文部科学省ナノテクノロジープラットフォーム

第18回ナノテクノロジー総合シンポジウム

JAPAN NANO 2020

"Quantum Science, Biotechnology and AI Technology driven by Nanotechnology"

Nanotechnology

Proceedings

Date: **January 31st (Fri), 2020**

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

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Center for Nanotechnology Platform, National Institute for Materials Science (NIMS)

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文部科学省ナノテクノロジープラットフォーム

第18回ナノテクノロジー総合シンポジウム

JAPAN NANO 2020

「ナノテクノロジーが切り拓く量子・バイオ・AI 技術」

Nanotechnology

講演予稿集

開催日： 2020年1月31日（金）

会　場： 東京ビッグサイト
会議棟１階レセプションホール A（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

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January 31st (Fri.), 2020, Reception Hall A
2020年1月31日（金）　会議棟1階レセプションホール A

10:00-10:30【Opening Remarks / 開会挨拶】

10:00 - **Ministry of Education, Culture, Sports, Science and Technology**/ 文部科学省

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）

10:30-11:05【Plenary Lecture / 基調講演】

Hiroshi Amano (Nagoya University, Japan)
天野 浩（名古屋大学）
“En Route to Realize Zero Carbon Emission”
「カーボンエミッションゼロを目指した取り組み」

11:05-11:40【Special Lecture / 特別講演】

Jinichi Igarashi (COCN(Council on Competitiveness-Nippon))
五十嵐 仁一（一般社団法人 産業競争力懇談会）
“Launching the MI platform program toward energy innovation”
「エネルギー革新に向けた MI 基盤の構築」

11:40-12:30【Session 1】

Quantum Science & Biotechnology / 量子と生命科学

11:40 - **Mutsuko Hatano** (Tokyo Institute of Technology)
波多野 睦子（東京工業大学）
“The potential of diamond solid-state quantum sensors”
「ダイヤモンド量子センサの可能性」

12:05 - **Ichio Aoki** (National Institutes for Quantum and Radiological Science and Technology)
青木 伊知男（量子科学技術研究開発機構）
“Nano- and Quantum Technology-based MR Imaging for Life Science”
「生命科学を革新するナノおよび量子技術による磁気共鳴イメージング」

12:30 - 13:30　Lunch / 昼食

13:30-13:55【Session 2】

nanotech 2019 award lecture / nano tech 大賞2019講演

13:30 - **Toru Ushirogochi** (Ricoh)
後河内 透（株式会社リコー）
“Prospects for Digital Print Manufacturing of Lithium-ion Batteries”
「リチウムイオン電池のデジタル印刷を目指して」

13:55-14:25【Session 3】

Overseas Nanotechnology User Facility Programs / 海外ナノテク共用施設・研究成果紹介

13:55 - **Daniel J. C. Herr** (Joint School of Nanoscience and Nanoengineering, USA)
"The National Nanotechnology Coordinated Infrastructure (NNCI) and Selected Convergent Technologies."
「NNCI とコンバージェントテクノロジー」

14:25 - 14:40 Coffee Break / 休憩

14:40-15:45【Session 4】

Topics and future perspectives of nanotechnology platforms / ナノテクノロジープラットフォームの成果と将来展望

14:40 - "Introduction"
「イントロダクション」

14:45 - **Yasutaka Matsuo** (Hokkaido University)
松尾 保孝（北海道大学）
"Biotechnology research by using a nano, micro structural analysis with electron microscope"
「電子顕微鏡による構造解析手法を用いたバイオ研究」

15:05 - **Kentaro Totsu** (Tohoku University)
戸津 健太郎（東北大学）
"R&D support by open collaboration based on shared facilities"
「共用設備を基盤としたオープンコラボレーションによる研究開発支援」

15:25 - **Yoshinobu Baba** (Nagoya University)
馬場 嘉信（名古屋大学）
"Research Support for the Interdisciplinary Research between Nanotechnology, Biotechnology, Quantum Technology, and AI, and Future Perspective for Nanotechnology Platform"
「ナノテクノロジーとバイオ・量子・AI 融合領域の支援成果とナノテクノロジープラットフォームの将来展望」

