文部科学省ナノテクノロジープラットフォーム

第20回ナノテクノロジー総合シンポジウム

JAPAN NANO 2022

"From a Nanotechnology Platform to a Materials DX Platform
~Aims of Advanced Research Infrastructure for Materials and Nanotechnology~"

Proceedings

Nanotechnology

Date: **January 28th (Fri.), 2022**

Venue: **Tokyo Big Sight, Conference Tower(Tokyo)**
※Online

Sponsored by

Nanotechnology Platform by the Ministry of Education, Culture, Sports, Science and Technology(MEXT)
Center for Nanotechnology Platform, National Institute for Materials Science (NIMS)

The Institutions, participating in the Nanotechnology Platform:

Hokkaido University, Chitose Institute of Science and Technology,
Tohoku University, University of Tsukuba,
National Institute for Materials Science,
National Institute of Advanced Industrial Science and Technology,
The University of Tokyo, Tokyo Institute of Technology,
Waseda University, Shinshu University,
National Institutes of Natural Sciences Institute for Molecular Science,
Nagoya University, Nagoya Institute of Technology,
Toyota Technological Institute, Kyoto University,
Japan Advanced Institute of Science and Technology,
Nara Institute of Science and Technology, Osaka University,
Japan Atomic Energy Agency,
National Institutes for Quantum and Radiological Science and Technology,
Hiroshima University, Yamaguchi University,
Kagawa University, Kyushu University,
Kitakyushu Foundation for the Advancement of Industry Science and Technology

NanotechJapan
Nanotechnology Platform

文部科学省ナノテクノロジープラットフォーム

第20回ナノテクノロジー総合シンポジウム

JAPAN NANO 2022

「ナノテクノロジープラットフォームからマテリアルDXプラットフォームへ
～マテリアル先端リサーチインフラの目指すもの～」

講演予稿集

Nanotechnology

開催日：2022年1月28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7階 国際会議場（東京都江東区有明）

主　催：文部科学省ナノテクノロジープラットフォーム
国立研究開発法人物質・材料研究機構ナノテクノロジープラットフォームセンター

文部科学省ナノテクノロジープラットフォーム参画機関：
北海道大学、公立千歳科学技術大学、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、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、山口大学、香川大学、九州大学、北九州産業学術推進機構

NanotechJapan
Nanotechnology Platform

January 28th (Fri.), 2022, International Conference Hall
2022年1月28日（金）　会議棟7階 国際会議場

10:00-10:10【Opening Remarks/ 開会挨拶】

10:00-10:05	**Kazuhito Hashimoto** (President, National Institute for Materials Science, Japan) 橋本 和仁（物質・材料研究機構理事長）
10:05-10:10	**Ministry of Education, Culture, Sports, Science and Technology** 文部科学省

10:10-12:00【Session 1】

10-year Achievements of Nanotechnology Platform Japan/ナノテクノロジープラットフォーム事業10年間の成果

10:10-10:35	**Yasuo Koide** (National Institute for Materials Science) 小出 康夫（物質・材料研究機構） “Center of Nanotechnology Platform” 「ナノテクノロジープラットフォームセンター 10 年間の成果」
10:35-11:00	**Daisuke Fujita** (National Institute for Materials Science) 藤田 大介（物質・材料研究機構） “Advanced Characterization Nanotechnology Platform” 「微細構造解析プラットフォーム 10 年間の成果」

11:00 - 11:10　Break / 休憩

11:10-11:35	**Hiroyuki Akinaga** (Kyoto University) 秋永 広幸（京都大学） “Nanofabrication Platform” 「微細加工プラットフォーム 10 年間の成果」
11:35-12:00	**Toshihiko Yokoyama** (National Institutes of Natural Sciences Institute for Molecular Science) 横山 利彦（自然科学研究機構 分子科学研究所） “Molecule & Material Synthesis Platform” 「分子・物質合成プラットフォーム 10 年間の成果」

12:00 - 13:10　Lunch / 昼食

13:10-15:30【Session 2】

Material Data Strategy to Strengthen Material Innovation Force/ マテリアル革新力強化に向けたマテリアルデータ戦略

13:10-13:45【Plenary Lecture / 基調講演】

Teruo Kishi (Innovative Structural Materials Association)
岸 輝雄（新構造材料技術研究組合理事長、東京大学名誉教授）
“Expectations for the Material DX Platform to Strengthen Materials Innovations”
「マテリアル革新力強化に向けたマテリアル DX プラットフォームへの期待」

13:45-14:20【Special Lecture/ 特別講演】

Taro Hitosugi (Tokyo Institute of Technology)
一杉 太郎（東京工業大学）
"Research Transformation Driven by Open Facility Platform"
「マテリアル先端リサーチインフラが牽引するリサーチトランスフォーメーション
～実験装置に加え、データ・知識の共有へ～」

14:20 - 14:30　Break / 休憩

14:30-15:30【Overseas Invited Lectures / 海外招待講演】

14:30-15:00　**Martin L. Green** (National Institute of Standards and Technology, USA)
"Autonomous (AI-Driven) Experimental Materials Science"
「AI 駆動自立型実験による材料科学」

15:00-15:30　**Claudia Draxl** (Humboldt University, Germany)
"FAIRmat's Approach toward Enabling Data-Centric Science"
「データセントリック科学構築に向けた FAIRmat の取り組み」

15:30 - 15:50　Coffee Break / コーヒーブレイク

15:50-17:05【Session 3】

Importance of Data Utilization in Material Strategy/ マテリアル戦略におけるデータ利活用の重要性

15:50-16:15　**Toyotaro Suzumura** (The University of Tokyo)
鈴村 豊太郎（東京大学）
"Accelerating Interdisciplinary Research between Material Science and Computer Science on the *mdx* Data Science Platform"
「データ活用社会創成プラットフォーム mdx における材料科学と情報科学の学際研究の促進に向けて」

16:15-16:40　**Masahiko Demura** (National Institute for Materials Science)
出村 雅彦（物質・材料研究機構）
"Materials Research in the Data Era: A NIMS Challenge"
「データ時代の材料研究：NIMS の取り組み」

16:40-17:05　**Shingo Ichimura** (Waseda University)
一村 信吾（早稲田大学）
"Standardization of Output Data Format for Measurement and Analysis Instruments: Current Situation and Future Plan"
「計測分析装置の出力データフォーマット標準化：現状と展望」

17:05-17:10【Closing Remarks / 閉会挨拶】

Yasuo Koide (Chairperson of the Organizing Committee of JAPAN NANO 2022 / Director, Center for Nanotechnology Platform, National Institute for Materials Science, Japan)
小出 康夫（JAPAN NANO 2022 組織委員長、物質・材料研究機構ナノテクノロジープラットフォームセンター長）

Contents / 目次

Overseas Invited Lectures / 海外招待講演

Session 3 : Importance of Data Utilization in Material Strategy / マテリアル戦略におけるデータ利活用の重要性

Session 1
【10-year Achievements of Nanotechnology Platform Japan / ナノテクノロジープラットフォーム事業10年間の成果】

“Center of Nanotechnology Platform”

「ナノテクノロジープラットフォームセンター 10年間の成果」

Yasuo Koide (National Institute for Materials Science)
小出 康夫（物質・材料研究機構）

“Advanced Characterization Nanotechnology Platform”

「微細構造解析プラットフォーム 10年間の成果」

Daisuke Fujita (National Institute for Materials Science)
藤田 大介（物質・材料研究機構）

“Nanofabrication Platform”

「微細加工プラットフォーム 10年間の成果」

Hiroyuki Akinaga (Kyoto University)
秋永 広幸（京都大学）

“Molecule & Material Synthesis Platform”

「分子・物質合成プラットフォーム 10年間の成果」

Toshihiko Yokoyama (National Institutes of Natural Sciences Institute for Molecular Science)
横山 利彦（自然科学研究機構 分子科学研究所）

Center of Nanotechnology Platform
ナノテクノロジープラットフォームセンター 10年間の成果

Yasuo Koide

Center for Nanotechnology Platform, National Institute for Materials Science,
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Abstract

The Nanotechnology Platform Japan (NPJ) is a 10-year project of the Ministry of Education, Culture, Sports, Science and Technology (MEXT), which was launched in 2012 as a shared research infrastructure consisting of a network of universities and national and public research institutes in Japan, and is an evolutionary successor to the Nanotechnology Network projects launched in 2002. The purpose of this project is to promote joint use by users in industry, academia, and government by establishing a nationwide research platform through close collaboration among research institutions with cutting-edge research facilities and know-how in nanotechnology.

