using machine learning to bridge the domain gap. Designing data generation workflows that ensure the scalability and transferability to downstream domains is essential in overcoming limited data resource in material researches.

**References**

[1] Hayashi et al., *npj Comput Mater* 8, 222 (2022).
[2] Wu et al., *npj Comput Mater* 5, 66 (2019).
[3] Yamada et al., *ACS Cent Sci* 5, 1717-1730 (2019)
[4] Minami et al., *arXiv*, arXiv:2408.04042 (2024).

<Name> Ryo Yoshida
<Affiliation> The Institute of Statistical Mathematics

<CV>
Ryo Yoshida is a Professor at the Institute of Statistical Mathematics, Research Organization of Information and Systems. He also serves as the Director of Research Center for Materials Informatics within the institute. He leads an industry-academia consortium comprising two national research institutes, nine universities, and 37 companies, advancing the joint development of the polymer computational experiment automation software RadonPy and a comprehensive polymer property database.

# 【Special Lecture / 特別講演】

# “The Designing Materials to Revolutionize and Engineer Our Future (DMREF) Program at the National Science Foundation (NSF)”

**John A. Schlueter**
**(Program Director, DMREF, NSF)**

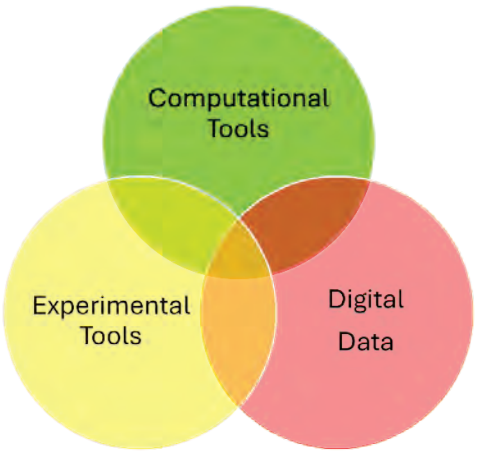
# The Designing Materials to Revolutionize and Engineer Our Future (DMREF) Program at the National Science Foundation (NSF)

**John Schlueter**

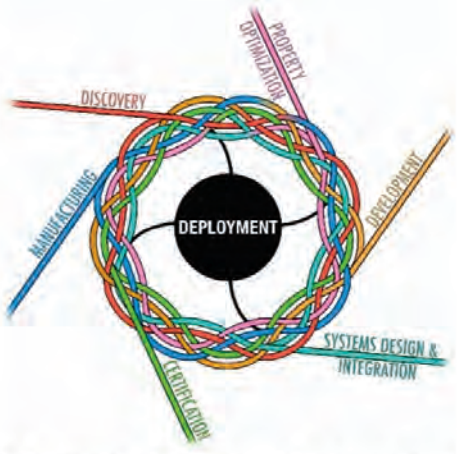
Designing Materials to Revolutionize and Engineer our Future (DMREF)
U.S. National Science Foundation (NSF)
2415 Eisenhower Ave Alexandria, VA 22314, USA

## Abstract

The United States' Materials Genome Initiative (MGI) is a multi-agency partnership that seeks to accelerate the progression of materials research across the Materials Development Continuum for the benefit of society. By coupling a predictive, computationally led and data-driven approach with experimental synthesis and validation via an iterative feedback loop, MGI promotes the rapid design, discovery, development, and deployment of advanced materials. After a decade of progress that has witnessed a paradigm shift in philosophy of materials research, the second MGI Strategic Plan was released in 2021 defining three primary goals for the next five years: 1) Unifying the Materials Innovation Infrastructure, 2) Harnessing the Power of Materials Data, and 3) Educating, Training, and Connecting the Materials Research and Development Workforce. The Designing Materials to Revolutionize and Engineer our Future (DMREF) program at the National Science Foundation (NSF) involves eight divisions in four directorates at the NSF, and partners with seven federal and four international agencies to promote these objectives. This talk will provide an overview of the DMREF program and MGI-related programs sponsored by the NSF. DMREF is a biannual program with a current competition in 2025. Additional information about DMREF can be found at DMREF.org.




Materials Innovation Infrastructure




Materials Development Continuum

DMREF
MATERIALS FOR OUR FUTURE

John Schlueter
Program Director,
Designing Materials to Revolutionize and Engineer our Future (DMREF)
U.S. National Science Foundation (NSF)

Dr. John Schlueter joined the National Science Foundation (NSF) in December 2013 as a Program Director in the Division of Materials Research, Directorate of Mathematical & Physical Sciences, where he manages the Designing Materials to Revolutionize and Engineer our Future (DMREF) program. DMREF is the primary program by which the NSF participates in the Materials Genome Initiative (MGI). He received his B.S. from Valparaiso University (Valparaiso, IN) in 1987 with majors in Chemistry and Physics and a minor in Mathematics. He then earned his Ph.D. in Inorganic Chemistry from Northwestern University (Evanston, IL) in 1992 under the direction of thesis advisor Prof. Tobin Marks. After spending three years as a Postdoctoral Chemist at Argonne National Laboratory with Dr. Jack Williams, he became an Assistant Chemist in the Chemistry and Materials Science Divisions in 1995 and was promoted to Chemist in 1999. Schlueter's experimental research includes the guided synthesis, crystallization, and characterization of molecule-based materials with emergent electronic and/or magnetic properties, including the development of multifunctional materials with applications in magnetism, superconductivity, spintronics, and multiferroics. Through the use of intermolecular interactions, such as hydrogen bonds, he has discovered new classes of superconductors and investigated pressure-induced phase transitions in magnetic coordination polymers. Dr. Schlueter was elected as a Fellow of the American Physical Society in 2015 and received NSF's Meritorious Service Award in 2022. He has chaired and serves on the Advisory Boards for several international conferences. Schlueter has co-authored over 400 publications (H-index 52) and delivered in excess of 75 invited presentations and seminars at international conferences and institutions. He has mentored 6 postdoctoral scholars and over 75 undergraduate students.

# Session 1

## Progress in Materials DX Platform Initiatives
## マテリアル DX プラットフォーム構想の進展

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**“DX of Fabrication Processes Accelerating Development of Diverse Devices”**
「多様なデバイス開発を加速させる加工プロセスデータ収集・利活用の取り組み」
**Kentaro Totsu (Tohoku University)**
戸津 健太郎（東北大学）

**“Nagoya University ARIM Hub for Accelerated Data-Driven R&D of Biomaterials and Biodevices”**
「名古屋大学 ARIM ハブ拠点におけるバイオマテリアル・バイオデバイスのデータ駆動型研究開発支援」
**Yoshinobu Baba (Nagoya University)**
馬場 嘉信（名古屋大学）

**“The Future of Data-Driven Materials Research Enabled by Materials DX Platform Integration”**
「マテリアル DX プラットフォーム連携が切り拓くデータ駆動型材料研究の未来」
**Satoshi Minamoto (National Institute for Materials Science)**
源 聡（NIMS）

**“Global Trends and Future Prospects for Data- and Robot-Driven Materials Science”**
「データ・ロボット駆動材料科学の世界的動向と将来展望」
**Taro Hitosugi (The University of Tokyo)**
一杉 太郎（東京大学）

**“DX Approaches for Structural Materials Research Incorporating Microstructures”**
「材料ミクロ組織を取り入れた構造材料研究のための DX アプローチ」
**Kyosuke Yoshimi (Tohoku University)**
吉見 享祐（東北大学）

# DX of Fabrication Processes Accelerating Development of Diverse Devices
# 多様なデバイス開発を加速させる
# 加工プロセスデータ収集・利活用の取り組み

**K. Totsu**

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## Abstract

The research and development of various devices are supported through microfabrication technologies in ARIM. However, due to the wide variety of materials, structures, and processes involved, a significant amount of information, particularly technical know-how, is required. To address this need, a DX environment is being developed to enable the search and recommendation of process flows and recipes tailored to individual device development. Data related to microfabrication is being accumulated and utilized to assist users in achieving their development goals more efficiently and promptly.