15:45-16:35【Session 5】

Beyond Nano・AI / ナノテクノロジーのシステム化と産業応用

15:45 - **Daisuke Okanohara** (Preferred Networks)
岡野原 大輔（株式会社 Preferred Networks）
"Materials Discovery Using Machine Learning: Latest Trends and Future Prospects"
「機械学習を使った材料探索の最新動向と今後の展望」

16:10 - **Hirohito Hirata** (TOYOTA)
平田 裕人（トヨタ自動車株式会社）
"Nanotechnology in automobiles : Nanomaterials in parts and units"
「自動車におけるナノテクノロジー：ナノマテリアルと部品・ユニット」

16:35-16:40【Closing Remarks / 閉会挨拶】

Shigeo Tanuma
(Chairperson of the Organizing Committee of JAPAN NANO 2020 / Director, Center for Nanotechnology Platform, National Institute for Materials Science, Japan)

田沼 繁夫（JAPAN NANO 2020 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）

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Session 5: Beyond Nano・AI / ナノテクノロジーのシステム化と産業応用

【Plenary Lecture / 基調講演】

“En Route to Realize Zero Carbon Emission”

「カーボンエミッションゼロを目指した取り組み」

Hiroshi Amano (Nagoya University, Japan)

天野 浩（名古屋大学）

EN ROUTE TO REALIZE ZERO CARBON EMISSION
カーボンエミッションゼロを目指した取り組み

Hiroshi Amano

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Abstract

The most important application of III nitrides is blue LEDs for full color displays and general lighting systems. Most of the commercially available blue LEDs are grown on foreign substrates such as sapphire, Si or SiC. In spite of high dislocation density over 10^8 cm^{-2}, wall plug efficiency (WPE) of blue LEDs exceeds 50%, which is extremely high compared with that of LEDs made by other III-V compound semiconductors such as GaAs or GaP. In case of other LEDs, WPE may be less than 1% if such a high density of dislocations exists in the crystal. One of the reasons of high-efficiency of blue LEDs based on III nitrides is short diffusion length of minority carriers in GaN and InGaN. By 2020, more than 70% of the general lighting system will be replaced from the conventional incandescent lamps or fluorescent lamps to LED lamps, by which about 7% of the total electricity consumption can be saved. In this presentation, history and future prospects of the development of the blue LEDs will be discussed.

AlGaN-based deep-UV (DUV) LEDs on sapphire substrates are effective for the efficient and long-life devices for sterilization and purification of water compared with conventional UV germicidal lamps. UNICEF reported that 844 million people still lack access to safe drinking water and 2.3 billion people do not use safe sanitation facilities. New water sterilization and purification systems have been commercialized, in which AlGaN-based high-power DUV LEDs are installed. Other applications of DUV LEDs include as a sterilizer for sanitation facilities, resins and the curing of inks in large printers, detecting forged banknotes, photolithography for manufacturing semiconductor devices, and treating skin disease, which is called dermatology.

Microwave high-electron mobility transistors (HEMT) based on AlGaN/GaN on SiC substrate works well in spite of high dislocation density over 10^8 cm^{-2} because high-density two-dimensional electron gas induced by polarization of these materials is used, therefore Fermi level in the channel layer is very high and scattering by the dislocation is small. Majority of high-power amplifier in base station of smart phone have been replaced from multichip GaAs-based HEMT to single chip GaN-based HEMT.

Breakdown field of GaN is one order of magnitude higher than that of Si. Therefore, we can reduce not only the size of the transistors, but also power loss to one tenth. If we replace all the Si based transistors such as insulated gate bipolar transistors to GaN based transistors in the invertor circuits, we can reduce 9.8% of the total electricity consumption in Japan. For power device applications, vertical structure is more feasible to operate high current. Low defect density crystal is essential for realizing low current leakage at high voltage. Therefore, requirement specification for the substrate and epitaxial layer is much higher than that of LEDs and microwave devices. In this presentation, substrate and epitaxy issues for the future power devices based on III nitrides will be discussed.