The NPJ is constructed by alliance of 25 institutes which make up one platform for promoting collaboration among industry, government, and academia, interdisciplinary research in nanotechnology, mobilization of human resources, and collaboration between three technological areas including nano-characterization and analysis, nanofabrication, and molecular synthesis and analysis. Figure 1 shows a NPJ organization of 25 institutes from 2012 to 2021. The 25 institutes are placed nationwide from Hokkaido to Kyushu Island in Japan.

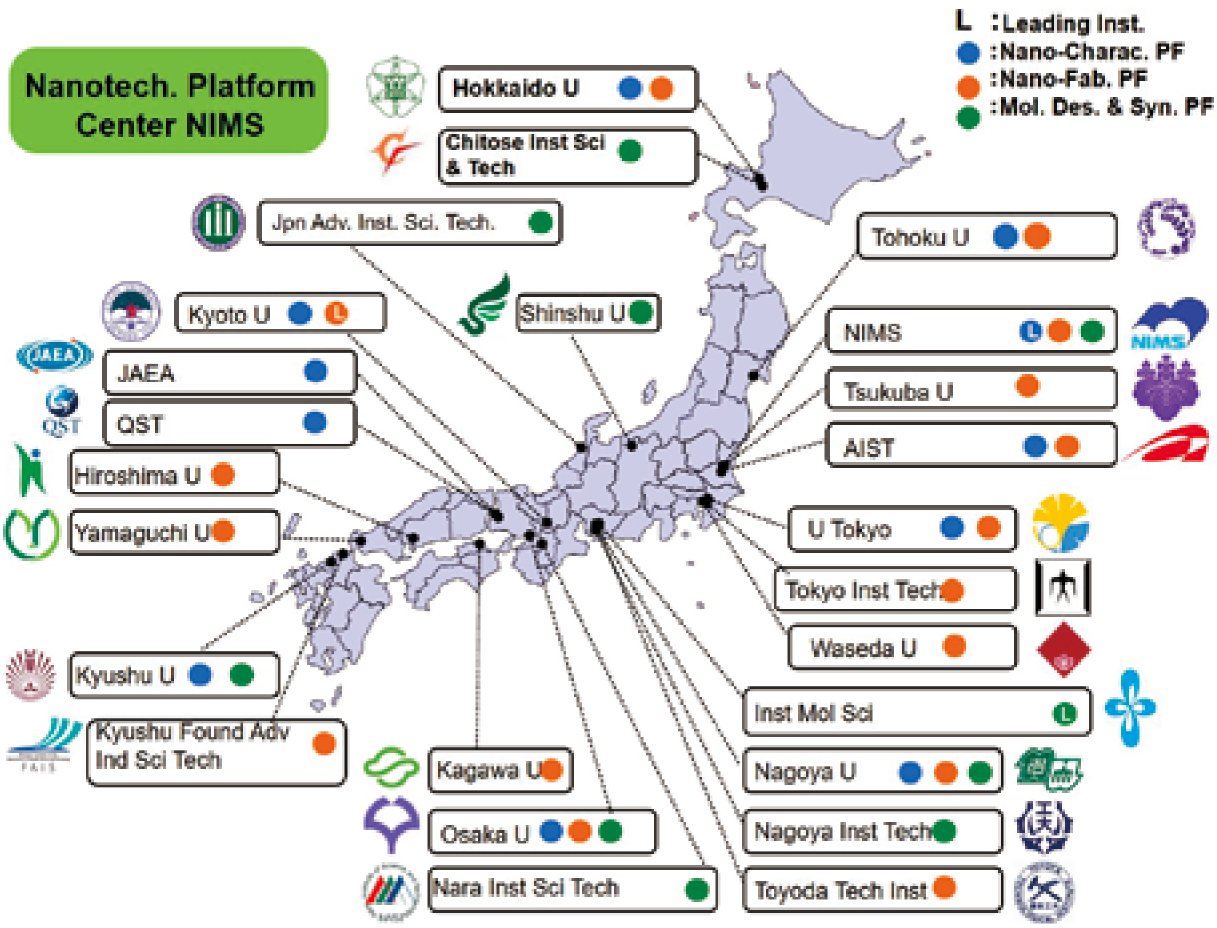

Fig. 1 NPJ organization from 2012 to 2021.

The aim is to maximize the efficiency of investment in research and development by industry, academia, and government related to nanotechnology, materials, and devices. It provides the shortest possible approach to solving problems that users are struggling with, and promotes industry-academia-government colla-boration, interdisciplinary fusion, and human resource development. For this purpose, a platform for sharing advanced facilities (hereinafter referred to as PF) covering three technological areas, namely, advanced characterization nanotechnology, nanofabrication, and molecule & material synthesis, has been established in order to make it widely available to users throughout Japan, based on the principle of democratic access. As shown in Figure 1, a total of 25 institutes and 37 centers are participating in the PF, including 11 institutes in the advanced characterization nanotechnology PF, 16 institutes in the nanofabrication PF, 11 institutes in the molecule & material synthesis PF, and one center.

The NPJ center is responsible for overall coordination and promotion of the program, external collaboration among sectors and developing new users, information service for users, and organizing workshop and symposium and exchange programs for education and training purposes of researchers, technical staffs, and students. Figure 2 indicates the relationship between NPJ center and three technology PFs.

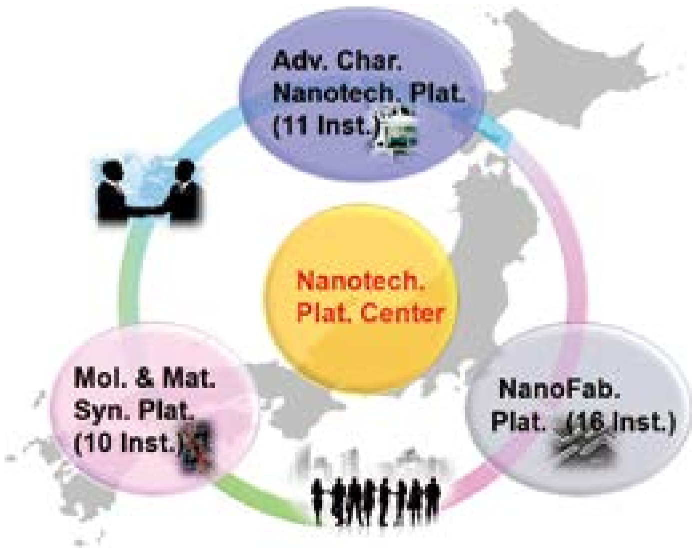

Fig.2 Relationship between NPJ center and three technology PFs

The total number of shared equipment is about 1,100, and the annual number of applications and users is about 3,000 and 20,000, respectively, with 870 professional staff supporting the project. The distribution of users is as follows: industry 30%, universities 60%, public institutions 7%, and others 3%, and we have been supporting the development of not only academia but also private companies. The impact factor of the papers published by the users has been calculated from the analysis of famous journals, and it is equivalent to that of famous universities in Japan, indicating that we are promoting high-level academic research support. Every year, we award the Grand Prize and Excellence Prize for outstanding research results, and we are promoting development support for academia and start-up companies while creating outstanding research results. The next phase of the shared use project, which will evolve into a nanotechnology data platform for sharing data from advanced equipment, will start in 2021, and is expected to develop further.