## I. INTRODUCTION

Since 2010, Tohoku University has been offering Hands-on-access Fab. services as part of the current ARIM with approximately 150 tools for microfabrication. Based on the concept of open collaboration, various process-related information obtained by users and staff has been organized and shared with users through the respective equipment managers[1]. For example, in etching processes, information such as differences in etching rates depending on materials or uniformity has been collected and made available. While the structures and applications of specific devices often cannot be disclosed, individual process recipes are generally open for sharing. In ARIM project, Tohoku University, serving as the hub for the Advanced Device Group, cooperates with University of Tsukuba, Toyota Technological Institute, Kagawa University and other institutions to accelerate DX in the development of diverse devices.

## II. DX ACTIVITIES

Many of the fabrication tools used in device development cannot output process parameters and other data in electronic form. To address this, Excel template files called Fabrication Data Log (FDL) are prepared for processes, allowing data to be manually input and collected. The FDL contents are divided into process data and flow (sequence) data. Process data consists of input sheets for each process, such as photolithography. Additionally, mask pattern data and images of resist patterns after processing, such as those captured with optical or electron microscopes, can be registered as attached files. Flow data, on the other hand, represents the sequence of fabrication steps involved in device fabrication. Specifically, it arranges the data IDs from the process data in the order of the fabrication steps required for a particular device.

To promote data utilization, our staff are collecting standard structural and process data for frequently requested components in devices, such as piezoresistive elements. Piezoresistive elements are particularly applied in pressure sensors and are also included as themes in student training programs[2]. Using IntelliSuite, a commercially available MEMS design integration software, enables the review of processes and mask designs, as well as the 3D modeling of MEMS structures within the software. This approach enhances the efficiency and accuracy of design and process validation.

**References**

[1] K. Totsu, M. Moriyama and M. Esashi, *Nat. Electron.* 2 (2019), pp.134-136.
[2] K. Totsu, M. Moriyama *et al*., *Sens. Mater.* 31 (2019), pp.2555-2563.

| | A | B | C | D | E | F | G | H | I | J | K | L | M |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | 未入力の項目があります | あにスクロールしてください～ | RDE項目 | 入力必須 | Input/入力欄 | Input/入力欄 | Input/入力欄 | Input/入力欄 | Input/入力欄 | Unit/単位 | Note/備考 | |
| 2 | RDE取り込み列 | | | | | Example | ※ | ※ | ※ | ※ | | 提供しないデータは※を取る | |
| 3 | ID, date, environment/ID, 作業日, 環境 | Data ID | Data ID | ※ | ※ | P_sens_Litho_230411-1 | | | | | | 任意の文字列 | |
| 4 | | Date yyyy/mm/dd | 作業日 | ※ | ※ | 2023/4/11 | | | | | | 年/月/日 | |
| 5 | | Time hh:mm | 作業時間 | | | 15:00 | | | | | | 時分 | |
| 6 | | Temperature | 室温 | | | 22.0 | | | | | ℃ | | |
| 7 | | Humidity | 湿度 | | | 26 | | | | | % | | |
| 8 | | | | | | | | | | | | | |
| 9 | Substrate/基板 | Material | 材料 | ※ | ※ | SI | | | | | | | |
| 10 | | Size | 大きさ | ※ | ※ | 4Inch | | | | | | | |
| 11 | | Thickness | 厚さ | ※ | ※ | 525.0 | | | | | um | | |
| 12 | | Material-top surface | 基板表面の主な材料 | ※ | ※ | Al | | | | | | | |
| 13 | | Quantity | 枚数 | ※ | ※ | 1 | | | | | pcs | | |
| 14 | | | | | | | | | | | | | |
| 15 | Coating/塗布 | Equipment | 装置 | | ※ | B-13_Coater/Developper_SUSS_ACS200Gen3 | | | | | | 装置名 | |
| 16 | | Equipment (ARIM No.) | 装置(ARIM No.) | ※ | | TU-062 | | | | | | ARIM設備ID(自動入力) | |
| 17 | | Material | 塗布材料 | ※ | ※ | TDMR-AR80_6cp | | | | | | | |
| 18 | | Target thickness | 塗布狙い膜厚 | ※ | ※ | 1.5 | | | | | um | | |
| 19 | | Recipe name | レシピ | | | 8003_COAT_HDMS60deg060sec_AR80_6cp2500rpm_BAKE90deg090sec | | | | | | Coater developer only | |
| 20 | | HMDS treatment | HMDS処理 | ※ | ※ | Yes | | | | | | ←Yes/No | |
| 21 | | Main rotation | 主回転数 | ※ | ※ | 3000.0 | | | | | rpm | | |
| 22 | | Baking temperature | ベーク温度 | ※ | ※ | 110.0 | | | | | ℃ | | |
| 23 | | Baking time | ベーク時間 | ※ | ※ | 300.0 | | | | | sec | | |
| 24 | | Other info | その他情報 | ※ | ※ | | | | | | | | |
| 25 | | | | | | | | | | | | | |
| 26 | | Equipment | 装置 | | ※ | B-14_i-line stepper_Canon_FPA-3030i5+ | | | | | | 装置名 | |
| 27 | | Equipment (ARIM No.) | 装置(ARIM No.) | ※ | | TU-063 | | | | | | ARIM設備ID | |
| 28 | | Minimum pattern size | 最小パターンサイズ | ※ | ※ | 1.5 | | | | | um | | |
| 29 | | Job name-stepper | ジョブネーム-ステッパ | ※ | | | | | | | | Stepper only | |

ver.情報 | Process flow | Wet cleaning_etch | Lithography | Oxidation_diffusion | Implantation | Annealing | CVD | Sputtering | Evaporation | Plating | ALD | DRIE | RIE | Dry cleaning | CDE | Io

**Fig. 1**
Excel template of Fabrication Data Log (FDL), including process data and flow (sequence) data.

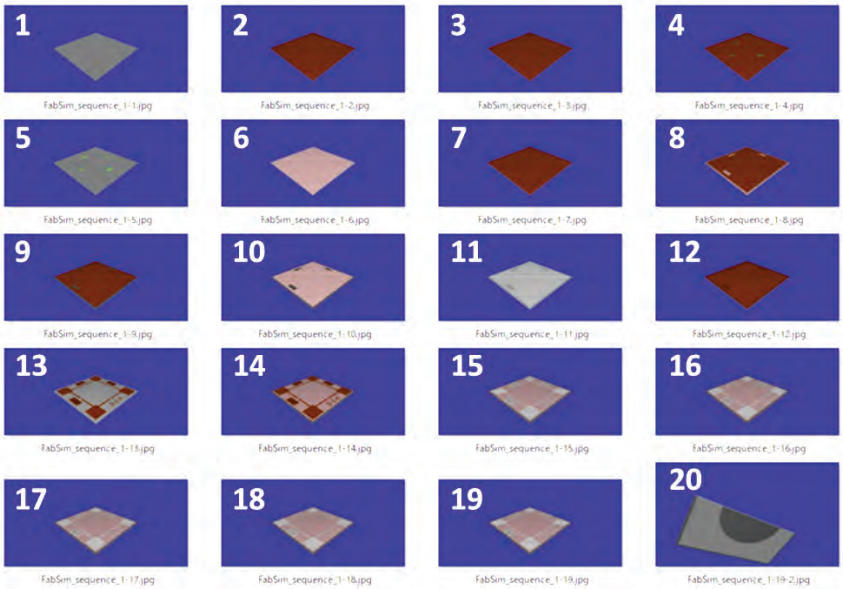


**Fig. 2**
3D modeling of fabrication process flow for silicon piezoresistive force sensor using IntelliSuite.

Kentaro Totsu, Micro System Integration Center, Tohoku University

Kentaro Totsu is the Director and a Professor of Micro System Integration Center, Tohoku University. He obtained Doctoral degrees from the Department of Mechatronics and Precision Engineering, Tohoku University in 2004. He served as an Associate Professor at the Micro System Integration Center (μSIC) from 2010 to 2020. Since 2010, he has also been the Director of the Hands-on-access Fabrication Facility at the Jun-ichi Nishizawa Memorial Research Center, Tohoku University. In 2021, he was appointed as the Director and a Professor at μSIC, where he currently oversees the research center and manages one of the largest open facilities for microsystem technologies. Under his leadership, the center has collaborated with over 300 partners since 2010, driving the industrialization of microsystems. Since 2024, he has chaired the Academia-Regional-Industry Collaboration Working Group for Semiconductor Human Resource Development under the Leading-edge Semiconductor Technology Center (LSTC).