This research is supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan, through its “Program for research and development of next-generation semiconductor to realize energy-saving society.

Hiroshi Amano joined Prof. Isamu Akasaki's group in 1982 as an undergraduate student. In 1985, while working on his master courses and PhD courses, Amano developed a metalorganic vapor phase epitaxy (MOVPE) process for low-temperature deposited buffer layers for the growth of GaN single-crystal films on sapphire substrates in 1985, which led to the realization of the first III-N semiconductor based light-emitting diodes and laser diodes. In 1989, he succeeded in growing the first conductive p-type GaN using Mg doping followed by low energy electron beam irradiation treatment and in fabricating p-n-junction GaN-based UV and blue light-emitting diodes for the first time in the world. After graduation, he has continued to independently do world-leading research on the growth, characterization and device applications of III –N semiconductors. Amano has independently led his own world-class research group since 1992 and he has moved to Nagoya University where continues to lead the world in the creation of high-performance DUV LEDs, UV photodetectors and power devices.

【Special Lecture / 特別講演】

“Launching the MI platform program toward energy innovation”

「エネルギー革新に向けたMI基盤の構築」

Jinichi Igarashi (COCN(Council on Competitiveness-Nippon))
五十嵐 仁一（一般社団法人 産業競争力懇談会）

LAUNCHING THE MI PLATFORM PROGRAM TOWARD ENERGY INNOVATION
エネルギー革新に向けたMI基盤の構築

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Abstract

Materials informatics (MI) is an emerging data-driven science, which is expected as a powerful tool for materials innovation. We targeted to develop the MI system to design novel functional polymer materials for energy-related devices as a benchmark of the MI-assisted materials science. With the use of the informatics techniques and a functional materials database originally developed through the collaboration of industry and academia, we have found intriguing highly ion-conducting polymeric materials for lithium-ion batteries. Based on these activities, we plan to create the open platform for the MI-assisted materials development within Waseda University. The open platform will include high-throughput synthesis and analysis, which largely enhance materials development. Education and development of MI human resource and difficulty in acquisition and accumulation of the experimental data for MI, which are buried and lost in industry, are also discussed.

I. INTRODUCTION

Recently, materials informatics have been attracting substantial attention to discover novel materials. Artificial intelligence (AI) analyzes and extracts the important trends of the big material databases automatically. The trained AI can predict the properties of materials with even new structures. Such capability has been partially pursued to discover novel ceramics, alloys, drugs, and functional molecules.
On the other hand, polymers have been still frontiers for AI, because they have highly complicated primary- and higher-order structures. Further, the system becomes much more complex when polymers having special functionalities such as electric or ionic conductivities are composited with additives to improve their performances. These features of polymeric materials with functionalities make it extremely difficult to design experimental polymer databases. Although databases for polymer informatics are under development, PoLyInfo[1,2] of National Institute for Materials Science (NIMS) is a world-leading big database of polymers including functional polymers.

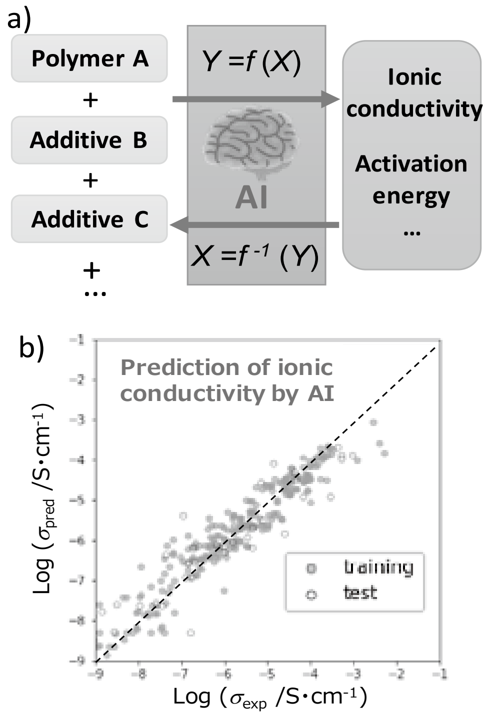

Fig. 1 MI-assisted discovery of ion-conducting polymers for lithium-ion batteries.

