

JAPAN  
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2023

# 文部科学省マテリアル先端リサーチインフラ 第21回マテリアル戦略 総合シンポジウム

マテリアル先端リサーチインフラが推進するマテリアル DX プラットフォーム構築

## 講演予稿集

### 開催日

2023年2月3日(金)



### 会場

東京ビッグサイト 会議棟1Fレセプションホール  
(東京都江東区有明)

### 主催

文部科学省マテリアル先端リサーチインフラ  
国立研究開発法人物質・材料研究機構  
マテリアル先端リサーチインフラセンター運営室

### 文部科学省マテリアル先端リサーチインフラ参画機関

北海道大学、公立千歳科学技術大学、山形大学、東北大学、  
筑波大学、物質・材料研究機構、産業技術総合研究所、  
東京大学、東京工業大学、早稲田大学、電気通信大学、  
信州大学、自然科学研究機構分子科学研究所、名古屋大学、  
名古屋工業大学、豊田工業大学、京都大学、  
北陸先端科学技術大学院大学、奈良先端科学技術大学院大学、  
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、広島大学、香川大学、九州大学





2023年2月3日(金) 会議棟1階 レセプションホール  
February 3rd (Fri.), 2023, Reception Hall

10:00-10:10

開会挨拶 Opening Remarks

10:00-10:05

宝野 和博 (物質・材料研究機構理事長)

Kazuhiro Hono (President, National Institute for Materials Science, Japan)

10:05-10:10

文部科学省

Ministry of Education, Culture, Sports, Science and Technology

Session 1

10:15-11:30

10:15-10:50 【基調講演 Plenary Lecture】

雨宮 慶幸 (高輝度光科学研究センター理事長)

Yoshiyuki Amemiya (JASRI)

「マテリアル革新強化に向けた放射光情報計測学(放射光計測×情報科学)への期待」

"Expectations for Synchrotron-Radiation Intelligent Measurement Analysis to Strengthen Materials Innovations"

10:55-11:30 【特別講演 Special Lecture】

年吉 洋 (東京大学 生産技術研究所 教授)

Hiroshi Toshiyoshi (University of Tokyo)

「ナノテクノロジープラットフォームを活用したMEMS研究開発」

"A Case Study: MEMS R&D using Nanotechnology Platform"

11:30-13:00 【昼食 Lunch】

Session 2

企業におけるマテリアルDXの取り組み

13:00-13:50

Material DX Initiatives in Companies

13:00-13:25

村井 亮太 (AGC株式会社)

Ryota Murai (AGC)

「R&D-DXのためのインフラ基盤とその将来像」

"DX infrastructures and its future vision for materials R&D"

13:25-13:50

河野 禎市郎 (旭化成株式会社)

Teiichiro Kohno (Asahi Kasei)

「旭化成におけるR&D DXの取り組み」

"R&D DX in Asahi Kasei"

13:50-14:00 【休憩 Break】

Session 3

ARIM事業と重要技術領域

14:00-17:00

About ARIM Project and Key technology Area

14:00-14:15 【ARIM事業の概要と取り組み紹介 Overview of the ARIM Business and Initiatives】

曽根 純一 (科学技術振興機構、文部科学省マテリアル先端リサーチインフラPD)

Junichi Sone (Japan Science and Technology Agency, Program Director of ARIM MEXT)

「マテリアル先端リサーチインフラの概要と、マテリアルDXプラットフォームが目指すもの」

"Overview of advanced research infrastructure for materials and nanotechnology (ARIM) and aims of the material DX platform"

Session データ創出基盤とデータ活用研究開発プロジェクトの融合(その1)

**3-1** Integration of Data Creation Infrastructure and Data Utilization R&D Projects <Part 1>

14:15-14:40

沼田 圭司 (京都大学)

**Keiji Numata** (Kyoto University)

「バイオ・高分子材料のビッグデータ構築と材料開発への利用」

“Digital transformation in biological and polymeric materials.”

14:40-15:05

伊藤 浩志 (山形大学)

**Hiroshi Ito** (Yamagata University)

「高分子および高分子マルチマテリアルの成形加工におけるデータ活用とプロセス最適化への取り組み」

“Process optimisation through data utilisation in the molding process of polymers and polymeric multi-materials”

15:05-15:30

**Shuichi Takayama** (Georgia Institute of Technology, USA)

「ハイスループット3次元マイクロフィジオロジーシステム -標準化と情報化-」

“High-Throughput 3D Microphysiological Systems -Standardization and Informatics-”

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15:30-15:45 【 コーヒーブレイク Coffee Break 】

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Session データ創出基盤とデータ活用研究開発プロジェクトの融合(その2)

**3-2** Integration of Data Creation Infrastructure and Data Utilization R&D Projects <Part 2>

15:45-16:10

杉山 正和 (東京大学)

**Masakazu Sugiyama** (University of Tokyo)

「再生可能エネルギー最大導入を実現する電気化学材料開発」

“Development of Electrochemical Materials for the Maximum Dissemination of Renewable Energy”

16:10-16:35

塩見 淳一郎 (東京大学)

**Junichiro Shiomi** (University of Tokyo)

「データ創出・活用による巨大パラメータ空間での材料探索: 熱機能材料を例に」

“Exploring materials in a huge parameter space through data creation and utilization: Examples of thermal functional materials”

16:35-17:00

山田 淳夫 (東京大学)

**Atsuo Yamada** (University of Tokyo)

「多階層計算科学・機械学習を活用した蓄電池開発」

“Battery development based on multi-stage computational and machine-learning protocols”

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17:00-17:05

閉会挨拶 **Closing Remarks**

17:00-17:05

小出 康夫 (JAPAN NANO 2023組織委員長、マテリアル先端リサーチインフラ運営機構長)

**Yasuo Koide** (Chairperson of the Organizing Committee of JAPAN NANO 2023 / Director, Advanced Research Infrastructure for Materials and Nanotechnology)



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曽根 純一 (科学技術振興機構、文部科学省マテリアル先端リサーチインフラPD)

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山田 淳夫 (東京大学)

# Session 1

Plenary Lecture & Special Lecture

基調講演と特別講演



## **Plenary Lecture**

基調講演

### **“Expectations for Synchrotron-Radiation Intelligent Measurement Analysis to Strengthen Materials Innovations”**

「マテリアル革新強化に向けた放射光情報計測学(放射光計測×情報科学)への期待」

**Yoshiyuki Amemiya (JASRI)**

雨宮 慶幸 (高輝度光科学研究センター理事長)

## **Special Lecture**

特別講演

### **“A Case Study: MEMS R&D using Nanotechnology Platform”**

「ナノテクノロジープラットフォームを活用したMEMS研究開発」

**Hiroshi Toshiyoshi (University of Tokyo)**

年吉 洋 (東京大学 生産技術研究所 教授)

# Expectations for Synchrotron-Radiation Intelligent Measurement Analysis to Strengthen Materials Innovations

## マテリアル革新強化に向けた放射光情報計測学（放射光計測×情報科学） への期待

Y. Amemiya

Japan Synchrotron Radiation Research Institute (JASRI),  
1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan

### Abstract

Synchrotron radiation facility (SPring-8)<sup>1)</sup> and X-ray free-electron laser facility (SACLA)<sup>2)</sup>, both located at the same site, are actively used in the fields of materials science and life science as indispensable tools for measuring electron state, atomic and molecular structures and their dynamics with sub-nanometer spatial resolution and several femtosecond temporal resolution. The measurement methods using synchrotron radiation are mainly classified into three categories: scattering, spectroscopy and imaging methods, all of which have static and dynamic modes. Annually, approximately 14,000 researchers from universities, academic research institutes, and companies use the facilities and the number of research papers published exceeds 1,100, which is equivalent to about 1 % of all research paper publication in Japan. In order to continue to be the top research facilities in the world and to allow more researchers to use them, we plan to upgrade SPring-8 to make it 100 times brighter and aim for energy-saving operation in the near future.

Nowadays, with the advancement of computers and related technologies, information science has made remarkable progress. One of the CREST areas<sup>3)</sup> of JST<sup>4)</sup> that I supervise, called "intelligent measurement-analysis" methods or "information measurement" methods, aims to detect physical quantities/material states, their changes, and latent factors that could not be found in the past by combining measurement technologies with information science and statistical mathematics, and to deepen scientific knowledge and solve social problems.

The "intelligent measurement-analysis" methods widely include inverse analysis techniques such as Bayesian inference, data assimilation, sparse modeling, image analysis, and signal processing developed in information science and statistical mathematics.

When "intelligent measurement-analysis" methods are introduced to synchrotron radiation research, conventional measuring methods using synchrotron radiation will be empowered. For example, they will help us carry out *operando* measurement of hitherto intractable objects under moving and functioning conditions by processing large amounts of data at higher speed and with higher precision in order to obtain characteristics of objects of interest.