<CV>

Yasuo Koide, Dr.

Received Dr. degree from Nagoya University in 1988, Assistant Professor at the Graduate School of Engineering, Nagoya University in 1987, Associate Professor at the Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University in 1993, Senior Researcher of the National Institute for Materials Science (NIMS) in 2002, Group Leader in 2006, Director in 2014, and Executive Vice President in 2016, and has been in his current position, Director of NPJ center since 2020.

Advanced Characterization Nanotechnology Platform
微細構造解析プラットフォーム 10年間の成果

Daisuke Fujita

National Institute for Materials Science
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Abstract

Advanced characterization Nanotechnology Platform (ACNP) of the nanotechnology platform program of the Ministry of Education, Culture, Sports, Science, and Technology (MEXT) has started in FY 2012 as a 10-year national infrastructure program. Since FY 2021 is the final year, the achievements of the 10 years are overviewed. ACNP is composed of 11 major universities and national research institutes that lead cutting-edge materials research. It includes Hokkaido University, Tohoku University, NIMS, AIST, University of Tokyo, Nagoya University, Kyoto University, Osaka University, Japan Atomic Energy Agency, National Institutes for Quantum Science and Technology, and Kyushu University, which cover the whole country (Fig.1). While focusing on advanced transmission electron microscopes with extremely high user needs, the world's most advanced microstructure analysis equipment such as synchrotron radiation, strong magnetic field NMR, advanced SPM, Positron Probe Microanalyzer, and so on are complementarily combined. Our core competencies are advanced measurement device development capability, advanced characterization techniques, and analysis know-how. By supporting the solution of problems in the research and development of industry and academia, we have created plenty of dramatic knowledge and accelerated material innovation. We have built a mechanism for complementary cooperation in terms of geography or support fields and have responded to the user needs for advanced nano-characterization as a whole. Besides we have been working to develop human resources for highly skilled technical staff in collaboration with domestic and overseas organizations. To enhance visibility, we have been striving for attractive public relations and outreach. In conclusion, it can be said that ACNP has grown into an internationally open National Research Infrastructure by achieving research support of ~ 1000 cases/year, the utilization rate of industry ~ 30%, and supporting the use of domestic and even overseas researchers.

Fig 1. Configuration of the Advanced Characterization Nanotechnology Platform (ACNP) consisting of 11 institutions. Activities such as the collaboration with overseas institutions, fostering of highly-skilled technical staff, public relations and outreach are shown in insertions.

<CV>
Name: Daisuke Fujita

Current Positions (Main):
Director, Advanced Characterization Nanotechnology Platform (ACNP), MEXT
Office Chief, TIA Promotion Office, National Institute for Materials Science (NIMS)
Chair, Japan Committee for Versailles Project on Advanced Materials and Standards (VAMAS)
Chair, Japan National Committee for Standardization of Surface Chemical Analysis (JSCA)

Academic Degree:

1984 Bachelor's Degree, Department of Engineering, University of Tokyo
1986 Master's Degree, Graduate School of Engineering, University of Tokyo
1991 Doctor of Engineering, Graduate School of Engineering, University of Tokyo

Scientific Curriculum

1986-1991	Research Associate, Institute of Industrial Science, University of Tokyo
1991-2001	Senior Researcher, National Research Institute for Metals (NRIM)
2001-2004	Group Leader, National Institute for Materials Science (NIMS)
2004-2006	Associate Director, Nanomaterials Laboratory, NIMS
2006-2010	Managing Director, Advanced Nano Characterization Center, NIMS
2007-2010	Principal Investigator, WPI-MANA, MEXT
2010-2011	Director, Key Nanotechnologies Field, NIMS
	Managing Director, Quantum Beam Center, NIMS
2011-2016	Director, Advanced Key Technologies Division, NIMS
	Managing Director, Nano Characterization Unit, NIMS
2012-2022	Director, Advanced Characterization Nanotechnology Platform, MEXT, Japan
2016-2018	Executive Vice President, NIMS
2016-2021	Director, Res. Center for Advanced Characterization & Measurement, NIMS
2021-	Office Chief, TIA Promotion Office, NIMS

Prizes
2020: The Society Award, The Japan Society of Vacuum and Surface Science
2018: The Society Award (Seto Prize), The Japanese Society of Microscopy
2016: The Best Paper Award, The Surface Science Society of Japan
2016: Fellow, The Surface Science Society of Japan
2010: The Best Poster Award, The 18th International Vacuum Congress (IVC-18)
2009: Ichimura Science Award, The New Technology Development Foundation, Japan
1998: Murakami Award for 'Young Best Researcher', Murakami Foundation, Japan
1993: The Best Young Researcher Award in Materials Chemistry, Japan Institute for Metals
1993: The Best Paper Award in Materials Chemistry', Japan Institute of Metals
1993: The Best Paper Award for Young Researcher, The Surface Science Society of Japan

Scientific Activities
• More than 200 publications in the distinguished scientific journals including *Nature Materials, Nature Physics, Nature Communications, Scientific Reports, Nano Letters, ACS Nano, Physical Review Letters, Small, Nanoscale, Physical Review B*, *Nanotechnology*, *Applied Physics Letters.*
• More than 100 invited talks at the distinguished scientific meetings

Nanofabrication Platform
微細加工プラットフォーム 10年間の成果

Hiroyuki Akinaga

The administrative office of the Nanofabrication Platform Consortium, Kyoto University,
Research Bldg. No.1/Project Lab.301, Yoshida-Honmachi, Sakyo-ku,
Kyoto 606-8501, Japan

First of all, we would like to thank all the users who have used our platform during the 10-year project period. Without everyone's use, this project would not have been successful. The reason for this success is attributed to the change in the way of researchers thinking about renting shared equipment from owning the equipment, and the strong will of assistive engineers with advanced technologies and experiences to realize the mission. As shown in Figure 1, approximately 10,000 users have used our platform. One of our valuable achievements was the establishment of this relationship, “KIZUNA”.

Manufacturing is a major driver of sustainable and economic development of our society, as claimed in Sustainable Development Goals (SDGs) Goal 9. Manufacturing technology has made continuous progress over the years and has brought about innovations in various industrial fields. Elemental technologies such as thin film deposition, lithography, etching, cleaning, measurement / analysis, and database-driven design have been developed on a nanoscale. Thus, nanotechnology in fabrication processes is a fundamental and indispensable to spur the development, and further stimulate academic research.

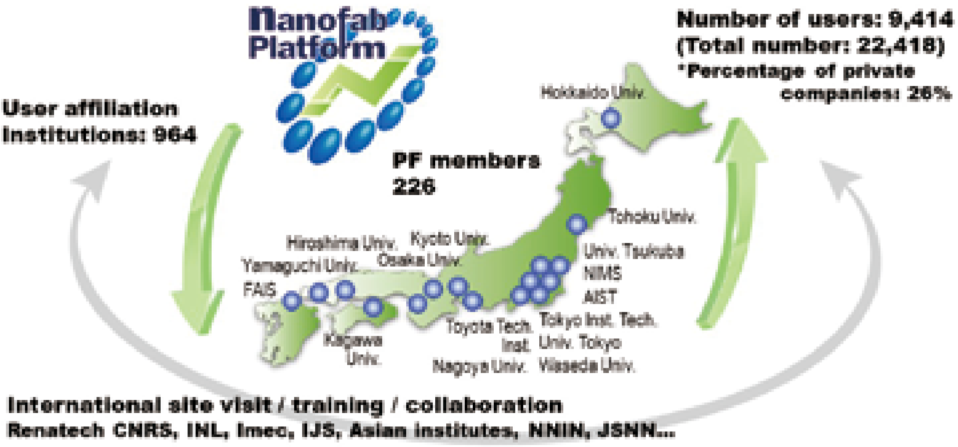

Fig. 1 Nanofabrication platform built by users and 226 project members of 16 institutions (as of July 30, 2021).