II. DEVELOPMENT OF MI SYSTEM FOR FUNCTIONAL MATERIALS DESIGN

A research group in Waseda University developed AI to explore new polymeric lithium-ion conductors for solid-state secondary batteries (Fig. 1).[3,4] A new database was created from data in public literatures (with >10^2 scientific articles) and contained more than 10^4 cases of the experimental ionic conductivity data. The relationships among the chemical structures and their conductivity were trained with the AI. The prediction was successful not only for homopolymers but also for copolymers and even for composite materials. AI predicted the untrained performances of the recently reported conductors accurately, which suggested the high-level predictable capability of the present MI system. Several next-generation conductors were also proposed by the AI. Some of the conductors were actually synthesized and successfully examined. Such automatic screening shortens the period of exploring new materials dramatically, which would facilitate future high throughput production of functional materials. Thus, the MI tool developed by the group in Waseda University based on a small-medium database can be a powerful tool for materials innovation.

III. CONCLUSIONS

Based on the activities described above, we are planning to create the open platform for the MI-assisted materials development within Waseda University. The open platform will include high-throughput synthesis and analysis which, along with the MI system, largely enhance materials development. Since education and development of MI human resource are urgently required, Waseda University launched the new curriculum for MI in their graduate school in last fall. We will also discuss the difficulty in acquisition and accumulation of the experimental data for MI, which are buried and lost in industry.

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[4] K. Oyaizu, et al., *Polymer Preprints, Japan*, vol. 68 (2019).

Dr. Jinichi Igarashi joined Nippon Oil Company in 1982, after he finished Graduate School of Engineering, Tokyo Institute of Technology. He is currently President of JX Nippon Research Institute. He also serves COCN as a member of Executive Committee.

Dr. Keisuke Nakayama joined Nippon Mitsubishi Oil Corporation in 1999, after he finished Graduate School of Applied Chemistry, the University of Tokyo. He is currently manager of new business Promotion group.

Kenichi Oyaizu is Professor at Waseda University. Ph.D. in 1995. Board Member of the Society of Polymer Science, Japan and the Chemical Society of Japan.

Kan Hatakeyama-Sato is Assistant professor at Waseda University. Ph.D. in 2018. Visiting Research Fellow at Texas A&M University, 2017.

Hiroyuki Nishide is Appointed Research Professor at Waseda University. Ph.D. in 1975. He is Past-President of the Federation of Asian Polymer Societies and Project Leader of COCN “MI toward Energy Innovation”.

Session 1
【Quantum Science & Biotechnology / 量子と生命科学】

“The potential of diamond solid-state quantum sensors”

「ダイヤモンド量子センサの可能性」

Mutsuko Hatano (Tokyo Institute of Technology)
波多野 睦子（東京工業大学）

“Nano- and Quantum Technology-based MR Imaging for Life Science”

「生命科学を革新するナノおよび量子技術による磁気共鳴イメージング」

Ichio Aoki (National Institutes for Quantum and Radiological Science and Technology)
青木 伊知男（量子科学技術研究開発機構）

The potential of diamond solid-state quantum sensors
ダイヤモンド量子センサの可能性

Mutsuko Hatano

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The electron systems localized at point defects in solid are stable sources of controllable spin states. Nitrogen-vacancy (NV) centers in diamond have superior physical properties at room temperature for quantum sensing of magnetic fields, electric field, strain, and temperature enabling scalable applications from atomic to macroscopic range. In this talk, we review the sensor materials, quantum control technology, and applications. The perfectly-aligned NV ensemble is well suited for sensing of biological/ medical systems and battery/ power energy electronics.