The field of "intelligent measurement and analysis" methods is a new field that is possible when researchers in measurement science and information science begin to collaborate, and is considered an interdisciplinary technology field that integrates traditional research fields.

In this symposium, an overview of the research based on the "intelligent measurement and analysis" method being conducted at SPring-8/SACLA and expectations for the future will be presented.

### References

- [1] <http://www.spring8.or.jp/en/>
- [2] <http://xfel.riken.jp/eng/index.html>
- [3] [https://www.jst.go.jp/kisoken/crest/en/research\\_area/ongoing/bunyah28-3.html](https://www.jst.go.jp/kisoken/crest/en/research_area/ongoing/bunyah28-3.html)
- [4] <https://www.jst.go.jp/EN/>



<Facial Photo>

<CV>

Fields of Research:

Synchrotron Radiation Research, X-ray Instrumentation,  
especially Small-Angle X-ray Scattering for Soft Materials, X-ray Detectors

Education/Career,

1979 Received the degree of Doctor of Engineering from The University of Tokyo

1982 Research Associate, Photon Factory, KEK

1988 Visiting Researcher, Brookhaven National Laboratory, USA

1989 Associate Professor, Photon Factory, KEK

1996 Associate Professor, Graduate School of Engineering, The University of Tokyo

1998 Professor, Graduate School of Engineering, The University of Tokyo

1999 Professor, Graduate School of Frontier Sciences, The University of Tokyo

2007-2009 Dean of Graduate School of Frontier Sciences, The University of Tokyo

2016-2021 Director, OIL Laboratory for Advanced Operando Measurement Technology, AIST and The University of Tokyo

2017- Professor Emeritus of The University of Tokyo

2019- President of JASRI (Japan Synchrotron Radiation Research Institute)

Award:

2001 The 1st Academic Award, Crystallographic Society of Japan

2019 Synchrotron Radiation Science Award, Japanese Society for Synchrotron Radiation Research,



# A Case Study: MEMS R&D using Nanotechnology Platform ナノテクノロジープラットフォームを活用したMEMS研究開発

H. Toshiyoshi

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## Abstract

MEMS (Microelectromechanical Systems) is a technology to create miniaturized machines using semiconductor fabrication processes. Since 1996, the author has been involved in industrial collaborations, developing MEMS devices for fiber-optic communications, automotive, medical diagnostic applications, and most recently vibrational energy harvesters. These devices are developed using a mix of in-house and shared manufacturing facilities, including the Nanotech platforms. We will discuss the significance of shared facilities using a MEMS device as an example.

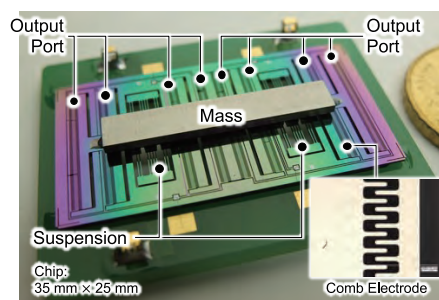
## I. INTRODUCTION

The successful installation of the internationally renowned semiconductor foundry is a good sign of the revival of Japan's hi-tech industry. We will soon see a rising demand for human resources in the field of microelectronics but it would take a few years or more for us in academia to produce a new generation of leading engineers and researchers. Perhaps it will take even longer to do so in the field of microelectromechanical systems or MEMS because of the wide variety range of processing techniques specifically tailored to each device. In this sense, the Nanotech-platforms will become more important as a training facility that provides practical experiences for more-than-Moore type engineering.

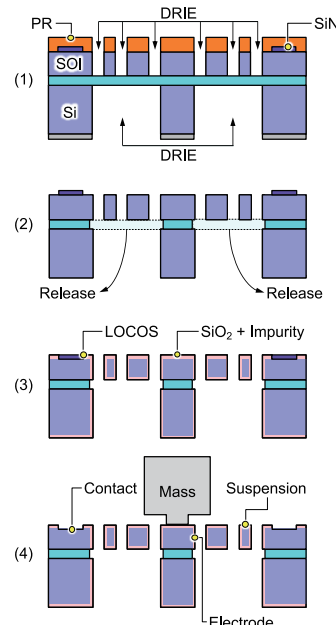
## II. MEMS BY ECCENTRIC PROCESSES

**Figure 1** is a good example that would have never been made if the fabrication had been restricted to either standard semiconductor processes or in-house fabs. This is a MEMS energy harvester that is designed to generate over 1 mW of electrical power from environmental mechanical vibrations in sub-gravity levels at frequencies of approximately 100 Hz [1][2]. The entire structure is made of silicon, and the surface skin of silicon oxide has been turned into an electret film, retaining a permanent electrical charge, which converts mechanical vibrations into electrical current through the mechano-electric coupling based on electrostatic induction.

The process steps are shown in **Fig. 2**; the silicon nitride is formed somewhere off-campus, and both surfaces of a silicon-on-insulator (SOI) wafer are processed using in-house photolithography and deep reactive ion etch (DRIE) to form fine patterns of electrodes and suspensions. Note that the impurity ions ( $K^+$ ) are intentionally included in the silicon oxide during the wet oxidation of step-3. As schematically illustrated in **Fig. 3**, the impurity source is carried



**Fig. 1**  
MEMS vibrational energy harvester



**Fig. 2**  
Silicon micromachining process for  
MEMS vibrational energy harvester

into the furnace by airborne droplets from the water bubbler of KOH. After the oxidation, the MEMS chip is removed from the furnace and charged by an externally applied voltage to form an electret film [3]. Any process handling alkaline metals is prohibited in the standard CMOS processes in order to avoid equipment contamination, so it is performed at the end of the MEMS process using the in-house fabs with a high degree of freedom.

### III. HINTS FOR SUCCESSFUL INDUSTRIAL-ACADEMIA COLLABORATION

The device shown here is just one example of the MEMS devices co-developed with industry over the last 20 years. What we have learned in common through industrial-academia collaboration can be summarized in the following three points:

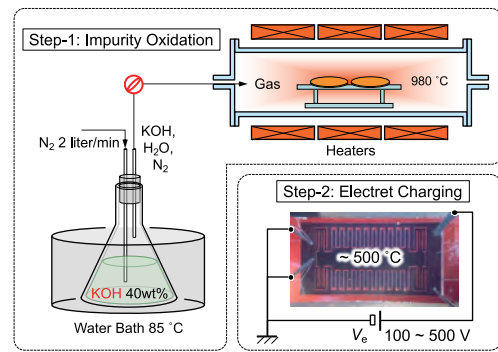
- (1) Industry should proactively set goals: University labs appear very attractive when they come with buzzwords like “MEMS.” They attract industrial researchers who anticipate fruitful results from just touching the new technologies in the lab but they ultimately find it a junk box rather than a treasure box, unless they had a clear vision on what they would make. Universities can help them solve their problems only if they clearly know what to solve.
- (2) Money cannot buy a result: “Outsourcing” used to be the word of justice in Japan but it brought with it a serious problem of not knowing how to build things from scratch. Industry may think that money can buy out the time of university students and researchers working for them. It is true, but they would simply leave the school in a few years, leaving nothing behind for the company. Industry should rather send their researchers to universities to train them for long term R&D. A university is a place of education after all.
- (3) Do not be overly defensive in the lab: Popular labs may accommodate many researchers from different companies, but try not to be overly defensive about intellectual property. Sharing lab utilities is like sharing know-how. Become part of the lab and co-develop what you can share. The real industrial competition begins after you are back in your company.

### IV. TAKE-HOME MESSAGE

Research utilities of the state-of-the-art are too expensive to afford for a single lab, regardless of university or company. Sharing the facilities is a natural consequence, and so is sharing experiences. The research environments supported by the Nanotech platform project is entering a new stage, and they should be designed as a gathering place for new-generation researchers who accumulate, share, and utilize hi-tech experience.

#### References

- [1] H. Honma, Y. Tohyama, H. Mitsuya, G. Hashiguchi, H. Fujita, and H. Toshiyoshi, “Power Enhancement of MEMS Vibrational Electrostatic Energy Harvester by Stray Capacitance Reduction,” *J. Micromech. Microeng.*, vol. 31, no. 12, 2021, p.125008 (11p).
- [2] H. Toshiyoshi, S. Ju, H. Honma, C.-H. Ji, and H. Fujita, “MEMS vibrational energy harvesters,” *Sci. Techno. Adv. Mater.*, vol. 20, no. 1, 2019, pp. 124-143.
- [3] G. Hashiguchi, D. Nakasone, T. Sugiyama, M. Ataka, and H. Toshiyoshi, “Charging mechanism of electret film made of potassium-ion-doped SiO<sub>2</sub>,” *AIP Advances*, vol. 6, no. 3, 2016, p. 035004-8.