# Nagoya University ARIM Hub for Accelerated Data-Driven R&D of Biomaterials and Biodevices

# 名古屋大学ARIMハブ拠点における バイオマテリアル・バイオデバイスのデータ駆動型研究開発支援

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Nagoya University is the Hub for next-generation biomaterials in the MEXT ARIM (advanced research infrastructure for materials and nanotechnology in Japan). We have been supporting the data-driven R&D for accelerated biomaterials and biodevices design, such as nanobiodevices for cancer diagnosis, quantum dots for *in vivo* imaging, biological quantum nanosensors, and bio-adaptive materials [1-16]. We have supported to develop nanowire devices, which are extremely useful to isolate extracellular vesicles from body fluids and vesicle-encapsulated microRNA analysis (Fig. 1). The device composed of a microfluidic substrate with anchored nanowires gives us highly efficient collections of extracellular vesicles in body fluids and *in situ* extraction for huge numbers of miRNAs (2,500 types) more than the conventional ultracentrifugation method. Nanowire devices gave us the miRNA date for several hundred patients and machine learning system based on these miRNA data enabled us to develop the early-stage diagnosis for lung cancer, brain tumor, pancreas cancer, liver cancer, bladder cancer, prostate cancer, diabetes, heart diseases, and Parkinson disease.

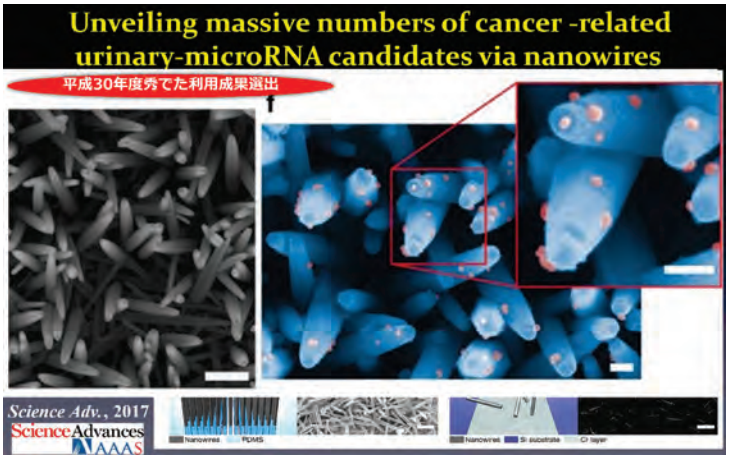


**Figure 1.** Nanowire devices for cancer diagnosis [1, 3]

We have been supporting data-drive R&D for biological quantum nanosensors. Nanodiamonds, with nitrogen-vacancy centers, and quantum dots are applied to develop quantum sensors for quantum switching *in vivo* imaging for iPS cell (induced pluripotent stem cells) based regenerative medicine, and quantum photo immuno-therapeutic devices for cancer (Fig. 2).

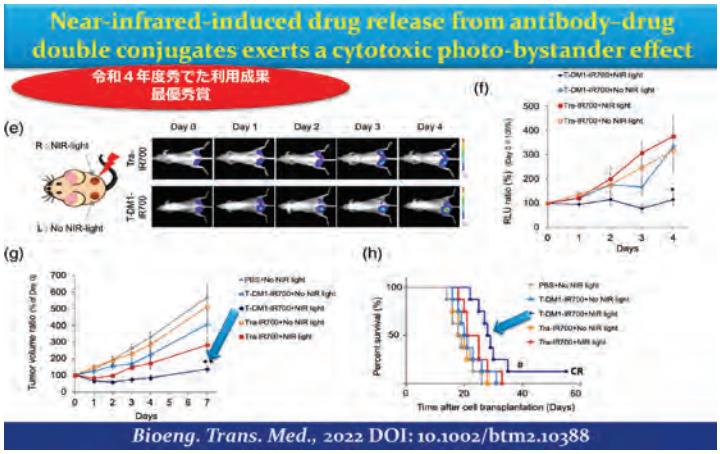


**Figure 2.** Quantum photo immuno-therapeutic devices for cancer [2, 6]

Since Kyoto University is the Hub for bio-adaptive materials in the MEXT DxMT (data creation and materials technology project), Nagoya University is collaborating with Kyoto University to support the data-driven R&D for accelerated bio-adaptive materials design. Cutting-edge MS technology enables us to collect big data for the amino acid sequences of proteins and peptides

isolated from spider's silk. These sequence data are applied to the data-driven development for sustainable textiles, fiber materials, and so on.

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| 1981-1986 | Department of Chemistry, Faculty of Science, Kyushu University, Ph. D. Degree in Chemistry |

**Research and Professional Experience**:

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| 1986-1986 | Postdoctral Fellowship at Kobe Women's College of Pharmacy |
| 1986-1990 | Assistant Professor at the Department of Chemistry, Oita University |
| 1990-1997 | Senior Lecturer. Associate Professor at Kobe Pharmaceutical University |
| 1997-2005 | Professor at the Department of Medicinal Chemistry, The University of Tokushima |
| 2004-2024 | Professor at the Department of Applied Chemistry, School of Engineering, Nagoya University |
| 2008-2024 | Professor at the Department of Medical Science, School of Medicine, Nagoya University |
| 2008-2012 | Presidential Advisor of Nagoya University |
| 2010-2015 | Director, FIRST Research Center for Innovative Nanobiodevices, Nagoya University |
| 2015-2019 | Director, ImPACT Research Center for Advanced Nanobiodevices, Nagoya University |
| 2017-present | Research Supervisor, JST CREST "Eextracellular fine particles" Project |
| 2018-2022 | Director, Institute of Nano-Life-Systems, Nagoya University |
| 2019-present | Director General, Institute for Quantum Life Science, National Institutes for Quantum Science and Technology (QST) |
| 2020-present | Project Leader, MEXT Q-LEAP Quantum Life Science |
| 2020-present | Fellow, Technology Strategy Center (TSC), NEDO |
| 2020-present | International Scientific Board, ONCOLille, l'Institut de recherches interdisciplinaires en cancérologie de Lille, France. |
| 2021-present | Project Leader, MEXT ARIM Next-Generation Biomaterials R & D Hub |
| 2024-present | Designated Professor, Research Institute for Quantum and Chemical Innovation, Nagoya University |
| 2024-present | Vice President of the Chemical Society of Japan (CSJ) |

# The Future of Data-Driven Materials Research Enabled by Materials DX Platform Integration

# マテリアルDXプラットフォーム連携が切り拓くデータ駆動型材料研究の未来

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**Abstract**

Data-driven research in materials science is pivotal for significantly enhancing the speed and accuracy of materials development, with the aim of strengthening Japan's industrial competitiveness and solving social issues. In particular, there is a need for the rapid development of new materials to address issues such as environmental and energy problems. In Japan, under the “Materials Innovation Strategy”, the National Institute for Materials Science (NIMS) is working to establish a materials data platform[1]. In collaboration with the Advanced Research Infrastructure for Materials and Nanotechnology (ARIM) and the Data-Creation and Application-Oriented Materials Research and Development Project (DxMT). Through the operation of DICE[2], this platform aims to drive digital transformation (DX) in materials science by optimizing the collection, management, and analysis of materials data, while also enabling efficient data sharing among researchers

The DICE system comprises three main components: MatNavi, RDE, and MInt. In addition, the development of pinax, a platform for AI analysis, is currently in progress. MatNavi is the culmination of the materials database that NIMS has accumulated over many years, and it covers a wide range of materials, encompassing a diverse range of materials such as metals, inorganic substances, organic materials, and polymers, and includes physical property data and structural information. Researchers can access material data collected using various methods through MatNavi, and obtain insights for new material design. RDE (Research Data Express) is a platform to enhance data sharing among researchers to facilitate research DX. Measurement data and data analysis results are stored in a form suitable for data-driven materials research through structured processing, and an environment is provided that allows easy access. This enables smooth information exchange between different research groups, and facilitates joint research. In addition, the process from data generation to analysis is recorded, which improves reproducibility and is expected to increase reliability in joint research. MInt (Materials Integration by networking technology) is an integrated system that supports the prediction of material performance and the optimization of process conditions. By combining advanced technologies such as computational science, databases, and machine learning, it is possible to simulate the properties of materials and manufacturing processes with precise. In particular, it is possible to design a model that links the “process-structure-properties-performance” of structural materials, and to propose new material design methods. In addition, pinax is a framework for applying machine learning technology to materials research. It is expected that machine learning technology will be used to extract meaningful patterns and laws from a vast amount of material data, and to design new materials and improve the performance of existing materials.