The NV center consisting of a nitrogen atom and a lattice vacancy in diamond (Fig. 1 (a)) preserves the quantum coherence even at room temperature under ambient conditions. The spin state of electrons localized at the NV center exhibits spin-1 triplet ground state (Fig. 1 (b)). The energy levels in the ground state are modulated by external magnetic field [1,2], electric field, strain, and temperature. In conjunction with spin state manipulation using microwave radiation, optically detected magnetic resonance (ODMR) can be utilized. The quantum state of the NV center can be detected by the red fluorescence difference between the quantum states m_s=0 and m_s =± 1 when excited by a green light source. The energy levels of the state m_s=± 1 split depending on the magnetic field due to the Zeeman effect, so the system is used as a highly sensitive magnetometer.

Table1 shows a comparison of the quantum magnetic sensors. The diamond sensors can operate at a wide temperature range (several mK - 700 K) and are superior in the dynamic range and the linearity to the magnetic field. The spatial resolution is scalable from nm to mm by using single to ensemble NV centers. The diamond sensors have the unique functions of the vector magnetic field imaging, as well as multi-modality such as temperature and magnetic fields. Due to the wide range of spatial resolution, the diamond quantum sensor has many potential applications, particularly well suited for sensing the magnetic field in the biological/ medical systems and battery/ power electronics (Fig. 2). Measurement set-up illustrations for magnetic field imaging of living cells are shown in Fig.3 as an example.

We will introduce the core technologies on material, devices, and sensor systems;

- Materials and devices [3-7]
  - Selectively-aligned NV ensemble formed by distinctive CVD-growth for scalable applications.
  - The heteroepitaxial growth of NV-contained diamond on Si substrate for large area and on chip integration.
  - Sensing devices by band engineering using pn junctions.
- Multi-scale and multi-modal sensor systems for biological and energy electronics applications. [8, 9]

This study was supported in part by MEXT Q-LEAP JPMXS0118067395,
and KAKENHI (17H01262 and 18H01472).

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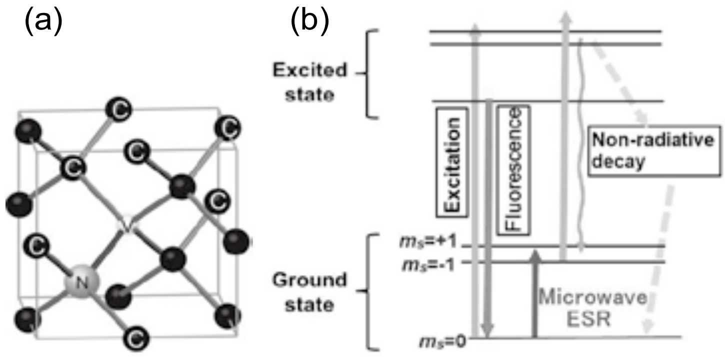

Fig. 1. Overviews of the NV center quantum system in daimond:
(a) Schematic of the NV center in diamond.
(b) Energy diagram of the NV center.
The energy levels in the grand state are modulated by external magnetic field, electric field, strain, and temperature.

Table 1 Comparison of quantum magnetic sensors.

Quantum sensor	Diamond (NV centers)	SQUID (Super-conductor)	Atomic Vapor cell
Sensitivity ($Hz^{-1/2}$)	~ pT→ fT • good Dynamic range • good Linearity	≈ fT	< fT
Spatial resolution	atomic to macro Scalability	>10μm	~ mm
Temp.	RT (mK-600K)	LT	>RT
Vector imaging	○	×	△
Temp. sensor	◎ (Temp.&Magnetic)	×	×
Miniaturization	◎ On-chip, Array, All electronics,	×	○