**Fig. 3**

Formation of electret by oxidation and charging.



Hiroshi Toshiyoshi received the M.E. and Ph.D. degrees in electrical engineering from The University of Tokyo, Tokyo, Japan, in 1993 and 1996, respectively. He joined the Institute of Industrial Science, The University of Tokyo in 1996 as a Lecturer. From 1999 to 2001, he was a Visiting Assistant Professor at the University of California, Los Angeles, CA, USA. In 2002, he became an Associate Professor at the Institute of Industrial Science (IIS), The University of Tokyo. From 2002 to 2007, he was a Codirector of LIMMS/CNRS-IIS UMI-2820, an international joint laboratory of the Centre National de la Recherche Scientifique, Paris, France. Since 2009, he has been a Professor at the IIS, The University of Tokyo. His research interests include optical MEMS, power MEMS, and CMOS-MEMS.



## **Session 2**

**Material DX Initiatives in Companies**

**企業におけるマテリアルDXの取り組み**



## **“DX infrastructures and its future vision for materials R&D”**

「R&D-DXのためのインフラ基盤とその将来像」

**Ryota Murai (AGC)**

村井 亮太 (AGC株式会社)

## **“R&D DX in Asahi Kasei”**

「旭化成におけるR&D DXの取り組み」

**Teiichiro Kohno (Asahi Kasei)**

河野 禎市郎 (旭化成株式会社)

# DX infrastructures and its future vision for materials R&D

## R&D-DXのためのインフラ基盤とその将来像

<sup>1</sup>R. Murai

<sup>1</sup>AGC Inc.

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### Abstract

AGC devotes to provide new values for our customers and society and obtain competitive advantages by accelerating digital transformation (DX). In the R&D-DX, utilization of data by applying materials informatics (MI) technologies can substantially improve the efficiency to find new materials. This talk introduces features and advantages of the database system, so-called ARDIS and the MI software, AMIBA, which are the in-house IT infrastructures for R&D-DX. In addition, a perspective for the technologies required in the advanced R&D is discussed.

### I. INTRODUCTION

An overview of our R&D-DX activities is shown in Fig.1. The infrastructures are electronic laboratory notebook (ELN), database (DB), and MI software. ELN/DB is used to collect and store usable data, easily, and these data are analyzed by MI software, quickly. We also educate researchers to master these IT tools for creating new values and businesses. For the success in R&D-DX, not only the IT infrastructures, but also the researchers who understand machine-learning technologies and importance of data management are indispensable. To use the tools for our daily research activities, developing highly usable IT tools that match procedures of a variety of experimental works is crucial. Therefore, the in-house IT tools would provide a competitive advantage by updating the functionals to evolve our R&D-DX.

### II. DX INFRASTRUCTURES

The IT tools for our R&D-DX is schematically shown in Fig.2. The DB system, ARDIS, efficiently and centrally stores data of our various business fields, as a web-based ELN. ARDIS can store text, figures, and electric files, in addition to numerical data. The experimental data stored is immediately analyzed by the MI software, AMIBA, with the use of machine-learning algorithms. This tool allows researchers to build machine-learning models and design experimental plans. By incorporating these tools into experimental works, the researchers can spontaneously record and utilize experimental data in a daily basis. A combination of these in-house tools is expected to maximize the value of data for expanding our future business.

### III. FUTURE OF R&D-DX

Recently, many industrial companies are adopting IT infrastructures to accumulate daily data as well as past data for R&D-DX. Developing automated experimental systems is another route to increase data of R&D. AGC now envisions moving from the first stage of R&D-DX to the next stage for creating new business based on the data accumulated by the infrastructures. Reusable and valuable data indeed provide us new business chances and competitive competencies, whereas each company now utilizes own data, solely, which might restrict the opportunity of new business. In the coming years, utilizing interoperable data among collaborative companies and customers will become essential for developing novel materials, products, and market. To do so, a technology for sharing confidential data is required. To prove the concept, we're extending ARDIS to share sensitive data among the companies and affiliates of AGC group. I'd like to discuss how to make a progress in R&D-DX by introducing such new technologies in this talk.



# R&D-DX Activity

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- Development digital tools for DX
- Implement Materials Informatics (MI) , Education of MI for researchers
- Accelerating R&D DX to utilize any data for our business and future

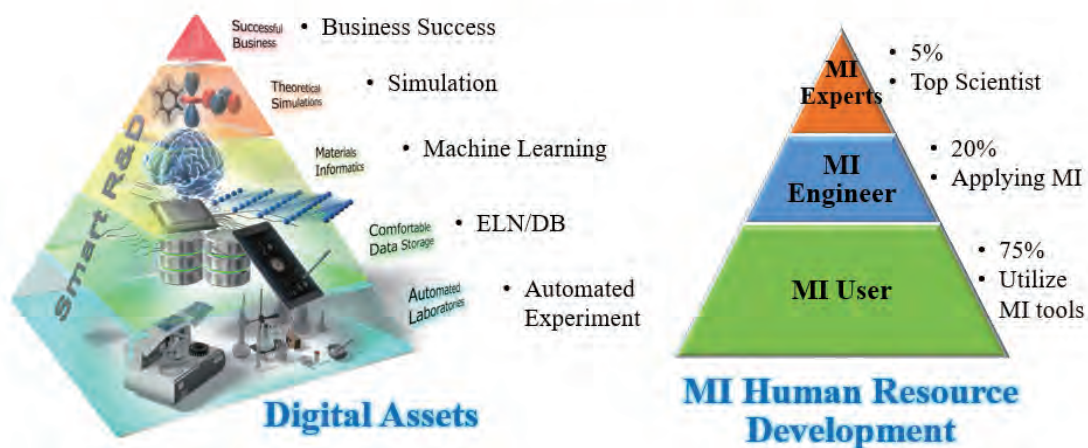


Fig 1. R&D-DX activity summary in AGC

# In-house DX tools

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- Development of in-house DX tools for AGC

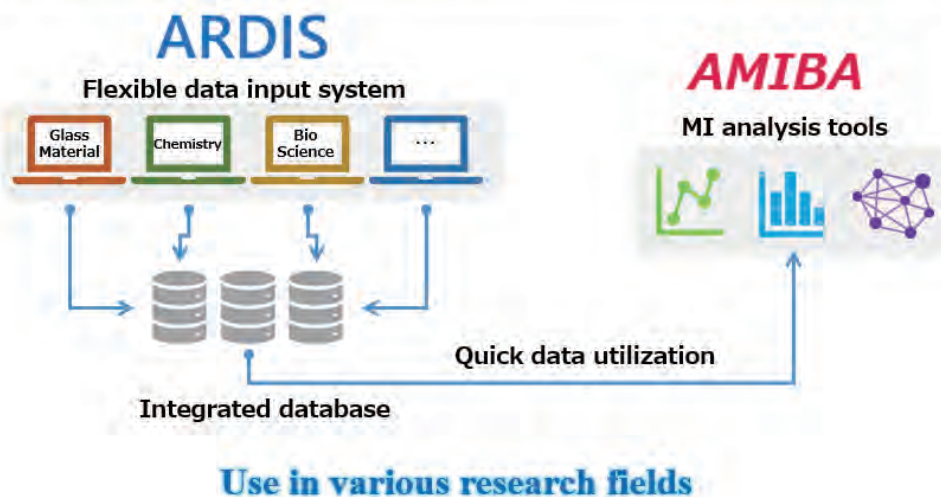


Fig 2. DX infrastructures



Ryota Murai, Manager  
Smart R&D Team, Tech. general division, AGC Inc.

# R&D DX in Asahi Kasei

## 旭化成におけるR&D DXの取り組み

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### Abstract

Since the Materials Genome Initiative was launched in 2011, the materials informatics (MI) has attracted great attention. Many initiatives and national projects have started in Europe, China, Korea [1-6]. Also in Japan, some national projects have started since 2014 and materials and of chemical researcher have been adopted MI in R&D [7-10]. Currently Japan has the international competitiveness in the field of material's R&D, however, the emergence of MI and other disruptive technology such as High Throughput Synthesis (HTS), High Performance Computing (HPC), and quantum computers, could be threat because the speed of R&D increases drastically, which might lead to the quick catch up of the emerging countries.

In order to cope with this possible threat, Asahi Kasei also started campaign to promote MI in various R&D projects in 2017. In early stage, we focused on creating successful model to gain wide recognition through company, then we made effort to extend MI to wide range of materials R&D fields, establishing use cases and implementation procedures that are suitable for corporate material development. On the other hand, we encountered several problems and obstacles in promotion of MI on the course of the campaign.