Figure 2 shows a brief history and the prospect of nanoscale fabrication technologies [1, 2]. With the development of IoT, nanofabrication technologies are expected to become more familiar. As mentioned above, nanotechnology is the foundation of various research and industrial fields, and we have cultivated the fertile soil that forms the basis of them. At the request of users, our platform members developed technologies to meet their purposes, which means that it was a technical competition and collaborative creation to improve our technical level to being high. These achievements contribute to society as an international standardized document [3] and are released as video contents for training engineers [4].

We have built a system that will strengthen the research function and industry-academia-government collaboration of each institution, through the exchange of diverse human resources and the aggregation of knowledge centered on shared facilities. We have fostered a culture to promote research and development efficiently by installing large and expensive equipment in the facility and using them by users. Our platform will continue to grow. The platform will promote shared use by diverse users of industry, academia and government, provide users with the shortest approach to problem solving, and will continue to promote their collaboration and interdisciplinary researches. Our platform must continue to grow. Digital transformation will make shared facilities smarter, enable high throughput and interoperability. By implementing machine learning, artificial intelligence, and informatics, we do develop our nanofabrication platform that provides users with new insights that can be obtained synergistically and emergently.

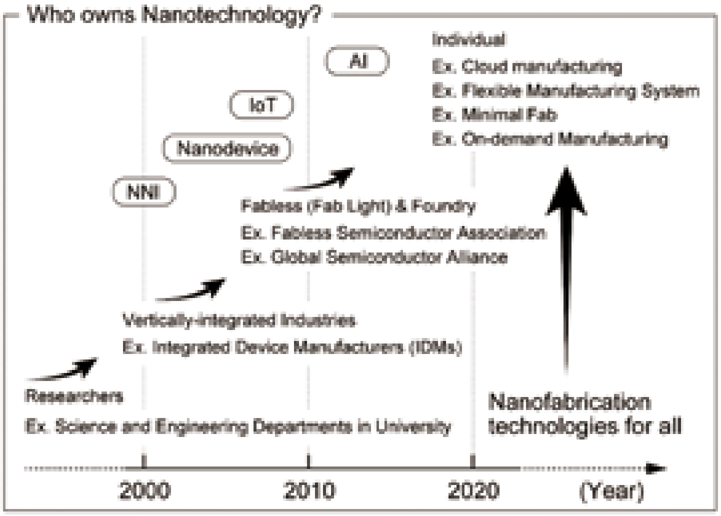

Fig.2 Who owns nanotechnology? Cloud manufacturing will spread widely by making access to nanotechnologies easy [2].

Acknowledgements

The author is deeply grateful for the active leadership of Prof. H. Kotera (RIKEN, Kyoto Univ.), the representative of this project. The author also appreciates the cooperation of the co-representative, Prof. H. Fujita (Tokyo City Univ., Univ. Tokyo), Prof. H. Misawa (Hokkaido Univ.), and Prof. S. Tanaka (Tohoku Univ.). The author sincerely thanks to have been able to collaborate with the coordinators of this project, K. Tomii, M. Matsumoto, S. Horiike (Kyoto Univ.), Y. Oonishi, and N. Shimamoto (Univ. Tokyo).

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[1] Special Issue on Advanced Nanofabrication Processes for Emerging Devices and Materials, Sens. Mater., 31 (2019), https://myukk.org/SM2017/index.php?vol=31&no=8&sub_no=2

[2] H. Akinaga, Nanofabrication Technologies for All, Sens. Mater., 31, 2477 (2019), https://myukk.org/SM2017/sm_pdf/SM1949.pdf

[3] Nanotechnologies - A guideline for ellipsometry application to evaluate the thickness of nanoscale films, IEC TR 63258, https://webstore.iec.ch/publication/59663

[4] NanoFab Platform Youtube channel https://www.youtube.com/channel/UCk3zxbLOFMzAa5bY5yHeZpw

Hiroyuki Akinaga (Member, IEEE) received the B.E., M.E., and Ph.D. degrees from the University of Tsukuba, Ibaraki, Japan, in 1987, 1989, and 1992, respectively. Currently, his main affiliation is the Principal Research Manager, Device Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), and the deputy research supervisor of the project of scientific innovation for energy harvesting technology, Japan Science and Technology Agency (JST). He has been serving as a convenor at International Electrotechnical Commission (IEC), TC113 (Nanotechnology for electrotechnical products and systems). He is a fellow of Japan Society of Applied Physics. His current interests include nanoelectronics and open innovation platform.
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Molecule & Material Synthesis Platform
分子・物質合成プラットフォーム 10年間の成果

Toshihiko Yokoyama

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Abstract
Molecule & Material Synthesis Platform provides shared use opportunity of highest research facilities in the research institutes to industrial, academic and public agency's researchers. We have supported molecule and material synthesis, structural analysis, and molecular design to explore and develop organic, inorganic materials, nanomaterials that have unique functions and/or superior characteristics. We have accepted and conducted more than 5,000 research proposals for these nine years. In this talk, I will show some of the most outstanding scientific/technological achievements in this platform.

Molecule & Material Synthesis (M&MS) Platform consists of ten research organizations: Chitose Institute of Science and Technology (CIST, Chitose, Hokkaido), National Institute for Materials Science (NIMS, Tsukuba, Ibaraki), Shinshu University (Nagano), Nagoya University (Nagoya, Aichi), Nagoya Institute of Technology (NIT, Nagoya, Aichi), Japan Advanced Institute of Science and Technology (JAIST, Nomi, Ishikawa), Osaka University (Suita, Osaka), Nara Institute of Science and Technology (NAIST, Ikoma, Nara), Kyushu University (Fukuoka), and Institute for Molecular Science (IMS, Okazaki, Aichi). IMS is a representative organization. We have been providing many kinds of material synthesis and analysis techniques to domestic and international industrial and academic researchers in extremely wide scientific and technological fields such as solid-state physics, semiconductors, magnetic materials, catalysts, batteries and cells, organic and inorganic materials, polymers, earth and space science, pharmacy, physiology and medicine, and so forth. Details of our shared equipment, user reports, and other useful information can be seen in the web page of https://mms-platform.com/. In this platform, we are supporting not only the sophisticated material characterization using shared equipment but also the material synthesis collaboration such as organic synthesis of important compounds. The latter is a quite unique program in equipment sharing projects, leading to many kinds of important and interesting scientific/technological results.

In every year, Advisory Committee in Nanotechnology Platform selects five to six outstanding achievements, and our M&MS Platform was awarded the outstanding achievement 15 times in these nine years. The research proposal title of these outstanding achievements selected are listed in Table 1. I am convinced that the Nanotechnology Platform program will be successfully terminated from the qualitative and quantitative points of view. I will briefly review these outstanding achievements in this talk.

Although the present Nanotechnology Platform program is completed in this fiscal year 2021, the equipment sharing supported by the Ministry of Education, Culture, Sports, Science and Technology, Japan (MEXT) continues in the successive program of Advanced Research Infrastructure for Materials and Nanotechnology in Japan (ARIM). In this program, we will provide not only shared equipment and material synthesis but also structured material database for the development of new functional materials. I believe that in the next ARIM program would be successfully conducted to provide many kinds of harmonious materials that exhibit high performance, excellent safety, and satisfactory reliability for our future lives.