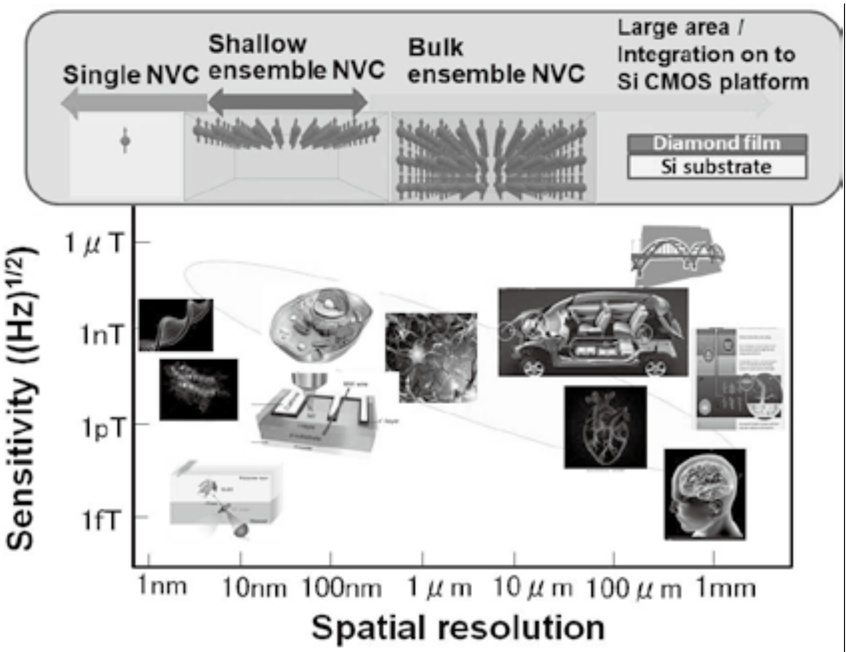

Fig.2. Potential on the scalable application of diamond quantum sensors and quantum materials by CVD technologies.

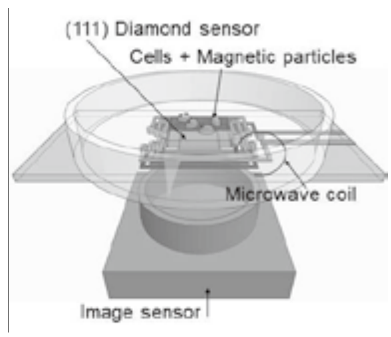

Fig.3. Potential on the scalable application of diamond quantum sensors and quantum materials by CVD technologies.

Mutsuko Hatano received the Ph.D. degree from Keio University. She joined Central Research Laboratory, Hitachi Ltd., Tokyo, Japan, and was engaged in research and development on the superconducting devices, mobile displays, and power electronics. She was a chief researcher at the CRL and the project manager of the environment electronics. She was a visiting researcher at the University of California, Berkeley from 1998 to 2000. In 2010, she joined Tokyo Institute of Technology as a professor of Electrical and Electronic Engineering. Her main research field is wide-gap semiconductor devices for power electronics and for quantum sensing. She is a member of the Science Council of Japan, a fellow and a vice president of the Japan Society of Applied Physics, and a council of Tokyo Institute of Technology.

生命科学を革新するナノおよび量子技術による磁気共鳴イメージング
Nano- and Quantum Technology-based MR Imaging for Life Science

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Abstract

ナノ粒子を使った造影剤の進歩は、MRI 診断技術に大きな発展をもたらしている。ナノ粒子をプラットフォームとした薬剤送達システム（DDS）は、治療だけでなく、生体イメージング等の画像診断のツールとして大きな貢献が期待される。MRI で可視化できるナノ粒子は、病巣内に送達される薬剤の濃度推定や、患者間の分布の差異を治療開始前に可視化できるため、臨床での治療効果の最適化のみならず、薬剤の開発段階においても重要な技術である（コンパニオン造影剤）。加えて、従来の造影剤の感度を理論値で 10 万倍まで向上させる「超偏極」という量子技術が注目されている。本講演では小動物を対象とした前臨床 MRI において、高解像度の MRI とナノ粒子造影剤の応用例を、最近の進歩と我々の取り組みを中心に紹介し、加えて、超高感度を実現する超偏極 MRI とナノ技術の組合せがもたらす将来を展望したい。