In this talk, we will explain 1) the typical use cases of MI in Asahi Kasei. Then we will introduce 2) a couples of applications of MI, then describe the problems and obstacles that hinder the enhancement and the spread of MI. In order to deal with these problems and obstacles, we are working on 3) promoting "R&D digital transformation (R&D DX)", which mainly consists of a "Digital Platform (DPF)" that integrates and unifies formats and terminology of data, "Smart Laboratory system" that are generates huge number of data autonomously at high throughput, and "MI human resource development program" that aims to train researcher in material field so that they acquire skills and knowledge of machine learning and related digital technologies. Finally we emphasis the importance of organization culture in order to proliferate and promote MI companywide and activate the activities heading for R&D DX.

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Teiichiro Kono is Senior General Manager of Informatics Initiative, Digital Value Co-creation at Asahi Kasei Corporation. His original background is materials and semiconductors analysis as well as R&D of them. The current mission is digital transformation in R&D, and strengthen the businesses using various informatics including data analysis, optimization, simulation and mathematical model. The e-mail address is [kohno.tb@om.asahi-kasei.co.jp](mailto:kohno.tb@om.asahi-kasei.co.jp)



## **Session 3**

About ARIM Project and Key technology Area

ARIM事業と重要技術領域



## **Overview of the ARIM Business and Initiatives**

ARIM事業の概要と取り組み紹介

### **“Overview of advanced research infrastructure for materials and nanotechnology (ARIM) and aims of the material DX platform”**

「マテリアル先端リサーチインフラの概要と、マテリアルDXプラットフォームが目指すもの」

**Junichi Sone (Japan Science and Technology Agency, Program Director of ARIM MEXT)**

曾根 純一（科学技術振興機構、文部科学省マテリアル先端リサーチインフラPD）



# Overview of advanced research infrastructure for materials and nanotechnology (ARIM) and aims of the materials DX platform

## マテリアル先端リサーチインフラの概要と、マテリアル DX プラットフォームが目指すもの

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### Abstract

The Advanced Research Infrastructure for Materials and nanotechnology (ARIM) which started in FY2021 as a 10-years program of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) succeeds the Nanotechnology Platform Project of the MEXT, which ended in FY2021 with 10 years of activities of sharing state-of-the-art equipment and technical support for users by highly specialized engineers. At the same time, ARIM will take on two important new challenges. One is to collect materials and process data continuously produced by state-of-the-art equipment and provide it to users in a reusable form. The second is to work together with users to promote seven important technological areas that are vital to strengthening Japan's R&D and industrial competitiveness through a hub-and-spoke structure of 25 participating universities and national laboratories that make up ARIM. The following is a brief overview of these two challenges.

ARIM will introduce new remote, automated, and high-throughput advanced equipment, and will collect materials and process data generated by the use of the equipment. The collected data will be structured according to the format defined by ARIM and stored as a database in a cloud computer at the National Institute for Materials Science (NIMS), which plays the role of the center hub in ARIM. We aim to establish an environment in which these structured data can be utilized nationwide, and to start providing data services to the Japanese research community in the middle of FY2023. Furthermore, in collaboration with the "R&D Projects for Materials-Data Creation and Utilization" by MEXT and the "Materials Data Platform Center" by NIMS, the three parties will build a "Materials DX Platform" to collaborate with each other on materials data, thereby contributing to further strengthening Japan's materials innovation capabilities. Figure 1 shows a conceptual diagram of the Materials DX Platform and the roles to be played by the above three parties.

The 25 universities and national laboratories that make up the ARIM will share their roles and support Japan's R&D in seven important technological areas in the materials field by forming hub & spokes structure. The seven hubs consisting of Tohoku University, NIMS, the University of Tokyo, Nagoya University, Kyoto University, and Kyushu University provide advanced facilities with strengths in each important technological area of responsibility. NIMS is responsible for promoting two important technological area, "Quantum and Electronic Functional Materials" and "Technology for Advanced Circulation of Materials". Each spoke with distinctive equipment and technologies is linked to one of those hubs and promotes each important technological area through supporting the corresponding hub. Figure 2 shows the seven important technological areas and the hub-and-spoke structure that is responsible for promoting them.

The foundation of this project, which are the nationwide state-of-the-art shared facilities and the expert engineers providing advanced technical support, have been cultivated through the 10-years of "Nanotechnology Platform Project," which had been implemented since 2012. While fully utilizing these foundations, we will create new perspectives of data collection and utilization and promotion of important technological areas, and take on the challenge of new initiatives for the next 10 years starting in 2021.