Table 1. List of the awarded outstanding achievements in M&MS Platform (2015-2022). For details, see the web page: https://www.nanonet.go.jp//magazine/feature/excellent-result/

Research Title	User Affiliation	Support	Year
Development of synthesis techniques for useful proteins using cultured plant cells	Ishikawa Pref. Univ.	JAIST	2015
Characteristic electron spin resonance of molecular magnet of endohedral fullerene molecular complexes	Kyoto Univ. Univ. Tsukuba, JST	IMS	2015
Vacuum ultraviolet light source and photodetectors using fluoride thin films	Tokuyama Co. Kyushu Inst. Tech. Tohoku Univ.	NIT	2015
Synthesis and analysis of designated dangerous drugs of 3,4-dichloromethylphenidate	Nat. Res. Inst. Police Science	IMS	2016
Development of chiral chromatographic supports that can freely reverse the elution sequence	Kanazawa Univ.	Nagoya Univ.	2016
Misfolding of protein onsetting neurodegenerative disease	Keio Univ.	IMS	2017
Successful development of adhesive material that can be used at high temperature and be peeled off with light	Kyoto Univ. Nagoya Univ.	Nagoya Univ.	2017
Development of nanotechnical prevention method against sessile organisms with low environmental loads for the application on the surface of marine equipment	Asahikawa Medical Univ.	CIST	2018
Molecular profiling of small extracellular vesicles via charge-based capture using oxide nanowire microfluidics	Kyushu Univ., Osaka Univ., Nat. Cancer Center Japan	Nagoya Univ.	2019
Spin structures in BiFe1-xCoxO3 thin films	Tokyo Inst. Technol., Kyushu Univ.	NIT	2020
Preparation of double coating nano particles and its commercialization as cosmetics	Adv. Pharma Japan Inc.	Kyushu Univ.	2021
Short and Unified Chemo-Enzymatic Synthesis of Spiroketals, and the Structural Elucidation by the Crystalline Sponge Method	Univ. Graz	IMS	2021
Chirality induced spin selectivity in inorganic chiral crystal	Osaka Pref. Univ., Toho Univ., Open Univ. Japan	IMS	2022
Structural determination of photosensitive compounds containing heteroatoms and application to anti-cancer photodynamic therapy	Osaka Pref. Univ., Nara Women's Univ., Nagoya City Univ.	Nagoya Univ.	2022
Ultrahigh sensitive fast detection of COVID-19 virus using gold nanostructures	Shanghai Inst. Ceramics	NIT	2022

<CV>

Toshihiko YOKOYAMA, Prof. Dr.

Received PhD degree from the University of Tokyo in 1991. Research Associate in Hiroshima University (1987-1993), Research Associate, Lecturer, and Associate Professor in the University of Tokyo (1993-2001), and Professor in Institute for Molecular Science (2002-present). Director in Department of Materials Molecular Science in IMS (2011-). Director of Instrument Center in IMS (2014-). Representative of Molecule & Material Synthesis Platform (2012-2021). President of the Japanese Society for Synchrotron Radiation Research (2021-).

Session 2
【Material Data Strategy to Strengthen Material Innovation Force / マテリアル革新力強化に向けたマテリアルデータ戦略】

【Plenary Lecture / 基調講演】

“Expectations for the Material DX Platform to Strengthen Materials Innovations”

「マテリアル革新力強化に向けたマテリアルDXプラットフォームへの期待」

Teruo Kishi (Innovative Structural Materials Association)

岸 輝雄（新構造材料技術研究組合理事長、東京大学名誉教授）

Expectations for the Material DX Platform to Strengthen Materials Innovations
マテリアル革新力強化に向けたマテリアル DX プラットフォームへの期待

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Abstract

Nanotechnology and materials science and technology have been focused on R & D investment in various countries around the world as leading technological innovations in a wide range of industries such as resources, environment, energy and life science as well as academic science. In the United States, President Bill Clinton delivered a speech on the National Nanotechnology Initiative at the California Institute of Technology in January 2000. In this speech, he stated that one of his specific goals was to "contain all the books in the Library of Congress in a memory element equivalent to one sugar cube." In July 2000, the National Nanotechnology Initiative: The Initiative and Its Implementation Plan was announced, and in December 2003, the 21st Century Nanotechnology Research and Development Act was signed by President George W. Bush. In Japan, the Atom Project carried out by NEDO started in 1993 prior to the United States, and the nanotechnology and materials field was positioned as one of the four priority promotion fields in the Second Science and Technology Basic Plan from 2001 and Third Science and Technology Basic Plan from 2006.

Industry-academia-government was required to work closely together to carry out research and development in order to make the best use of limited research resources such as human resources and experimental facilities, and the Nanotechnology Support Project supported by MEXT (Ministry of Education, Culture, Sports, Science and Technology) was started in April 2002 with a five-year plan. Targeting nanotechnology research and development at universities, public research institutions, and private research institutes, this project conducted both of shared use of 14 large and special research facilities nationwide and support of nanotechnology information. The Nanotechnology Support Project has been linked to MEXT's "Nanotechnology Network" project from 2007 and also to MEXT's "Nanotechnology Platform" project from 2012. In addition, these projects are also an opportunity to create large national projects in elemental strategies and structural materials.

Nanotechnology is considered to be a cross-disciplinary technology field that crosses conventional research fields as well as being the basis for creating innovative technologies in the 21st century. In this symposium, I will give an overview of Japan's national nanotechnology projects, which began with the Nanotechnology Support Project, and I will describe my expectations for the Material DX platform which is the next nanotechnology platform shared project.

<CV>
Fields of Research:
materials science, especially fracture mechanics and
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Education/Career:
1969 Received the degree of Doctor of Engineering from the University of Tokyo
1974 Associate Professor, the Institute of Space and Aeronautical Science (ISAS), the University of Tokyo
1988 Professor, the Research Center for Advanced Science and Technology (RCAST), the University of Tokyo
1995 Director General of RCAST
1997 Director General of the National Institute for Advanced Interdisciplinary Research, Ministry of International Trade and Industry (METI)
2001-2009 President of the National Institute for Materials Science (NIMS)
2009- Emeritus of the National Institute for Materials Science (NIMS)
2014-2019 Program Director for SIP (Cross-ministerial Strategic Innovation Promotion Program) at Cabinet Office
2015-2020 Science and Technology Advisor to the Minister for Foreign Affiars
2013- President of Innovative Structural Materials Association

Awards:
Officier de l'Ordre National du Mérite, France (2004)
Honda Memorial Award, Honda Foundation (2006)
Barkhausen Award, Dresden, Germany (2007)
Distinguished Life Membership, ASM, USA (2010), etc.

【Special Lecture / 特別講演】

“Research Transformation Driven by Open Facility Platform”

「マテリアル先端リサーチインフラが牽引するリサーチトランスフォーメーション
～実験装置に加え、データ・知識の共有へ～」

Taro Hitosugi (Tokyo Institute of Technology)
一杉 太郎（東京工業大学）

Research transformation driven by open facility platform
マテリアル先端リサーチインフラが牽引する
リサーチトランスフォーメーション
～実験装置に加え、データ・知識の共有へ～

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Abstract

The emergence of an "autonomous materials laboratory" using machine learning and robots is shifting a paradigm in materials science. Here, the impact of autonomous labs to open facility platforms is discussed. The platform powered by autonomous labs strongly affects the way we conduct research and our mindset toward research.