Strengthening the functionality of individual platforms is undoubtedly crucial. However, significant advancements in digital transformation (DX) for materials research can be realized in DX for materials research by integrating these platforms through technologies such as APIs and ontologies. For instance, AI analysis can be conducted by leveraging data from MatNavi, RDE, and even external sources, while the AI analysis models can be employed to perform comprehensive simulations for material performance evaluation using MInt. This data-driven, collaborative platform approach aims to transform material development from a traditional hypothesis-driven, trial-and-error methodology to a more precise and efficient design process utilizing data and artificial intelligence.

This initiative aims to accelerate materials development by streamlining the collection, accumulation, and analysis of materials data, facilitating data sharing among researchers, and leveraging AI for materials design support. Additionally, this initiative will also play a role in strengthening industry-academia-government collaboration in Japan. By utilizing the NIMS platform, researchers in materials science are expected to foster open innovation and enhance Japan's overall materials research capabilities. The 'Materials DX Platform Development' by NIMS is intended to contribute to the enhancement of international competitiveness and the resolution of societal challenges by advancing and optimizing materials science research in Japan. The effectiveness of this platform has already been demonstrated in the development of high-performance magnetic materials and the exploration of novel polymer materials. Future plans involve expanding its application to areas of significant social demand, such as the development of new materials that address environmental and energy challenges and the design of biomaterials.

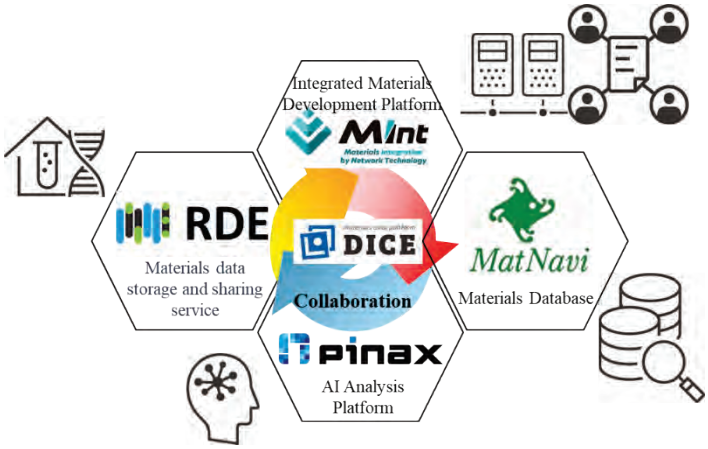


Fig. 1 Formation and collaboration of material data platforms

**References**

[1] https://www.nims.go.jp/rnfs/en/materials-data-platform/ (accessed on 1st Dec. 2024)
[2] https://dice.nims.go.jp

<Minamoto Satoshi>
<National Institute for Materials Science (NIMS)>

<CV>

Received his Ph.D. from Tokyo Institute of Technology in March 2008 for his thesis on STM observation of Ag/Si surface structures; worked on thermodynamic calculations using ab initio and CALPHAD methods from 2000 to 2015; engaged in the development of the “MInt system” for structural materials research at NIMS since February 2015; since April 2018, he has been engaged in the development of fundamental technologies for the materials data platform; and since April 2024, he has been in his current position (Platform Director).

# Global Trends and Future Prospects for Data- and Robot-Driven Materials Science
# データ・ロボット駆動材料科学の世界的動向と将来展望

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## Abstract

Advances in digital technologies are accelerating the evolution of materials science. There is a growing trend to incorporate autonomous synthesis and characterization (Fig. 1). This shift requires the integration of machine learning, robotics, and data analytics.[1]

Here, we present global trends and our recent achievements in autonomous materials exploration. Our system is designed to fully automate the processes of sample handling, thin-film deposition, and growth condition refinement (Fig. 2). By using Bayesian optimization with robotic automation, we facilitate high-throughput experimentation and generate extensive datasets that cover many aspects of synthesis and evaluation. We demonstrate the synthesis and optimization of electrical conductivity in oxide thin films and solid electrolytes.[2, 3]

This presentation concludes with a brief discussion of the prospects and implications of this innovative research methodology for accelerating advances in materials science.

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[3] Autonomous exploration of an unexpected electrode material for lithium batteries, S. Kobayashi, R. Shimizu, Y. Ando, T. Hitosugi, ACS Mater. Lett. 5, 2711–2717 (2023).

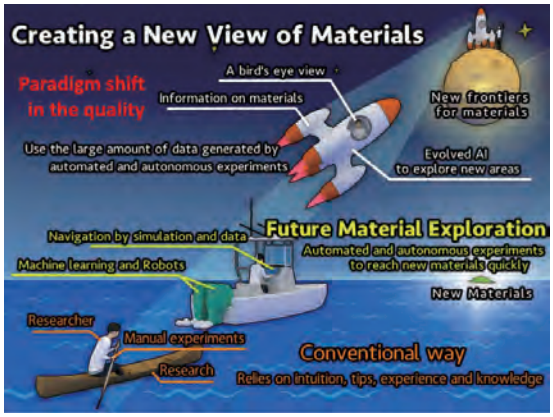



**Fig. 1** Vision of the data- and robot-driven science.

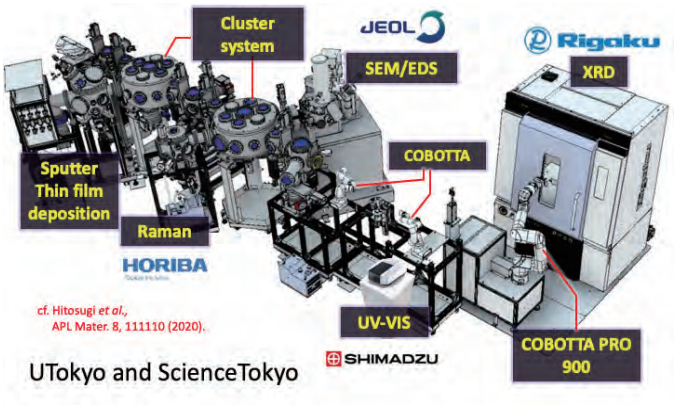
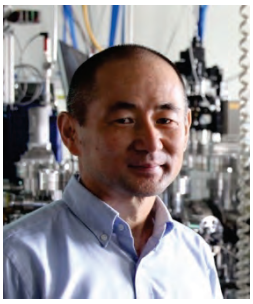



**Fig. 2** Autonomous synthesis and characterization system for thin-film material exploration.



Taro Hitosugi
The University of Tokyo

He received his PhD (Doctor of Engineering) from The University of Tokyo in 1999 and worked at Sony Corporation. Then, he served as an Assistant Professor at The University of Tokyo from 2003 and an Associate Professor at the Tohoku University from 2007. He was appointed a full professor at the Tokyo Institute of Technology in 2015. From 2022, he is a full professor at The University of Tokyo, Department of Chemistry. He specializes in solid-state chemistry. His research interests involve surfaces and interfaces of materials for electronics and energy applications. He has recently succeeded in autonomous materials synthesis by machine learning and robotics, aiming to accelerate materials science research. He has published more than 200 refereed papers in leading academic journals.