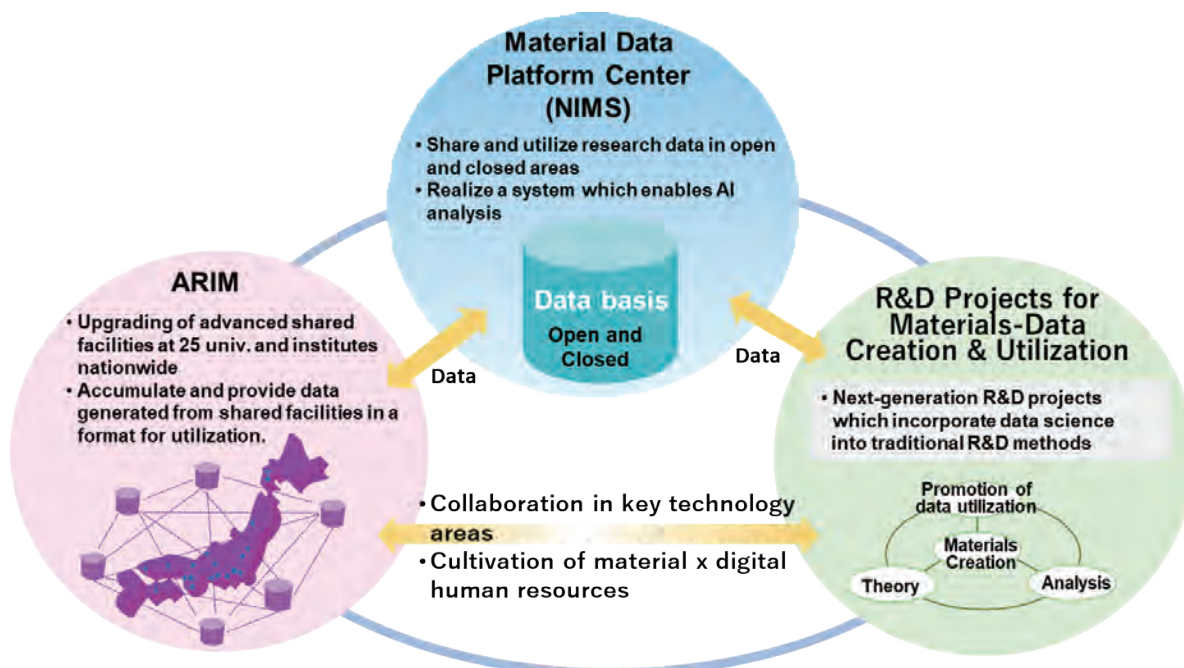


Fig.1 Materials DX Platform Cooperation Concept

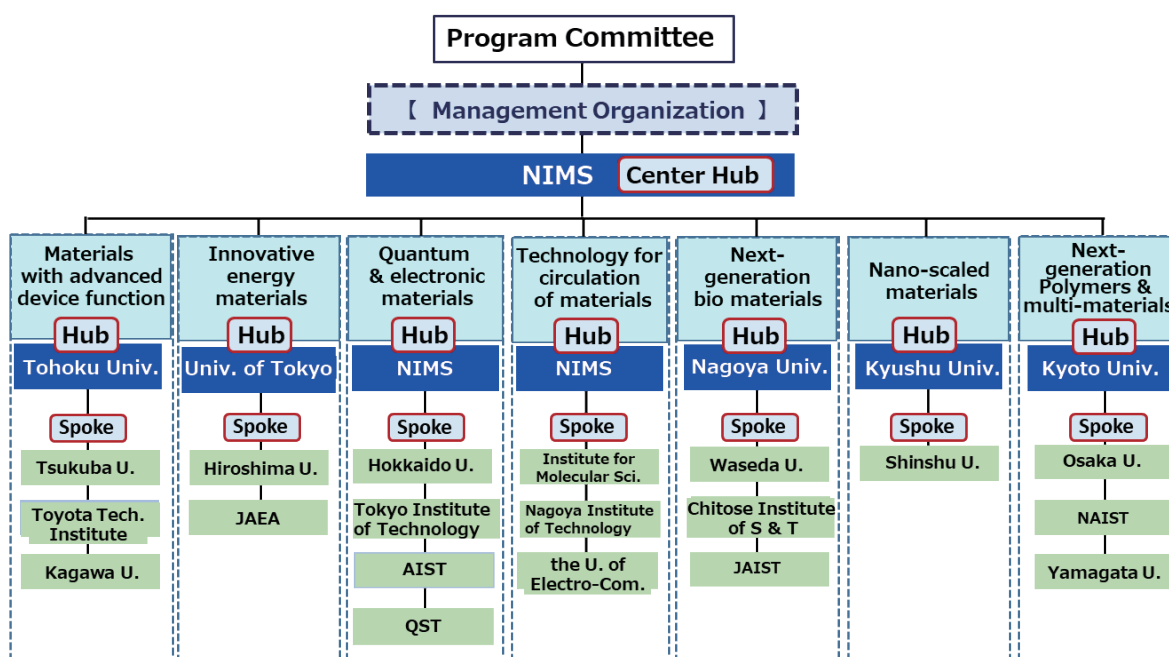


Fig.2 ARIM Hub & Spokes Management Structure

<CV> Jun'ichi Sone

After graduating from the master course of the Science Department of the University of Tokyo in 1975, he joined NEC Corporation as a research staff of the Central Research Laboratories. He got the Doctor degree of science in 1983 from the University of Tokyo. He became a General Manager of NEC Fundamental Research Laboratories and later a Vice President of NEC Central Research Laboratories. In 2008, he obtained concurrent position of Research Supervisor of the JST's CREST program of nanosystems. In 2010, he joined NIMS as Executive Vice President. He served the Society of Nanoscience and Nanotechnology in Japan as President from 2012 to 2016. He joined Center for Research and Development Strategy of JST as Principal Fellow in 2015. He was awarded JSAP Fellow in 2008. He is an Executive Vice President Emeritus of NIMS.





## **Session 3-1**

### **Integration of Data Creation Infrastructure and Data Utilization R&D Projects <Part 1>**

**データ創出基盤とデータ活用研究開発プロジェクトの融合(その1)**



**“Digital transformation in biological and polymeric materials.”**

「バイオ・高分子材料のビッグデータ構築と材料開発への利用」

**Keiji Numata (Kyoto University)**

沼田 圭司（京都大学）

**“Process optimisation through data utilisation**

**in the molding process of polymers and polymeric multi-materials”**

「高分子および高分子マルチマテリアルの成形加工におけるデータ活用とプロセス最適化への取組み」

**Hiroshi Ito (Yamagata University)**

伊藤 浩志（山形大学）

**“High-Throughput 3D Microphysiological Systems**

**-Standardization and Informatics-”**

「ハイスループット3次元マイクロフィジオロジーシステム -標準化と情報化-」

**Shuichi Takayama (Georgia Institute of Technology,USA)**

# Digital transformation in biological and polymeric materials. バイオ・高分子材料のビッグデータ構築と材料開発への利用

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Our Material DX research project ([http://pixy.polym.kyoto-u.ac.jp/ku\\_numata/index.html](http://pixy.polym.kyoto-u.ac.jp/ku_numata/index.html)) aims to solve the issues on material design and synthesis, and hence we will establish a material research and technical platform based on polymer database. We will design and develop bioadaptive materials with biological functions and self-healing ability, including high toughness/environmentally friendly polymers, circular polymers, Quality Of Life (QOL) biomaterials, and carbon dioxide capture materials, which are important application areas. In the polymer science field, the structural property correlation using material informatics (MI), its methodology, and the use of big databases have not progressed significantly these days. Although the development of MI-driven materials is essential in bioadaptive materials research fields, it has not been possible to come up with effective countermeasures due to the lack of human resources and research systems for polymer MI. Under these research circumstances, the MI-driven polymer material science project based on polymer database just started in Kyoto University<sup>1,2</sup> and will become an indispensable research base for materials science in Japan, and can greatly contribute to its international competitiveness.

Structural protein is an eco- and bio-friendly polymer as well as one of the key factors to realize the unique properties and functions of natural tissues and organisms.<sup>3,4</sup> However, use of structural proteins as structural materials in human life is still challenging. Spider silks are among the toughest known materials and thus provide models for renewable, biodegradable and sustainable biopolymers. However, the entirety of their diversity still remains elusive, and silks that exceed the performance limits of industrial fibers are constantly being discovered. We obtained transcriptome assemblies from 1,098 species of spiders to comprehensively catalog silk gene sequences and measured the mechanical, thermal, structural, and hydration properties of the dragline silks of 446 species.<sup>1</sup> The combination of these silk protein genotype-phenotype data revealed essential contributions of multicomponent structures in high-performance dragline silks as well as numerous amino acid motifs contributing to each of the measured properties. We hope that our global sampling, comprehensive testing, integrated analysis and open data will provide a solid starting point for future biomaterial designs.

One of the major drawbacks of protein/polypeptide-based materials is their limited synthesis/process method. My research group is interested in marine purple photosynthetic bacteria as ideal organisms and platforms for production of useful materials to reduce production costs and to contribute sustainable society, because they can utilize sun energy, seawater and carbon dioxide and nitrogen gas in the air for their growth. My research group studies on the photosynthetic bacteria to produce spider silk-like polymers. *Rhodovulum sulfidophilum*, a marine purple non-sulfur photosynthetic bacterium, was genetically engineered for the production of synthetic spider dragline silk protein. The successful construction of photosynthetic microbial host for silk production could reduce the production cost, especially the marine photosynthetic bacteria can fix CO<sub>2</sub> and N<sub>2</sub> with using seawater as a cheap culture medium. To establish the fundamental platforms for photosynthetic bacterial technology, we are currently developing peptide-mediated transformation and protein introduction methods for alga and photosynthetic bacteria.<sup>5-7</sup> These new methodologies will be able to support the high-throughput characterizations for biopolymer productions. My research group also reported the new finding in spider silk spinning, which is



essential to clear the hierarchical structure of spider silk. The scalable and sustainable synthesis method along the clarified structure-function relationship of natural proteins provides a new insight for structural and functional material design of amino acids-based polymers.<sup>8-10</sup>



**Fig. 1** Sustainable biopolymer design and biosynthesis based on spider silk spinning and amino acid sequences.

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Keiji Numata earned his Ph.D. (2007) with a thesis centered on enzymatic degradation and synthesis with hydrolases of biopolymers, especially poly(hydroxyalkanoate), under the supervision of Prof. Yoshiharu Doi, Tokyo Institute of Technology. His Ph.D. thesis includes works on enzymatic polymerization to synthesize branched biopolymers, which has been performed in Royal Institute of Technology (Sweden) under the supervisions of Prof. Ann-Christine Albertsson and Prof. Anna Finne-Wistrand. He worked as a JSPS Postdoctoral Fellow for Research Abroad at Tufts University (USA) where he studied biosynthesis of silk-based polymers via bacterial pathways as well as silk-based gene carriers in the laboratory of Stern Family Professor in Engineering David L. Kaplan. He moved to RIKEN as a Senior Scientist in 2010 to start up a laboratory to investigate biosynthesis and material design of structural proteins and poly(amino acid). He has been a Team Leader (PI) of the lab since 2012 and Research Director for JST-ERATO Numata Organelle Reaction Cluster Project (2016-2023), Research Director for JST-COI-NEXT, Research Director for MEXT Program: Data Creation and Utilization-Type Material Research and Development Project (2022-). In 2020, he moved to Department of Material Chemistry, Kyoto University, as a full professor. He received Nagase Prize from the frontier salon foundation (2022), the 2020 *ACS Macro Letters/Biomacromolecules/Macromolecules* Young Investigator Award (American Chemical Society, 2020), SPSJ Asahi Kasei Award (2019), Award for Encouragement of Research, Japanese Society for Plant Cell and Molecular Biology, Japan (2019), Bio-Environmental Polymer Society Outstanding Young Scientist Award, USA (2018), The Young Scientists' Prize for Minister of MEXT, Japan (2018), and so on. He was appointed as an associate editor of *Polymer Journal* (2018-2020) and is currently an associate editor of *ACS Biomaterials Science and Engineering*.

# Process optimization through data utilization in the molding process of polymers and polymeric multi-materials

## 高分子および高分子マルチマテリアルの成形加工におけるデータ活用とプロセス最適化への取組み

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### Abstract

Thermoplastic polymer materials such as plastics are molded into a variety of components through the processes of melting, flowing, forming, and solidifying. These plastics are molded under non-isothermal and non-isotropic conditions such as rapid cooling, high pressure, and high shear stress. It is therefore important to understand the history of these pressures, temperatures, and shear stresses in the relevant process stages. From the complex process history, the higher-order structures, such as the orientation of molecular chains and crystalline state of plastics and polymer composites developed during these processes, also influence the final physical properties. In order to clarify the correlation between the history of the molding process, the higher-order structure formed and the final physical properties, various measurement techniques have been developed, such as visualization and in-situ observation techniques. Furthermore, attempts to understand complex forming phenomena through numerical analysis are actively being conducted, and numerical analysis techniques are becoming more important in the future.