I. INTRODUCTION

The materials that humanity has synthesized to date represent just a tiny fraction of all possible compounds, which by some estimates may include 10^{60} possible materials.[1] Thus, before us lies a vast search space for new materials, many of which should be useful in addressing the problems that society faces. Therefore, materials exploration is a frontier for humanity, like space or deep-sea exploration.

Then, a question arises. How can we "quickly and systematically" find unexpected materials within this vast search space? For this purpose, materials science needs a tool that serves as a "materials explorer," like a spaceship or a deep-sea exploration vessel. There are limits on the amount and quality of research conducted when relying on human capabilities alone.

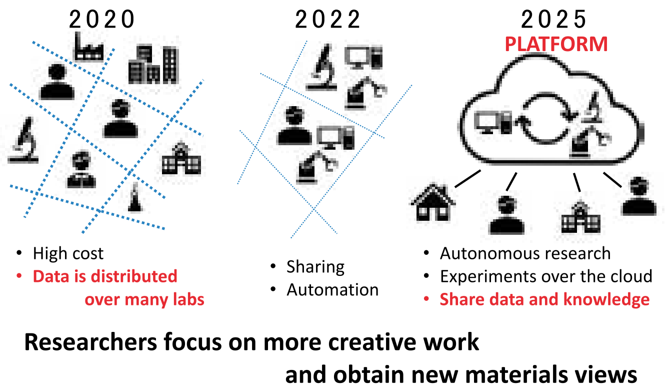

Fig. 1
An open facility platform equipped with autonomous systems enables to share data and knowledge with many researchers.

II. A PLATFORM EQUIPPED WITH AUTONOMOUS EXPERIMENT SYSTEMS

The core of the "materials explorer" is an autonomous experiment system. Here, the term autonomous means that a computer algorithm decides what experiment to do next, and robots proceed with the experiment. No human intervention is required; this approach is called closed-loop experiments [2].

When this materials explorer is implemented to an open facility platform, users can log in to this system via the internet and fabricate and evaluate materials. In addition, due to the high-throughput experiments, a large amount of data will be accumulated on the platform. Then, the data is shared with many researchers to stimulate discussions (Fig. 1). The new platform is not just about shortening time and improving efficiency but sharing data and knowledge with many researchers to obtain new materials views.

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＜CV＞

Professor, Tokyo Institute of Technology
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Degrees:

Bachelor of Engineering 1994, Department of Applied Chemistry, The University of Tokyo
Master of Engineering 1996, Department of Superconductivity, The University of Tokyo
Doctor of Engineering 1999, Department of Superconductivity, The University of Tokyo

Awards

2010 The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (MEXT), Japan
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Professional Experience

1996-1999	Predoctoral Fellow, Advanced Research Laboratory, Hitachi, LTD.
1999-2003	Researcher, Core Technology Development Group, Sony Corporation.
2003-2007	Assistant Professor, Department of Chemistry, The University of Tokyo
2007-2015	Associate Professor, Advanced Institute for Materials Science, Tohoku University
2015-2016	Professor, Department of Applied Chemistry, Tokyo Institute of Technology
2016-	Professor, School of Materials and Chemical Technology, Tokyo Institute of Technology

【Overseas Invited Lectures / 海外招待講演】

“Autonomous (AI-Driven) Experimental Materials Science”

「AI駆動自立型実験による材料科学」

Martin L. Green (National Institute of Standards and Technology, USA)

“FAIRmat’s Approach toward Enabling Data-Centric Science”

「データセントリック科学構築に向けたFAIRmatの取り組み」

Claudia Draxl (Humboldt University, Germany)

Autonomous (AI-Driven) Experimental Materials Science
AI駆動自立型実験による材料科学

Martin L. Green

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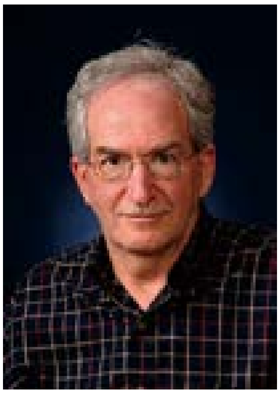
Several critical technologies are currently materials-limited, awaiting novel materials solutions for advancement, e.g., transportation (light-weight, high-strength alloys, and corrosion resistant coatings), sustainable energy (earth-abundant catalysts for solar fuel production), and nanoelectronics (low-energy/operation integrated circuit devices). A fundamental obstacle to efficient discovery of novel materials and processing schemes is the large number of candidate materials, and their associated processing parameters. Modern materials scientists train for decades in the fundamentals of the field to develop the knowledge and intuition required to discover new materials. They must then plan and conduct a series of experiments to test their hypotheses, analyze the resultant data, generate new hypotheses based on the knowledge gained, and plan the next series of experiments. They are constrained to study relatively simple materials (e.g., those that may contain ≤ 4 elements and involve ≤ 2 processing parameters). This is because while the number of variable parameters (n) increases linearly, the number of candidate materials/processing schemes increases exponentially ($\sim 10^{2n}$). I will discuss the development of a novel NIST platform which will place artificial intelligence in charge of materials optimization and discovery, thereby transforming "dumb" instrumentation into "intelligent" systems capable of planning, executing, analyzing, and extracting knowledge from experimental and modeling data. The marriage of artificial intelligence and materials science will result in a sea-change, enabling a $10^2 – 10^4$ acceleration of materials discovery and process optimization.



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EDUCATION
Ph. D., Materials Science, Massachusetts Institute of Technology, 1978
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EMPLOYMENT
2003 - present: Leader, Materials for Energy and Sustainable Development Group, NIST
2001 - 2003: SEMATECH Assignee (from Agere Systems) to IMEC, Belgium
1978 - 2003: Research Scientist, Bell Laboratories/Lucent Technologies/Agere Systems
1966 - 1970: Co-op Student, Naval Applied Science Laboratory

AWARDS
Plenary Speaker, IUMRS (2016)
MRS Fellow (2011)
Department of Commerce Bronze Medal (2010)
President of the MRS (2001)
AMAX Fellow at MIT (1974-1977)
Kurtz Memorial Visiting Scientific Fellow, Technion, Israel (1977)

FAIRmat’s approach toward enabling data-centric science
データセントリック科学構築に向けたFAIRmatの取り組み

Claudia Draxl

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Abstract

High-throughput studies provide much information but will never cover the vast chemical and structural space of materials. Thus, Artificial Intelligence (AI) must enhance our research of tomorrow – starting today. To predict novel candidate materials for a given application, possibly even in regions of the materials space that no-one would think of, our goal is to build a general “map of materials properties”. A FAIR (findable and AI ready; an alternative interpretation of the original acronym) data infrastructure will be an important step for achieving this goal [1]. The NOMAD Laboratory [2] is a community effort and a living example for such infrastructure in computational materials science, comprising the NOMAD Repository (raw data) and its Archive (normalized, i.e. code-independent data), the NOMAD Encyclopedia, and the NOMAD Analytics Toolkit. A real breakthrough is, however, only possible if the combined insight from synthesis, experiment [3], theory and simulations are brought together. This is the concept of FAIRmat [4], a consortium of the German data-infrastructure project (NFDI), representing the research field of condensed-matter physics and the chemical physics of solids. I’ll review where we are on this road that requires an immense but rewarding effort of the wide community.