# DX Approaches for Structural Materials Research Integrating Microstructures
# 材料ミクロ組織を取り入れた構造材料研究のためのDXアプローチ

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**Abstract**

The properties and performance of inorganic structural materials are strongly dependent on their microstructure. Furthermore, since the microstructure has a hierarchical structure from the atomic to macro levels, the design of structural materials requires microstructure control on multiple scales. Therefore, in order to predict the properties and performance of structural materials, it is necessary to: 1. extract microstructural features at multiple scales, 2. identify the properties of each constituent phase by considering the equilibrium composition indicated by the phase diagram, and 3. model the hierarchical microstructure and assign properties to each constituent phase. In this talk, I will introduce the challenges of the Research Initiative of Structural Materials under Extreme Environments (RISME), which aims to establish the framework for structural materials research proposed above.

## I. MICROSTRUCTURE FEATURE EXTRACTION

The MoSiBTiC alloy, which has attracted attention in recent years as a novel ultrahigh temperature material, is composed of a Mo solid solution ($Mo_{ss}$), $Mo_5SiB_2$ ($T_2$), TiC, and the metastable phase $Mo_2C$, and has a very complex hierarchical microstructure. For this alloy, we have succeeded in segmenting scanning electron microscope images obtained at different magnifications using image processing and in extracting the microstructural feature values of each constituent phase.

## II. PHASE DIAGRAMS AND PROPERTIES OF CONSTITUENT PHASES

A thermodynamic database for the Mo-Ti-Si-C-B quinary system was created based on experimental phase equilibrium data and other information, and a calculated phase diagram that included the composition range of MoSiBTiC alloys was successfully created. The composition of each constituent phase was determined based on the phase equilibria shown in the experimental or calculated phase diagrams, and the mechanical properties of each constituent phase as a function of composition were obtained using the nanoindentation plastometry and molecular dynamics calculations using machine learning potentials.

## III. PREDICTION OF MECHANICAL PROPERTIES BY FINITE ELEMENT ANALYSIS

In order to evaluate the macroscopic material properties of MoSiBTiC alloys, which have a complex and locally heterogeneous microstructure, we applied the Representative Volume Element (RVE) method to obtain a solution using the Finite Element Method (FEM). The result is shown in Fig. 1. This not only allowed us to predict the macroscopic stress-strain curve of MoSiBTiC alloys, but also to clarify the local mechanical response within the microstructure. It is hoped that this framework will help to clarify the relationship between microstructural features and macroscopic and local mechanical responses.

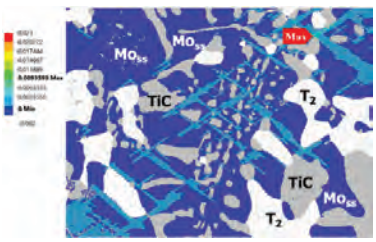


**Fig. 1**
FEM analysis using the RVE model for the MoSiBiC alloy.

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Apr. 2018 – Mar. 2024: Special Assistant to the President for Outreach Activity, Tohoku University, JAPAN.
Apr. 2013 – Present: Professor, Graduate School of Engineering, Tohoku University, JAPAN.
Oct. 2022 – Present: Director, Research Initiative of Structural Materials for Extreme Environments (RISME), Data Generation and Utilization Materials Research and Development Projects (DxMT), Ministry of Education, Culture, Sports, Science and Technology, Japan (MEXT).

# Session 2

## Promoting R&D via Materials DX Platform
## マテリアル DX プラットフォームを活用した研究開発の推進

MatISS 2025

**“Social Implementation of Ball SAW Sensors, a Palm Sized Gas Chromatograph”**

「ボール SAW センサの社会実装、超小型可搬ガスクロマトグラフ」

**Shingo Akao**
**(Ball Wave Inc.)**
赤尾 慎吾
（ボールウェーブ株式会社）

**“New Characterization Technology and Methods from ARIM- University of Tokyo”**

「ARIM 東京大学発の新しい評価技術と手法」

**Yuichi Ikuhara**
**(The University of Tokyo)**
幾原 雄一
（東京大学）

# Social Implementation of Ball SAW Sensors, a Palm Sized Gas Chromatograph
# ボールSAWセンサの社会実装、超小型可搬ガスクロマトグラフ

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## I. INTRODUCTION

There is a need for on-site analysis of a wide variety of volatile organic compounds (VOCs) in semiconductor manufacturing, bio-manufacturing, global environmental analysis for carbon neutrality, and pressurized environmental control for space activities. Gas chromatographs (GC) are effective for multi-species gas analysis, but are generally difficult to apply in the field due to their large size and the large number of utilities required. In contrast, we have developed a palm sized ball SAW GC by applying a ball SAW sensor that utilizes surface acoustic waves (SAWs) orbiting multiply on the surface of a spherical element [1,2]. The ball SAW sensor is shown in Fig.1. In this presentation, the structure of the developed palm-sized GC and its application to in-situ analysis in air will be reported.

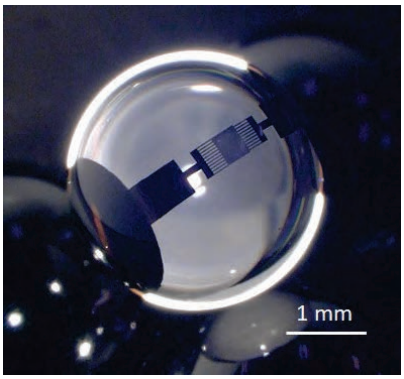


**Fig. 1 Ball SAW Sensor**

## II. Ball SAW GC

A schematic diagram of the ball SAW GC is shown in Fig. 2. The sample gas is drawn by a pump and collected in the pre-concentrator. Then, by switching the valve to rapidly increase the temperature of the pre-concentrator tube by resistive heater, the collected components are instantly heated and desorbed, and the hydrogen carrier gas flows introduced into the separation column in a backflush. Each component is separated in time by the difference in adsorption on the stationary phase coated on the inner surface of the column, and adsorbed on the sensitive film deposited on the ball SAW sensor, which is detected as SAW delay time change and amplitude change.

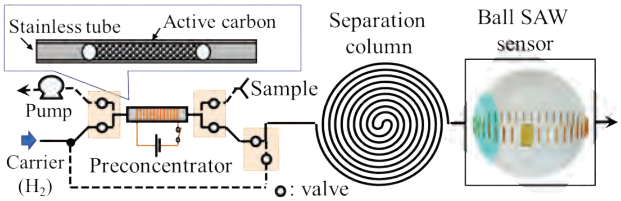


**Fig. 2 Schematic diagram of a ball SAW GC**

The palm-sized ball SAW GC fabricated in this study is shown in Fig. 3. This system is equipped with a hydrogen canister for gas supply, a pressure regulator, the pre-concentrator, the column, the ball SAW sensor, the valve manifold, the ball SAW drive circuit, and a valve drive and heater circuit, and can be connected to a PC via USB for control and analysis. The pre-concentrator was a stainless-steel pipe with an outer diameter of 1.61 mm and a wall thickness of

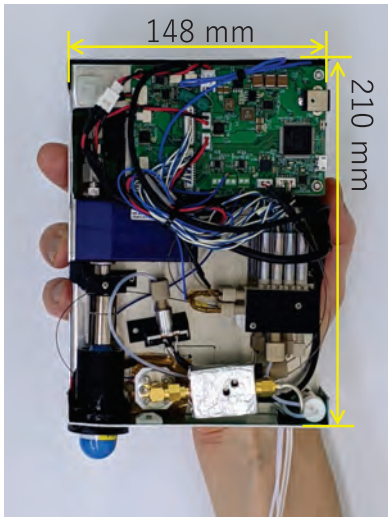


**Fig. 3 A palm sized ball SAW gas chromatograph**

0.18 mm, packed with approximately 2 mg of Tenax TA as the adsorbent, and wrapped around the periphery with nichrome wire for resistive heating. The column was a metal capillary, 30 m long Ultra-Alloy®, coated with polyethylene glycol as the stationary phase, and wound in a solenoid shape.