### I. Polymer flow in polymer processing

Higher-order structures of polymer materials develop in a flow field of polymer processing. Therefore, the understanding polymer flow behaviors such as rheological field is very important. Materials and process informatics in polymer processing require a material database of polymer rheology. Rheology is defined as the science of flow and deformation of materials that usually is used to describe the consistency of different molded parts in terms of viscosity and elasticity. The flow behavior plays a key role in polymer processing technology, mainly in process design, process monitoring and control, quality control, and problem solving in several polymer processing including precise injection molding [1]. Shear viscosity is given as the ratio of shear stress to shear rate, which is strongly dependent on the shear rate. A typical shear viscosity curve of polymer melt has four important regions: (1) 1st Newtonian (zero-shear viscosity) plateau, (2) transition region, (3) shear thinning region, and (4) 2nd Newtonian plateau, when all the molecules have disentangled (see Figure 1). In general, precise injection molding process such as micro/nano-injection molding is usually operated at the high shear rate regions [2]. However, it has not currently been reported on an appropriate model able to calculate the viscosity at ultra-high shear rates. For the viscosity at the nano scale, a precise instrument able to measure the real viscosity of the polymer melt is still not available. One approximation method to model the apparent viscosity considering the surface tension of the polymer melts and its contact angle on the wall of the flow channel as key factors has been proposed recently [3].

### II. Internal structure and morphology of polymers in injection molding

A multilayer so-called skin—core structure is formed inside of the injection molded parts. The skin layer and core layer are formed in the molded parts surface and the central portion in the

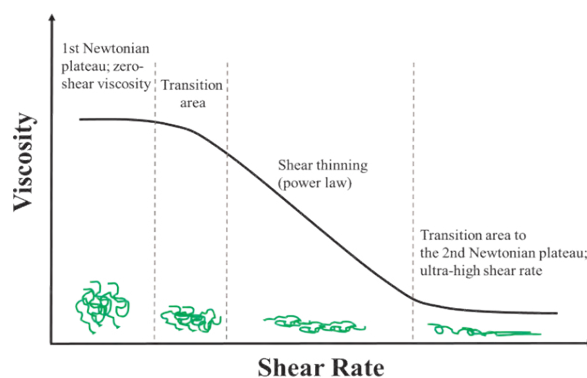


Figure 1 Typical viscosity versus shear rate curve.

thickness direction of the molded parts, respectively. Additionally, the shear layer having molecular orientation caused by the flow of polymer melt is formed between the skin layer and the core layer. The crystallization of a semi-crystalline polymer is induced by this molecular orientation. The crystallinity of a semi-crystalline polymer is affected by the degree of molecular orientation and the size of the spherulite. This molecular orientation and crystallization vary according to polymer materials, molding conditions, cavity thickness, etc. In micro/nano-injection molding, the surface features and the thickness of the molded parts are in the micro/nano scale; the ratio of skin-core layers the ratio of layer received the shear becomes higher than in conventional injection molding because a polymer melt is injected in a cavity by high injection speed and pressure.

### III. Computer Aided Engineering (CAE) for micro injection molding process

In micro injection molding process, both the injection step and cooling step of polymer materials progressed simultaneously because molten polymer is injected at high temperatures into a mold cavity at a low temperature. Therefore, surface layer solidification is expected to occur at the boundary area between mold wall surface and polymer (Figure 2). Formation of a solidified surface layer influences the injection ability of molten polymer, the shape accuracy, and features of the molded product. Therefore, it is difficult to transcribe micro/nanostructures perfectly at the mold surface. For thickness of the solidified surface layer that is sufficiently high against the gap of the mold cavity, a large pressure drop in the filling step occurs. For molecular orientation causes mechanical and optical anisotropy, it often disrupts reduction of the product quality of precision molded parts. For this reason, controlling the solidified surface layer growth becomes extremely important to improve the molded product quality. The other fatal issue is the air trap within the mold cavity. Simulation data that agree with the experimentally obtained results demonstrate the possibility of air trap generation during the filling step in the micro injection molding process (Figure 2) [4]. Results demonstrated that the air traps occurring during the filling step are strongly related to the replicated shape and replication rate.

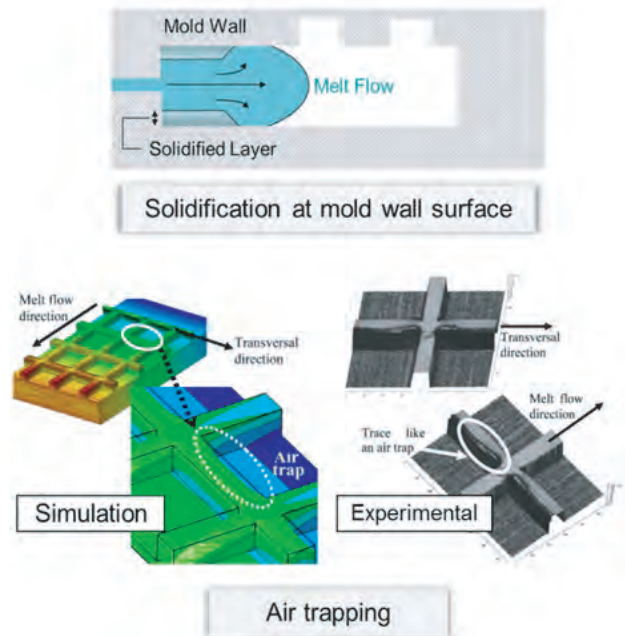


Figure 2 Surface solidification at mold wall (upper) and air trap difficulties (lower) in micro/nano-injection molding process.

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Dr. Ito's major research field is to clarify and control the development of higher-order structure in polymeric materials through experimental and theoretical studies on the polymer processing. His research projects cover several types of polymer processing and engineering properties of plastics. Research achievements have Patents and Awards, have published over 198 papers in International Academic Journal, 33 Book Chapters and have over 50 Invited lectures.

#### PROFESSIONAL EXPERIENCE

2018 – Present; Director Special Assistant, Yamagata University (YU)  
 2016 – Present; Dean, Graduate School of Organic Materials Science, YU  
 2015 – Present; Vice-Dean, Faculty of Engineering, YU  
 2015 – Present; Director of Research Center for GREEN Materials and Advanced Processing, YU  
 2010 – Present; Professor, Yamagata University (YU)



# High-Throughput 3D Microphysiological Systems -Standardization and Informatics-

ハイスループット3次元マイクロフィジオロジーシステム -標準化と情報化-

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## Abstract

This presentation will describe development of high-throughput (96 and 384 well format) 3D microscale models of the lung, kidney, and some cancers. The presentation will describe some of the underlying engineering technologies and materials science of the platforms along with accompanying biomedical applications of the technologies. Additionally, this presentation will discuss some of the standardization challenges for these systems along with some materials science and informatics solutions to these challenges.

## I. INTRODUCTION

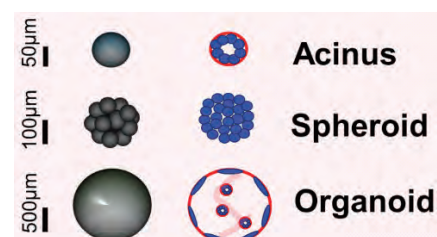
This presentation will describe the use of 384 hanging drop and ultra-low attachment plate 3D cell cultures. By changing the amount and method of extracellular matrix molecule manipulation, the type of culture obtained is very different ranging from space-filled spheroids to hollow epithelial organoids. Efforts for standardization and applications to disease modeling will be described.

## II. SPHEROIDS

The presentation will start with description of scaffold-free formation of spheroids in 384 hanging drop plates.<sup>1</sup> The platform is used to form space-filled balls of cancer cells in a one-drop, one-spheroid format. Due to oxygen and nutrient transport into the spheroid core, a hypoxic and necrotic core can form mimicking physiological cancer tissue.<sup>2-3</sup> These features of 3D spheroid cultures are not observed in 2D cultures and critically impacts how anti-cancer drugs affect cancer cells. Given the broad utility and accessibility of spheroid cultures, it is important to standardize spheroid cultures. A data bank for reporting of minimal information for reproducible spheroid experimentation called MISpheroid has been established and use of it by the community invited.<sup>4</sup>

## III. ORGANOIDS

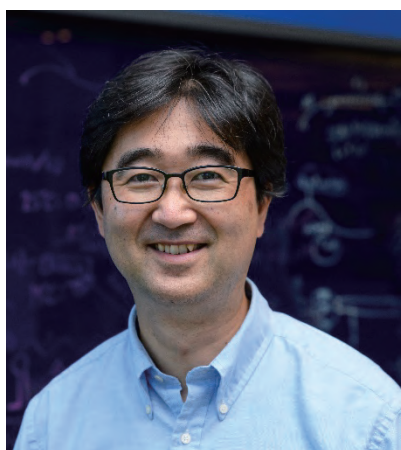
Another type of useful 3D cell culture is the formation of organoids, particularly epithelial cell-based organoids that mimic normal tissue. Most commonly, epithelial organoids are formed in scaffold-rich environments such as Matrigel domes. The organoids formed in such environments, however, can be varied in size, shape, and number of organoids formed per well. Furthermore, biological assays that require access to the apical surface of organoids are hindered by the apical side of the epithelium being hidden in the organoid interior.<sup>5</sup> Here, this presentation will describe formation of geometrically-inverted epithelial organoids in a one-well, one-organoid format with consistent organoid shape and size.<sup>6-8</sup> While these geometrically-inverted 3D cell culture platforms are still in early development, they provide unique features that complement existing organoid cultures.