Fig. 1: The structure of FAIRmat

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[3] A. Trunschke et al., Towards Experimental Handbooks in Catalysis, Topics in Catalysis, 1-17 (2020).
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Prof. Claudia Draxl

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Humboldt-Universität zu Berlin

Education

Studies of mathematics and physics, University Graz
PhD in solid-state theory

Professional Activities

July 2019	Fellow at the Max Planck Graduate Center for Quantum Materials
July 2014	Max-Planck Fellow at the Fritz-Haber Institute Berlin
November 2011	Einstein Professor, Humboldt-Universität zu Berlin, Germany
November 2005	Full professor, Montanuniversiät Leoben, Austria
2000 / 2001	Guest professor, Uppsala University, Sweden
1997	Associate professor, University Graz, Austria

Honors and Awards

2021	Lise-Meitner lecturer of the German and Austrian Physical Societies
April 2018	Corresponding member of the Austrian Academy of Sciences abroad
March 2014	Appointment as Max-Planck Fellow
December 2013	Caroline-von-Humboldt-Professor 2014 by the HU Berlin
April 2013	Paracelsusring by the City of Villach (video)
November 2011	Fellow of the American Physical Society
December 2008	Science Award of the Federal State of Styria
March 2008	Beller Lectureship of the American Physical Society
April 2005	Scientist of the month (FEMtech)
2000	Guestprofessorship by the Swedish Research Council NFR
January 2000	Honorary doctorate of Uppsala University, Sweden
September 1995	Ludwig-Boltzmann award for theoretical physics by the Austrian Physical Society

Session 3
【Importance of Data Utilization in Material Strategy / マテリアル戦略におけるデータ利活用の重要性】

“Accelerating Interdisciplinary Research between Material Science and Computer Science on the *mdx* Data Science Platform”

「データ活用社会創成プラットフォームmdxにおける材料科学と
情報科学の学際研究の促進に向けて」

Toyotaro Suzumura (The University of Tokyo)
鈴村 豊太郎（東京大学）

“Materials Research in the Data Era: A NIMS Challenge”

「データ時代の材料研究：NIMSの取り組み」

Masahiko Demura (National Institute for Materials Science)
出村 雅彦（物質・材料研究機構）

“Standardization of Output Data Format for Measurement and Analysis Instruments: Current Situation and Future Plan”

「計測分析装置の出力データフォーマット標準化：現状と展望」

Shingo Ichimura (Waseda University)
一村 信吾（早稲田大学）

Accelerating interdisciplinary research between material science and computer science on the *mdx* data science platform
データ活用社会創成プラットフォーム mdx における材料科学と情報科学の学際研究の促進に向けて

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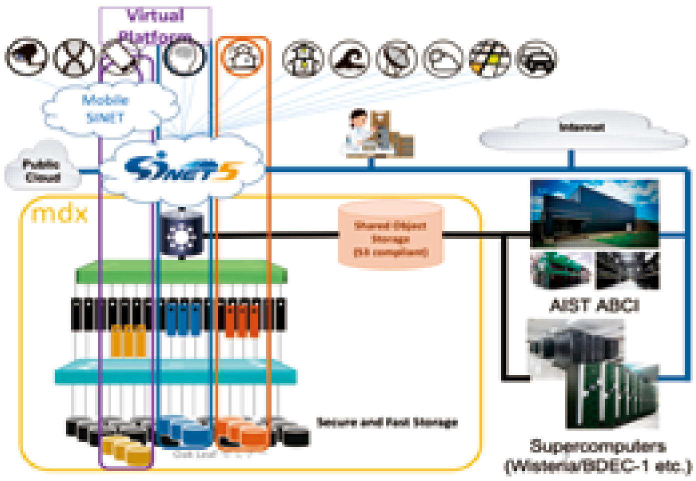
The mdx platform [1] has been jointly designed and operated by 11 research institutes including 9 national universities (Tokyo, Hokkaido, Tohoku, Tsukuba, Tokyo Tech, Nagoya, Kyoto, Osaka, Kyushu), NII (National Institute of Informatics) and AIST (National Institute of Advanced Industrial Science and Technology). The aim of the platform is to provide a nation-wide research cloud that accelerate interdisciplinary research collaborations on data utilization and data science. This platform is not limited to academic institutes, but also open to collaborations between private institutes, academia and governments.

The main important features that the mdx platform provide are listed as follows:



- To provide a cloud-like functionality that allows you to create your own virtualization environment by specifying required computing and storage resources. This is a different point than existing supercomputers where you cannot change various configurations such as OS, network, application package depending on your data science needs.
- To provide a high-speed network based on SINET and mobile SINET that can connect other computing/storage or IoT devices. You can establish your environment via L2VPN as well.
- To provide dedicated computing environments for users that have highly sensitive and confidential data such as personal data.
- To provide a single sign-on mechanism by leveraging an authentication service named "Gakunin"

As of this presentation in January 2022, the mdx platform is in the testing phase that allows you to test our the mdx platform for free and the production phase with billing mechanism plans to start around Fall in 2022.　On the top of the mdx platform, we have been starting to collaborate with material science researchers from various aspects including fundamental research around material informatics such as predicting material properties using graph neural networks and multi-task machine learning methods, and discuss how the mdx platform can be exploited as on-demand computing resources by coupling with a material research cloud platform that is led by NIMS (National Institute for Materials Science)

References

[1] Toyotaro Suzumura, et.al, The mdx Project Report 2021 A Large-Scale Platform for Accelerating Cross-Disciplinary Research Collaborations Towards Data-Driven Societies, December 2021, AXIES 2021

Prof. Toyotaro Suzumura is a professor at the University of Tokyo since April 2021. His current research interests are graph neural networks and their application to e-commerce, medical science, finance, and such. After obtaining a Ph.D. in computer science in 2004 from Tokyo Institute of Technology, he has 17-year experiences from 2004 to 2021 in IBM Research as a principal research scientist in global research labs including Tokyo(2004-2013), Dublin(2013-2015), and IBM T.J Watson Research Center and MIT-IBM Watson AI Lab in New York (2015-2021). As for his research achievements, he won an international competition related to large-scale graph processing named Graph500 10 times since 2014. He has published more than 90 papers to top-tier international conferences and journals and served as a PC chair of IEEE BigData 2017 as well as serving program committee members in numerous international conferences such as AAAI, ACM/IEEE Supercomputing, and IEEE Cloud.

Dr. Masatoshi Hanai is a Project Assistant Professor in the University of Tokyo. His research area is large-scale graph computing and analysis. He completed his Ph.D. in Tokyo Institute of Technology in 2016. After that, he was a research fellow in Nanyang Technological University, Singapore, and a Research Assistant Professor in Southern University of Science and Technology, Shenzhen, China.

Materials Research in the Data Era: A NIMS Challenge
データ時代の材料研究：NIMSの取り組み

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Abstract
Data-driven materials research is spreading to various areas at NIMS. The development of a data platform to support this research is progressing well. In the near future, it is expected that a materials DX platform will be realized to accelerate materials research in Japan.

I. INTRODUCTION

In the development of materials, one designs the optimal combination of elements and methods of processing from the desired performance. There are high expectations for data-driven approaches to change the ways of the materials development through making it possibe to search in the vast space[1]. In this talk, I will introduce data-driven research and its foundation, materials data platform, focusing on the efforts at NIMS.

II. ADVANCES IN DATA-DRIVEN RESEARCH

Data-driven materials research began with the combination of computational materials science typically using first-principles calculations; for example, the discovery of novel semiconductors[2] and the proposal of multiphase film structures for thermal radiation[3] are pioneering works. Then, researches utilizing an experimental database has been emerging like a good example of proposing a new polymer with high thermal conductivity[4] using PoLyInfo[5], which is the world's largest polymer database. Furthermore, there is another research example that explored the combination of elements with high thermal resistance by utilizing data in literatures[6], where Bi/Si was discovered to show the world best thermal resistance, demonstrating the usefulness of public data.
The data-driven approach has been expanding into more practical materials. Active learning can be applied to optimize materials and processes, and there are several examples such as process optimization of thermoelectric devices[7], development of new adhesives[8], search for new alcohol oxidation catalysts[9], and optimization of metal fine powder processing conditions[10]. Furthermore, materials and processes have been explored in combination with automated experiments[11], which is called Smart Laboratory. In the SIP project[12], a materials integration system (called MInt[13]) is developed as a computational method for predicting property and performance from process through microstructure, and based on this system, one can design materials and processes from the desired performance in industry.