## III. Toxic gas detection in outdoor environments

For the reliable management of industrial plants and predict their impact on the surrounding environment, analysis of multiple gases emitted from such plants using GCs is essential. A GC installed on a drone would be a solution for places at high altitudes and elevated temperatures or with hazardous gas emissions.

As shown in Fig. 4, white smoke was emitted from the top of the chimney. The drone was brought close to this point and made to hover so that the horizontal position of the tip of the sampling unit was inside the chimney opening. Under these conditions, the smoke emitted from the chimney was sucked in for 0.5 min at a flow rate of 20 mL/min through the sampling tube and 10 mL of smoke was collected in the pre-concentrator.

**Fig. 4 Collecting smoke from a chimney using a gas chromatograph installed on a drone.**

It is noted that, in the chromatogram in Fig. 5, propylene glycol (P) was detected near the peak corresponding to octane (C8). This substance is usually synthesized by hydrolyzing glycerin catalyzed by a copper-based compound and is not generated under normal plant operation. Therefore, the chromatogram in Fig. 5 shows the possibility that the ball SAW GC installed on a drone can separate and detect abnormal gases generated owing to plant malfunctions.

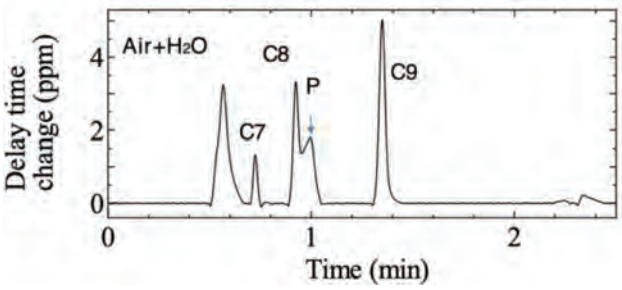


**Fig. 5 Chromatogram of gas components in smoke emitted from the chimney**

## IV. Conclusion

The palm-sized GC developed was designed and demonstrated for use on a drone to measure and analyze hazardous gases in the air as an example of its field application. This technology is expanding its range of applications to include not only robotics, but also airborne molecular contamination of advanced semiconductors, metabolic monitoring for biomanufacturing, behavior of volatile organic compounds in the Earth's troposphere, and analysis of pressurized environments for human activities in space.

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Shingo Akao

Ball Wave Inc.

1997: B. A. in Physics from Toho University. 1999: M. S. in Science and Engineering from Tsukuba University, and started his career in Research Center of Toppan Printing Co. 2003: Got involved in the R&D of ball SAW. 2009: Ph.D. in Department of Materials Processing, Graduate School of Engineering, Tohoku University. 2015: Co-founded Ball Wave Inc. as president and CEO.

# New Characterization Technology and Methods from ARIM-University of Tokyo
# ARIM 東京大学発の新しい評価技術と手法

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**[2]Masatoshi Hanai and [2]Kenjiro Taura,**

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**Abstract**
The University of Tokyo has intensively developed nanotechnology research, focusing on advanced microstructure analysis and microfabrication with core facilities at Asano Campus and Takeda Sentanchi Building. Over the years, the university has led major national initiatives, such as the Nanotechnology Network Project (2007–2011), the Low Carbon Research Network Project (2011–2016), and the Nanotechnology Platform Project (2012–2021), achieving globally recognized outcomes. Building on this foundation, the university was selected in 2021 for MEXT's Advanced Research Infrastructure for Materials (ARIM) Program and established "The University of Tokyo Advanced Research Infrastructure (ARIM)."
This program focuses on energy conversion materials to tackle environmental challenges and achieve carbon neutrality. By collaborating with Hiroshima University and the Japan Atomic Energy Agency, ARIM employs advanced microanalysis and microfabrication techniques to drive innovation. Additionally, the program leverages materials informatics and the ARIM-mdx data platform to enhance data collection, analysis, and utilization. This symposium will present cutting-edge technologies, methodologies, and examples of support provided by ARIM, highlighting advancements in energy conversion materials research.

## I. INTRODUCTION

### 1. Current Status and Support Examples of Microstructure Analysis

#### 1.1: Transmission Electron Microscopy (TEM) and Scanning TEM (STEM)

ARIM at the University of Tokyo operates 12 (S)TEM systems for analyzing diverse materials, from inorganic to biological samples. A recent addition, the JEM-F200 system, enables high-throughput, high-precision EDS analysis with minimal sample damage, thanks to two large-area silicon drift detectors (SDDs).
Improved sample preparation tools, such as the cooling-enabled ion milling system PIPSII, and advanced environmental controls, like holders for non-atmospheric exposure and cooling, support atomic-level analysis. For instance, atomic-resolution catalyst analysis conducted by experienced staff meets a wide range of research needs.

#### 1.2: Scanning Electron Microscopy (SEM)

The SEM division operates five SEM instruments designed for diverse analytical objectives, such as high-resolution or low-damage imaging. The JSM-IT800SHL and JSM-7800F enable non-atmospheric observations, which are further supported by enhanced capabilities this fiscal year.
For sensitive materials like lithium-ion and fuel cells, the IB-19520CCP cross-section polisher with cooling and non-atmospheric features minimizes thermal damage, allowing precise analysis of structures like fuel cell MEA layers. This helps assess bonding states and particle aggregation, critical for performance improvement.

#### 1.3: X-ray Diffraction (XRD)

ARIM operates three XRD systems and one single-crystal analysis system, supporting a variety of material types, including powders, thin films, and single crystals. Techniques like high-temperature and 2D detection meet diverse research needs.
A notable application is analyzing PZT ferroelectric films on Si wafers with $ZrO_2$ buffer layers, confirming epitaxial structures with orientation alignment. Additionally, beginner XRD workshops held in FY2023 attracted over 1,000 participants, promoting practical skills and earning high praise.

### 1.4: Secondary Ion Mass Spectrometry (SIMS)

The NanoSIMS 50L system supports high-sensitivity, high-resolution elemental and isotopic analysis for diverse samples, such as ceramics, semiconductors, and biological specimens.
A key application is high-resolution stable isotope imaging, revealing material reactions and pathways. For example, oxygen tracer distributions in SOFC/SOEC electrodes illuminate mechanisms, while oxygen movement in ceramic membranes provides insights into storage processes in catalysts.

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## II. Current Status of Data Collection and Utilization

ARIM's data division developed the "ARIM-mdx Data System" (https://arim.mdx.jp) in collaboration with the Graduate School of Engineering and the Information Technology Center. Fully operational since August 2023, this platform offers cloud storage and high-performance computing for data aggregation and analysis. With IoT-based remote data collection, the system supports over 900 academic and corporate users and is growing. Integration with theoretical research groups and supercomputers enables the combination of experimental and simulation data, creating a comprehensive system.
This interconnected platform accelerates materials research and fosters data-driven innovation. Moving forward, ARIM-mdx aims to enhance materials research and contribute to societal transformation through data-driven approaches.

Prof.Yuichi Ikuhara
School of Engineering, The University of Tokyo

Yuichi Ikuhara is Distinguished Research Professor of Institute of Engineering Innovation, School of Engineering at University of Tokyo. He graduated from Kyushu University with BS in 1983, and received Dr.Eng. from Department of Materials Sciences, Kyushu University in 1988. He then joined Japan Fine Ceramics Center (JFCC) as a researcher, and was the Division Manager at JFCC from 1993. In 1996, he joined University of Tokyo as an associate professor of Materials Sciences, and became a full professor since 2003. His current research interest is interface and grain boundary science, advanced transmission electron microscopy, high-temperature ceramics, dislocation technology and so on. Dr.Ikuhara is author and coauthor of about 960 scientific original papers in this field, and has more than 410 invited talks at international and domestic conferences. He received “Japan Academy Prize” (2023), Medal with Purple Ribbon” from the Emperor of Japan (2016), “Humboldt Research Award” from Alexander von Humboldt Foundation (2010) and so on. He is a fellow of the American Ceramics Society (2011), member of World Ceramic Academy (2014). He holds a group leader position at JFCC and WPI (World Premier International Research Center Initiative) professor at AIMR, Tohoku University concurrently.