**Fig. 1** Types of 3D cell cultures that can be formed from the same cells depending on materials manipulation.<sup>6</sup>

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B.S.& M.S., 1986-1994, Agricultural Chemistry, University of Tokyo  
Ph.D., 1994-1998, Scripps Research Institute, Chemistry  
Postdoc 1998-2000 Harvard University, Chemistry and Chemical Biology  
Prof. Shuichi Takayama's research interests started with bioorganic synthesis at the University of Tokyo and Scripps Research Institute. Subsequently he pursued postdoctoral studies in bioengineered microsystems at Harvard University as a Leukemia and Lymphoma Society Fellow. He spent 17 years at the University of Michigan in the Biomedical Engineering Department and Macromolecular Science and Engineering Program, then moved to the Wallace H. Coulter Department of Biomedical Engineering at the Georgia Institute of Technology and Emory School of Medicine in the summer of 2017. He is an associate editor of Integrative Biology and recipient of the Pioneers of Miniaturization Prize. He is also the Director of the Nakatani RIES Program which promotes international undergraduate student internships between the US and Japan.



## **Session 3-2**

### **Integration of Data Creation Infrastructure and Data Utilization R&D Projects <Part 2>**

**データ創出基盤とデータ活用研究開発プロジェクトの融合(その2)**





**“Development of Electrochemical Materials  
for the Maximum Dissemination of Renewable Energy”**

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**Junichiro Shiomi (University of Tokyo)**

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**“Battery development based on  
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「多階層計算科学・機械学習を活用した蓄電池開発」

**Atsuo Yamada (University of Tokyo)**

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# Development of Electrochemical Materials for the Maximum Dissemination of Renewable Energy 再生可能エネルギー最大導入を実現する電気化学材料開発

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## Abstract

To achieve net-zero emission of CO<sub>2</sub> by 2050, it is indispensable to introduce variable renewable energy sources (VREs) such as solar and wind power generation by almost 10 times larger capacity than the value that has been introduced so far in Japan. Balancing the demand and the supply of electricity is therefore a crucial technological bottleneck for the realization of net zero. Furthermore, the energy demand that cannot be electrified, including gas-firing power generation that provides adjustability in power generation, should use hydrogen as a fuel that does not emit CO<sub>2</sub> from production to usage.

Batteries for power storage and water electrolyzers for hydrogen production from decarbonized electricity are two essential technologies for the realization of net-zero (Fig. 1). The capacities required for these devices are tremendous and innovations are demanded so that they can be supplied massively without elemental constraint and at drastically low cost. For batteries, stationary use with a capacity over 1000 GWh is expected to use a vital role in providing adjustability for the power grid with ca. 70% share of VREs in the total electricity supply. Drastic improvement in cycle lifetime and reliability is highly expected rather than the pursuit of energy density. For water electrolyzers, novel combinations of electrode catalysts and electrolytes (i.e., ions added into water) are vital that are composed of abundant elements and can realize a long lifetime under mild pH conditions in contrast to the existing alkaline electrolysis. Alternatively, novel combinations of an ion-exchange membrane and catalysts are expected to mitigate the shortage of iridium for polymer electrolyte membrane (PEM) electrolyzers.

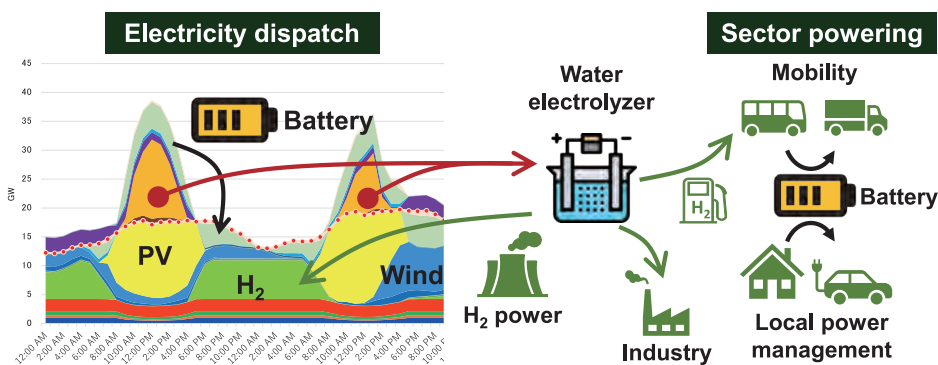
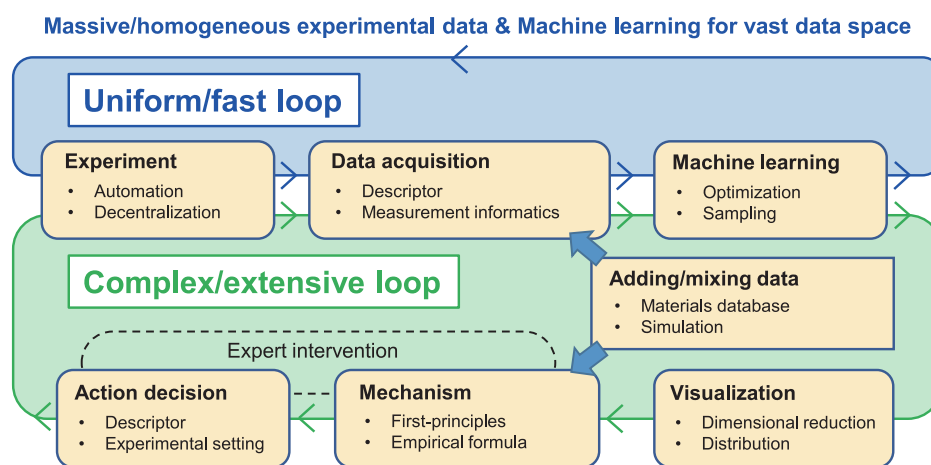


Fig. 1 The role of batteries and water electrolyzers in a decarbonized energy system

The project DX-GEM (Digital Transformation Initiative for Green Energy Material) started in 2022 to develop innovative materials for these electrochemical devices, batteries and water electrolyzers, through the best combination of experiment, theoretical calculation, and advanced characterization on the basis of data science. The function of electrochemical devices originates from the interface between an electrode and an electrolyte. The interface has a complex atomistic structure, which may change during electrochemical reactions.

The project aims at the establishment of novel approaches for the material development in such complex and dynamic electrochemical systems with the effective and efficient use of data science. Depending on the ease of gathering a vast number of experimental data that enables us to search

for new materials, two kinds of loops are proposed. When automated parallel experiments are possible, a quick loop is applied which is composed of high-throughput experiments and machine learning to suggest the next conditions for experiments. The approach fits the development of electrolytes to seek the best mixture of components. The development of electrode material, however, is inevitably time-consuming and elaborate choice of experimental conditions is important so that experimental data hits the essential points in the vast parameter space of materials. In such a complex and extensive loop of material development, theoretical calculations can provide supplemental data. It is also very important for data science to empower the imagination of researchers by “visualizing” the correlation among plural parameters including operating variables (material composition, fabrication condition, etc.), basic properties (material structure, charge distribution, etc.), and material performance. A combined approach using theoretical calculation, advanced characterization, and data science to make the results intuitively understandable to researchers is an indispensable step in this loop.



**Masakazu Sugiyama** is the director and a professor at Research Center for Advanced Science and Technology (RCAST), The University of Tokyo. He received the B.E., M.S., and Ph.D. degrees in Chemical Systems Engineering, all from the University of Tokyo, Japan, in 1995, 1997, and 2000, respectively. In 2000, he became a Research Associate at the Department of Chemical System Engineering, the University of Tokyo. In 2002, he joined the Department of Electronic Engineering as a Lecturer. He became an Associate Professor in 2005. In 2016, he was promoted to a full professor and then moved to RCAST in 2017.