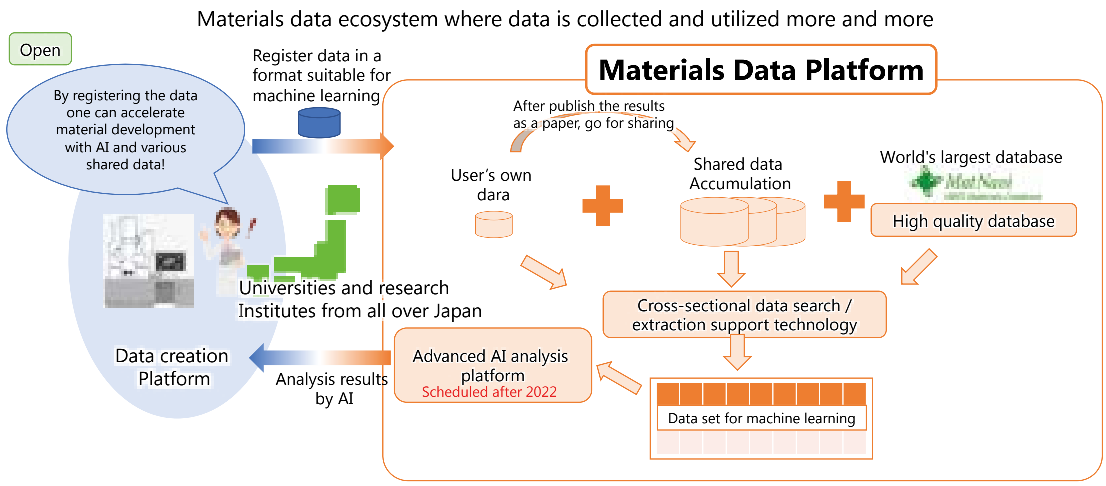

Fig. 1
Schematic draw for a concept of materials DX platform to accelerate R&D in Japan[21].

III. MATERIALS DATA PLATFORM

Based on our experiences in developing MatNavi[14], one of the world's largest materials databases, we have been developing a materials data platform for aggregating and utilizing materials data generated in daily research activities. It has been three years since the materials data platform project[15] started in 2017, and we have developed an automatic data collection system using the IoT[16], technology to improve the efficiency of curation of literature data by using natural language processing technology[17], and a data infrastructure system to aggregate data. Some of the systems are now in operation on a trial basis under the name DICE[18].

III. MATERIALS DX PLATFORM

Using the above-mentioned practices at NIMS as a template, the Materials DX Platform concept has been proposed, and its construction is being promoted as projects of the Ministry of Education, Culture, Sports, Science and Technology. NIMS will play the role of a data core center (Fig. 1[21]) that will consolidate data from materials research throughout Japan. This platform is supposed to enhance R&D capabilities.

Acknowledgements

This work was partly supported by Council for Science, Technology and Innovation (CSTI), Cross-Ministerial Strategic Innovation Promotion Program (SIP), "Materials Integration for Revolutionary Design System of Structural Materials" (Funding agency: JST).

References

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Masahiko Demura is Director of Research & Services Division of Materials Data and Integrated System at National Institute for Materials Science, Japan. He received his Dr. Eng. in Material Science and Engineering from U. Tokyo in 2003. His recent research interests include the digital transformation in materials research, particularly in the field of structural materials. Demura can be reached by email at DEMURA.Masahiko@nims.go.jp.

Standardization of output data format for measurement and analysis instruments: current situation and future plan
計測分析装置の出力データフォーマット標準化：現状と展望

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I. Request for a common output data format

The request for a common output data format for measurement/analysis instruments arises from the activity of the JSPS (Japan Society for the Promotion of Science) special committee on *Construction of Measurement/Characterization Platform Strategy for Open Innovation*. The discussion at the committee (FY2014-FY2017) highlighted the importance of combined/integrated analysis and application of artificial intelligence (AI) technologies to data obtained by various measurement instruments. It became clear that the output data of the instruments should be able to be used both inside of the instruments (i.e., use in physical space) and outside of the instruments (i.e., use in cyber space). The adaptability for the use in cyber space led the request of common output data format for various measurement instruments [1].

II. Development of a common output data format

The development of a common output data format was achieved through two NEDO (New Energy and Industrial Technology Organization) projects, i.e., *Research and development of innovative analysis/evaluation technology with adaptability to big data* (FY2016-FY2017) [2] and *Development of combined measurement and characterization systems to accelerate the development of energy-saving products* (FY2018-FY2019) [3]. In order to ensure the independent availability in cyber space of data obtained by various measurement instruments, information relating to measuring object, measurement methods, sample pretreatment, used instrument and analysist, etc., was added to a format named MaiML (Measurement, Analysis, Instrument Markup Language). The format is composed of four main tags of Document, Protocol, Data, and eventLog as schematically shown in Fig.1. Based on the format, output data converters of 14 analytical instruments were fabricated and tested. To ensure the confidentiality and safety of data collected in cyber space, the functions of recording data change and data locking are also integrated in the MaiML format.

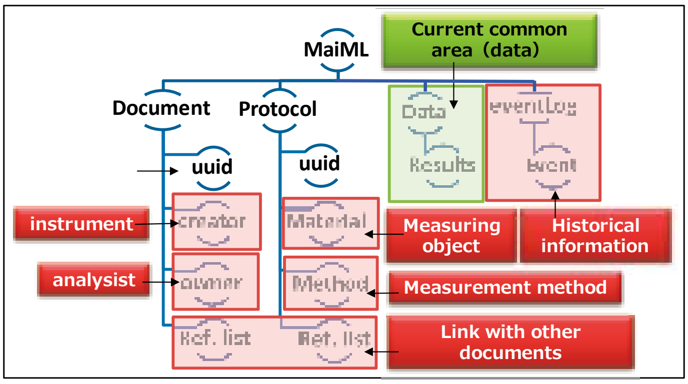

Fig. 1 Structure and main feature of the common output data format named MaiML.

III. Standardization of the common output data format

The standardization of the common output data format based on MaiML is in progress as a METI project (FY2020-FY2022). A Japanese Industrial Standard (JIS) for the format is planned to be published in 2023, and an ISO standard based on the JIS document is planned to follow it.

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[3] Development of combined measurement and characterization systems to accelerate the development of energy-saving products (FY2018-FY2019) Final Report, NEDO No. 20200000000670 (in Japanese)

Shingo ICHIMURA （一村信吾）

Shingo ICHIMURA is Professor and Associate Director of Research Strategy Center/Waseda University, and Special Emeritus Advisor of AIST (National Institute of Advanced Industrial Science and Technology). He also serves as Chairman of the JSPS (Japan Society for the Promotion of Science) 193 Committee on Measurement and Characterization Platform, and Chairman of the national mirror committee of ISO/TC 229 on nanotechnology.
Prior to the current position he had been working as Professor and Director of Strategic Innovation Office/ Nagoya University (from 2014 to 2018), and Vice and Senior Vice President of AIST (from 2007 to 2014). He started his research carrier at Electrotechnical Laboratory (ETL) in 1982, mainly in the fields of Applied Surface Science/Engineering and Extremely High Vacuum Technology. He is Fellow of American Vacuum Society and the Japan Society of Applied Physics, and Regional Editor of Surface and Interface Analysis.

組織委員会/Organizing Committee

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