# Session 3

## Material Innovation Accelerated by Data Driven Approaches
## データ駆動で加速するマテリアルイノベーション

MatISS 2025

**“Resonac's Data-Driven Materials Development DX Initiative and Expectations for the Materials DX Platform”**

「レゾナックでのデータ駆動型材料開発 DX の取組み紹介と
マテリアル DX プラットフォームへの期待」

**Yoshishige Okuno**
**(Resonac Corporation)**
奥野 好成
（株式会社レゾナック）

**“Machine Learning Technology in SiC Solution Growth Method”**

「SiC 溶液成長法における機械学習技術とその応用」

**Toru Ujihara**
**(UJ-Crystal Inc., Nagoya University)**
宇治原 徹
（株式会社 UJ-Crystal, 名古屋大学）

**“Materials Design and Process Development using Closed-Loop Digital Technology”**

「デジタル技術によるクローズドループを用いた材料設計とプロセス開発」

**Mikiya Fujii**
**(Nara Institute of Science and Technology)**
藤井 幹也
（奈良先端科学技術大学院大学）

# Resonac's Data-Driven Materials Development DX Initiative and Expectations for the Materials DX Platform

# レゾナックでのデータ駆動型材料開発DXの取組み紹介と マテリアルDXプラットフォームへの期待

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## Abstract

Collaboration between data scientists and experimentalists is necessary to accelerate material development, but differences in expertise can hinder the development of materials informatics. At Resonac Corporation, we accelerated the usage of materials informatics by deploying electronic laboratory notebooks, statistical analysis tools, and user-friendly web apps for experimentalists. This deployment has allowed them to focus on data organization and statistical analysis and to accelerate the development of new materials.

## I. INTRODUCTION

Using past experimental data is advantageous for material design, but constructing machine learning models based on this data poses challenges for experimentalists unfamiliar with machine learning. While many scientists are utilizing machine learning to predict material properties, the successful application requires careful model and attribute selection and hyperparameter tuning, which can sometimes yield inconsistent results. Although creating machine learning models is becoming more accessible, experimentalists often struggle with coding and tuning due to their lack of familiarity with these techniques. While data scientists excel in model development, they frequently need more domain-specific knowledge for materials design, leading to predictions that may seem unrealistic to experimentalists. To address these challenges, we have implemented electronic laboratory notebooks (ELN), statistical analysis tools, and user-friendly web applications to help experimentalists leverage machine learning insights while applying their expertise. Additionally, managing numerous machine learning models for over a hundred chemical products has resulted in the creation of a web app portal that facilitates data management and AI analysis, supporting data-driven research and development.

## II. RESONAC'S DATA-DRIVEN MATERIALS DEVELOPMENT DX INITIATIVE

To accelerate information sharing and statistical analysis knowledge, we introduced ELN developed by Biovia[1] and JMP software[2] developed by SAS Institute for statistical analysis. The distribution of these tools has steadily increased, enabling experimentalists to organize experimental data effectively.

We also developed AI web apps to predict the properties of various materials. We deployed over 50 apps with user-friendly interfaces, like polymer property prediction app[3], aluminum alloy prediction app[4], image analysis app, ChatGPT[5], molecular property prediction app, and others (**Fig. 1**)[6]. This system allows experimentalists to design materials independently, even without extensive data science knowledge. We also constructed a web app portal to make users available to these apps. Moreover, by implementing Machine Learning Operations[7,8], we efficiently managed numerous machine learning models and automated processes to update them as new experimental data became available.

To address data management challenges, we developed a data pipeline based on ELN (**Fig. 2**). This systematic approach helps convert scattered, unstructured data into structured data, facilitating

better data visibility and analysis. By fostering collaboration between data scientists and materials scientists, we have improved material informatics efficiency and streamlined the research process.

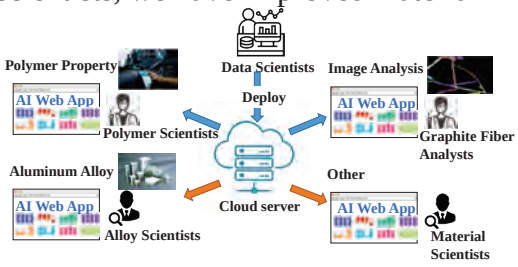


**Fig.1** Distribution of web apps.

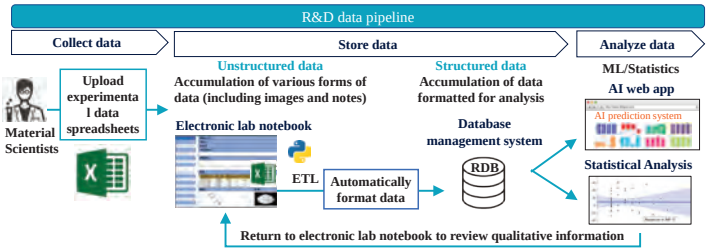


**Fig. 2** Data Pipeline by using ELN

## III. EXPECTATIONS FOR THE MATERIALS DX PLATFORM

We hope that the Materials DX Platform enhances data integration and management, accelerates materials development through digital tools and AI, enables advanced simulations and predictions, promotes collaboration across disciplines, improves sustainability in materials selection and processes, and provides educational resources for the next generation of researchers and engineers. At Resonac Corporation, we have prioritized solving individual challenges and advancing the development of specialized apps. However, ideally, we want to unify these apps onto a single platform. That said, it is also a fact that there are challenges that we need to overcome to achieve this, and we are hopeful we will find solutions to those challenges shortly.

## IV. CONCLUSION

Resonac Corporation's initiative on data-driven materials development represents a significant step forward in integrating machine learning into materials science. By addressing the challenges experimentalists face in utilizing past experimental data, this initiative fosters collaboration between data scientists and experimentalists, ultimately enhancing the accuracy and relevance of material predictions. Implementing electronic laboratory notebooks, statistical analysis tools and user-friendly web apps has empowered experimentalists to organize and analyze data effectively, allowing them to focus on their core expertise while leveraging advanced analytical tools.

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[8] Microsoft Azure: https://azure.microsoft.com/

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# Machine Learning Technology in SiC Solution Growth Method
# SiC溶液成長法における機械学習技術とその応用

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## Abstract

Materials development requires both material discovery and process optimization. While materials informatics has advanced the discovery stage, optimizing manufacturing processes remains challenging. To address this, we developed process informatics based on digital twin modeling for virtual process simulation. The digital twin enables optimization beyond physical constraints, enhancing innovation. This approach was applied to silicon carbide (SiC) crystal growth, crucial for next-generation power devices. Defect reduction is essential for SiC wafers, and the solution-growth method offers high-quality potential under near-equilibrium conditions. Using a digital twin, we optimized temperature, concentration, and flow distributions to control macrosteps on the crystal surface, reducing defects. Two objective function strategies were employed: leveraging basic research insights and adapting small-diameter growth parameters to large-diameter crystals. These efforts resulted in the successful growth of 8-inch SiC crystals, showcasing the potential of digital twin-driven process informatics for scalable, high-quality production.

## I. Materials Development and Process Informatics

Materials development is a complex process that requires a lot of time and effort. The process can be divided into two major categories: research and development of new materials and material process development to realize the new materials as specific manufacturing processes. In particular, in the initial stage of searching for new materials, it is necessary to find appropriate combinations from a vast number of material candidates, and in this stage, early materials informatics has made great achievements. On the other hand, the manufacturing process itself needs to be optimized in order to bring the materials into a manufacturable form. To solve this challenge, we have been working on the development of process informatics.