# Exploring materials in a huge parameter space through data creation and utilization: Examples of thermal functional materials

## データ創出・活用による巨大パラメータ空間での材料探索： 熱機能材料を例に

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Materials informatics (MI), which efficiently develops materials by creating and utilizing materials data with informatics methods, has widely spread in order to accelerate the development of materials. Many of the approaches have been inherited from bioinformatics, but the recent rapid growth of MI is attributed to the quantitative and qualitative improvement of materials databases, which was made possible by the development in standardized first-principles computations and automated experiments. The database provides an environment in which researchers can utilize computational and experimental data, for instance, to quickly determine phase diagrams, predict material properties, and efficiently control material processes by using the data and applying machine learning.

The Laboratory of Thermal Energy Engineering at the University of Tokyo, together with the collaborators, has been studying the application of MI to heat transfer materials for the last decade. Our series of research started with the JST project (2015-2020) *Materials Integration Initiative (Mi<sup>2</sup>i)*, which was a human resource hub project to promote MI research in the three outlets of battery materials, magnetic materials, and heat-transfer materials. The heat transfer materials had unexpectedly good affinity with MI. It led us to find or design materials with high/low thermal conductivity, thermoelectric conversion with high performance, and wavelength-selective thermal radiation, in response to social needs such as thermal management of electronic devices and optical sensors, power sources for IoT sensors and communication devices, and energy saving by thermal radiation cooling, etc [1-6].

While many of the above works were driven by computed data, the next non-trivial challenge has been to create and utilize large scale experimental data. The difficulties are to assure uniformity of the data to reduce noise and to include process data for descriptors. This is one of the targets of the MEXT project *Advanced Research Infrastructure for Materials and Nanotechnology (ARIM)* and the developed infrastructure will be used in the research project *Data Creation Infrastructure and Data Utilization R&D Projects (DxMT)*. We intend to contribute to these projects in two aspects. (1) Since the material search space, consisting of parameters axes concerning structures, properties, states, processes, etc, is expected to be extremely large and sometimes continuous, we develop an MI methodology that performs modelling and search in massive continuum parameter space. (2) Since, in many cases, the experiment-based-MI will still lack in uniformity and filling rate of data, high-quality human input will be essential, and for that, we develop an MI methodology that mutually adopts predictability and understandability. In the talk, I will discuss these aspects with thermal functional materials as examples.

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Junichiro Shiomi is Professor in Institute of Engineering Innovation, School of Engineering, the University of Tokyo. He received B.E. (1999) from Tohoku University, and Ph. D. (2004) from Royal Institute of Technology (KTH), Sweden. Leading the Thermal Energy Engineering Lab, he has been pursuing research to advance thermal management, waste heat recovery, and energy harvesting technologies based on nano-to-macro innovation in materials, structures, and systems.

Prof. Shiomi has been leading several projects including Grant-in-Aid for Scientific Research (S) (JSPS), Core Research for Evolutional Science and Technology (JST-CREST), Precursory Research for Embryonic Science and Technology (JST-PRESTO), and New Energy and Industrial Technology Development Organization (NEDO) projects. He is Fellow of Japan Society of Mechanical Engineers and Member of Science Council of Japan. He serves as an editor of *Nanoscale and Microscale Thermophysical Engineering*.

He is a recipient of the Zeldovich Medal from the Committee on Space Research, the Young Scientists' Prize, the Commendation for Science and Technology by the Minister of Educational, Culture, Sports, Science and Technology, the Academic award of Heat Transfer Society of Japan, the Academic Award of Thermoelectric Society of Japan, the JSPS Award, and the Nukiyama Memorial Award.

# BATTERY DEVELOPMENT BASED ON MULTI-STAGE COMPUTATIONAL AND MACHINE-LEARNING PROTOCOLS

## 多階層計算科学・機械学習を活用した蓄電池開発

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Battery is a complicated materials system composed of several chemical/electrochemical reaction steps, that can not be represented by a simple “cause-result” type problems. Also, each component and reaction step are to be described with essential scientific terms which are strongly correlated with each other with several issues occurring in multiple time- and special- scales. This led me to propose a concept, “multi-stage computational and machine learning protocols” with suitable/timely contribution of human brains, of which schemes are drawn in Figure 1.

Big data, that can be obtained both experimentally and computationally, may be categorized into a suitable stage or layer as a part of “scientific” body of knowledge for whole battery system, then followed by a machine learning analysis for the several cause-result issues between each stage. The accumulation of the essential relationships will form “understandable”, “flexible”, and “resilient” artificial intelligence (AI) that include rationally hieratical parameters to which a human can access easily.

As a successful example, a long-term mystery in electrochemistry, “origin of huge electrode-potential shift depending on electrolyte”, was addressed. We applied machine learning regression analysis to lithium battery electrolytes by gathering several explanatory variables such as composition, solution structures, interatomic distances, electronic structures, and molecular properties, obtained by molecular dynamics (MD) simulation and DFT calculation [1]. Obviously, neutral solvent related structure, inherent properties such as LUMO HOMO levels, obtained by DFT, are not so important. On the other hand, structural factors obtained by MD simulation, particularly for lithium-anion and lithium-lithium (inter-ionic) distances are higher-ranked and very influential to the electrode potential. The hierarchical analysis has stimulated my brain and led to propose the new scientific concept of “liquid Madelung potential” that can quantitatively explain the potential shift and identify several promising electrolytes [2]. The concept of liquid Madelung potential has been extended to optimize several new promising battery systems, realizing hitherto unrealized high-performance with outstanding stability [3].

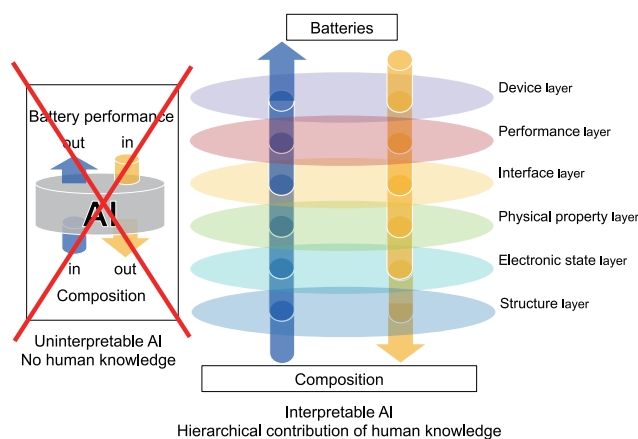


Fig. 1 Schematic derivation of the concept, “multi-stage computational and machine learning protocols”

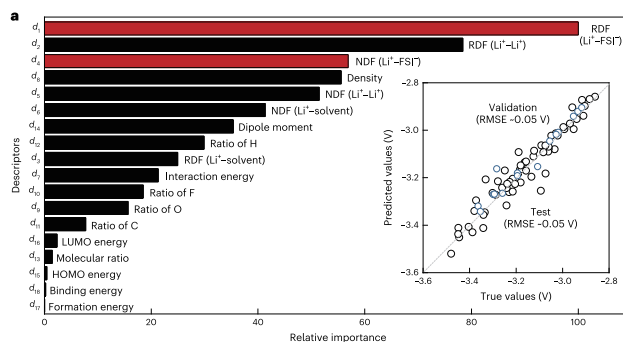


Fig. 2 Machine-learning regression for lithium electrode potential with electrolyte descriptors obtained by MD or DFT calculations.

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Atsuo Yamada has unique career covering both academic and industrial research. After serving as a laboratory head of Sony Research Center, he was immediately appointed as an associate professor at Tokyo Institute of Technology in 2002, a full professor of the University of Tokyo in 2009. During the period, he joined the John. B. Goodenough's lab. in University of Texas at Austin as a visiting scholar for one year, and was called for sabbatical stay from University of Bordeaux as an invited professor to enhance research communication with Dr. Claude Delmas in ICMCB/CNRS.

His diverse research works on battery materials, particularly recognized for sophisticated approaches for structure-property relationships, include very early-stage exploration/optimization of LFP and more recently, identification and understanding of several functional electrolytes. He holds 90 patents, published 25 chapters and well over 260 refereed journal papers with total citation exceeding 28,000, delivering 125 plenary/keynote/invited presentations, and ranked as a Highly Cited Researcher by Clarivate Analytics.

Over the last decade, Atsuo has led the important Japanese national research programs called "Elements Strategy Initiative for Catalysts and Batteries", "Specially Promoted Research", "Core Research for Evolutional Science and Technology", as well as "Data Creation and Utilization Type Materials Research and Development Project", and now serving for the scientific advisory board of Advanced Energy Materials.

Among his many honors, Atsuo has been awarded the Spriggs Award and the Purdy Award from American Ceramic Society (2010, 2016), the Scientific Achievement Award from ECS Japan (2016), IBA Research Award from International Battery Association (2016), and ECS Battery Division Research Award from the Electrochemical Society (2022).

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