Process Informatics is a methodology that utilizes machine learning to improve the efficiency and accuracy of material processes. This methodology can be divided into two main categories: first, it utilizes Bayesian optimization and other techniques to efficiently predict optimal process parameters from experimental data. The second is a digital twin approach. In this approach, the process is modeled and a virtual experimental environment is created. By using this digital twin, the specifications and constraints of the equipment are also used as parameters, allowing for a higher degree of freedom of trial and error in the virtual environment and optimization beyond the limits of the actual equipment.

## II. Development of SiC Solution Growth Method Using Digital Twin

In this study, we applied this method to the growth process of silicon carbide (SiC) crystals in particular to further technological innovation: SiC has attracted considerable attention as a semiconductor for next-generation power devices. In SiC wafers, defect reduction is an extremely important issue, and its solution directly improves the quality of the entire manufacturing process. The solution-growth method is attracting attention as a method that is expected to produce high-quality crystal growth because it can grow crystals under near-equilibrium conditions.

Of particular importance in the solution growth method is the control of macrosteps on the crystal growth surface. Success in this control is the key to reducing defect density and obtaining high-

quality crystals. Proper control of the distribution of temperature, concentration, and flow in the solvent is essential for macrostep control. To optimize these distributions, we took advantage of the digital twin. In this virtual environment, we are attempting to optimize crystal growth conditions by predicting various distributions in the solvent based on physical models.

In the first approach, we used the knowledge from our basic research to define the distribution conditions for high quality crystal growth as objective functions. The second approach was to design an objective function based on the conditions that had been used to achieve high-quality crystals in small-diameter growth, so that it could be applied to large-diameter growth. This made it possible to find optimal parameters for crystals of different diameters with similar distribution conditions inside the solvent. As a result of using these techniques, we have succeeded in growing 8-inch SiC crystals.

Prof. Toru UJIHARA
IMaSS, Nagoya University, UJ-Crystal, U-MAP, Aixtal

Prof. Toru Ujihara is a professor at Nagoya University's Institute of Materials and Systems for Sustainability and serves as the director of the Deep Tech Serial Innovation Center. He specializes in semiconductor material science and crystal growth technology, with a particular focus on developing high-quality crystal growth technologies for next-generation semiconductor materials, such as silicon carbide (SiC), which have earned him recognition both domestically and internationally.

Born in 1970, he graduated from the Department of Materials and Engineering at Kyoto University and obtained his Ph.D. in engineering from the Graduate School of Engineering at the same university. After serving as an assistant professor at the Institute for Materials Research at Tohoku University, he joined Nagoya University as an associate professor in 2004, eventually advancing to his current position.

In his research, he employs solution growth methods for SiC to facilitate the practical application of energy-efficient materials for power devices. He is also advancing the development of cutting-edge materials, such as high-thermal-conductivity aluminum nitride (AlN). Furthermore, he has pioneered research in process informatics, incorporating data-driven approaches into crystal growth technologies, enabling efficient and high-precision process development.

In education, he has dedicated himself to mentoring many graduate and undergraduate students, fostering the next generation of researchers and engineers. He is also actively involved in establishing and managing startup companies. As CEO of UJ-Crystal, a university spin-off, he has been driving the social implementation of his research results, establishing a successful model for university-originated ventures.

# Materials Design and Process Development using Closed-Loop Digital Technology
# デジタル技術によるクローズドループを用いた材料設計とプロセス開発

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**Abstract**

Recently, the closed-loop development of materials leveraging digital techniques such as AI and simulations has garnered significant attention. In this talk, I will present two studies: the first focuses on process optimization for copolymerization, while the second explores the inverse design of inorganic materials by using virtual closed-loop modeling.

## I. Process Optimization in Copolymization

First, the properties of polymers are highly dependent on the combination and composition ratio of the monomers used to prepare them; however, the large number of available monomers makes an exhaustive investigation of all the possible combinations difficult. In the present study, five binary copolymers were prepared by radical polymerization using a flow reactor (Fig. 1), and the extrapolation regions for the estimation of the monomer conversion and monomer composition ratio in the polymer. Especially, in the extrapolation region, the model that included explanatory variables corresponding to quantum chemical calculation values representing the energy related to the radical reactions such as energies of transition states and radicals showed a high prediction accuracy [1]. Besides, we will make a presentation about Bayesian optimization to synthesize a desired copolymer by optimizing the process variables [2]. Here, optimization of copolymization of synthesis of styrene-methyl methacrylate by using Bayesian optimization (BO) in a flow system were conducted. Initial trials with four candidate points per cycle achieved optimization within five cycles, while a second trial with 40 points identified multiple processing conditions yielding target compositions and variations in physical properties. Data analysis revealed that the solvent-to-monomer ratio plays a key role alongside styrene proportions as well as temperature and reaction time. The results demonstrate that machine learning can precisely control copolymer composition and offer insights into reaction mechanisms. Future use of multi-objective BO for simultaneous optimization of composition and physical properties will be also presented.

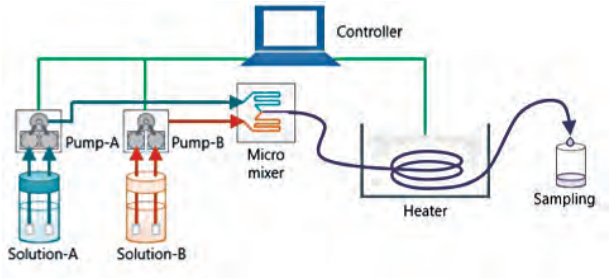


Fig. 1 Schematic representation of radical polymerization using a flow reactor

## II. Inverse Material Design of Inorganic Materials

Second, Materials development requires advanced knowledge and creativity, with designing materials to achieve desired properties—an inverse problem—being particularly challenging. While traditionally reliant on researchers' creativity, combining materials data with machine

learning can greatly accelerate novel material design. Recently, Conditional GAN (CompGAN), proposed by Sawada et al., was shown to generate chemical compositions with desired properties using a conditional adversarial network and oxidation state balancing [3]. However, the lack of corresponding crystal structure information limited direct validation of these properties. We integrates CompGAN with a machine learning-based crystal structure prediction model (CSPML [4]) to predict crystal structures for generated compositions, followed by DFT-based property calculations. By incorporating the generated data into the training set and iterating data augmentation (closed-loop), retraining, and generation, the search space is expanded, allowing for more diverse material proposals (Fig. 2).

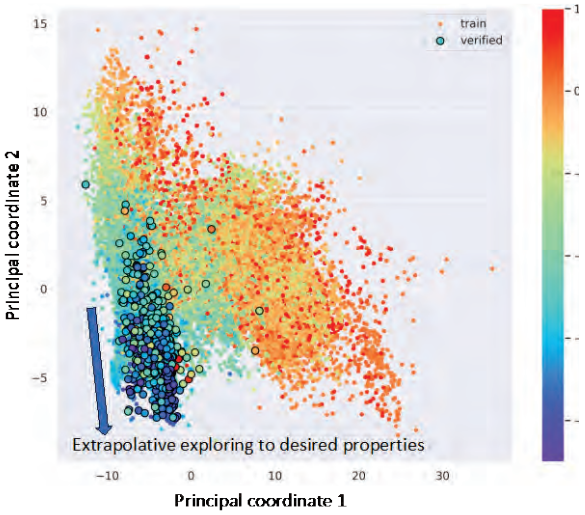


Fig. 2 Schematic representation of the extrapolative exploring

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MF received his Ph.D. from the University of Tokyo, Japan, in 2008. Following this, he worked as a postdoctoral researcher at the University of Tokyo from 2008 to 2009. In 2009, he transitioned to industry as a software engineer at Cybozu Inc., where he worked until 2010. He then returned to academia as an assistant professor at the University of Tokyo, a position he held from 2010 to 2017. In 2017, he joined Panasonic Corporation in Japan as a staff researcher and was later promoted to manager in 2019. Since 2021, he has been serving as a professor at the Nara Institute of Science and Technology in Japan.

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