I. INTRODUCTION

MRI は磁場中にある水プロトンが電磁波と共鳴現象を生じる核磁気共鳴（NMR）を利用した生体断層イメージング法であり、基本特性として、高空間分解能（マウスで 50 µm 程度）、軟部組織の高いコントラスト、放射線を使用しない無侵襲性などに加えて、生体の形状だけでなく機能（循環、血管、脳機能、線維走行など）や代謝など多様なイメージング法が可能であること等を特徴とする。臨床においても全国で６千台以上も普及し大半の病院で稼働するなど大きな市場性があり、また小動物を対象とした前臨床装置も研究用途に使われ、小動物から臨床への接続が比較的容易なモダリティであると言える。

II. MAIN TEXT

幾つかの技術革新が、最近の MRI に大きな進歩をもたらしており、その一つがナノ粒子を使った造影剤の進歩である。ナノ粒子をプラットフォームとした薬剤送達システム（DDS）は、治療だけでなく、生体イメージング等の画像診断あるいは体外診断のツールとして大きな貢献が期待され、多様な研究成果が報告されている。ナノ粒子の MRI への応用は、①ナノ粒子を MRI 造影剤で標識し動態を観察する「コンパニオン診断」（1）、②ナノ粒子中に造影剤と薬剤の両方を包含する「セラノスティクス」（2）、③MRI 造影剤に標的性を持たせる「標的性造影剤」、④生体や病巣の環境に応答して信号を変化させる「反応性造影剤」（3,4）、⑤感度あるいは安全性を向上させる「高感度・高安全性型」などで進歩している。とりわけ、ナノ粒子による DDS を患者に応用する際、患者毎に病巣内の分布が大きく異なるなど、特有の現象が生じることが指摘されており、事前に可視化可能なナノ粒子を投与して、病巣内に送達される濃度を推定することは、臨床のみならず、開発段階においても重要な技術である。

さらに最近、量子技術の進展に注目が集まっている。量子とは「粒子と波の性質をあわせ持った物質やエネルギーの単位」のことで、原子・電子・中性子・陽子などを指す。第１次の量子革命は、1940 年代後半から始まったトランジスタや半導体に代表される技術で現在の MRI 技術もその範疇に入る。最近の進展は、第２次量子革命に繋がる技術革新として語られ、量子特有の性質である量子もつれや重ね合わせ等を利用して、これまでにない飛躍的な性能を持つコンピュータ、通信、暗号などを生み

出そうとする動きである。MRI に関連しては、従来の造影剤の感度を理論値で 10 万倍まで向上させる「超偏極（ちょうへんきょく）」という技術が注目されている。NMR や MRI では、信号に寄与する核スピンの数が磁場強度に依存しており、それゆえに高磁場の装置ほど信号雑音比が高くなる。一方、超偏極技術では対象となる化合物（例えば ^{13}C）の電子スピンを励起し、それを原子核スピンに遷すことで核スピンの大多数を励起できるため、磁場強度に非依存的で、劇的な信号上昇を可能とする。

本講演では、小動物を対象とした前臨床 MRI において、高解像度の MRI とナノ粒子造影剤の応用例を、最近の進歩と我々の取り組みを中心に紹介する（6）。併せて、次世代量子技術の一つに期待される超偏極を紹介し、ナノ技術と高感度 MRI がもたらす将来を展望したい。

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略歴：

福岡県北九州市出身。機能性MRI造影剤の研究でPhDを取得後、2000年から米国NIH/NINDSにおける機能分子イメージング研究室（Koretsky APディレクター）にて超高磁場MRIと機能性造影剤の生体適用を研究。帰国後2006年、放射線医学総合研究所・分子イメージング研究センター上席研究員、2007年よりチームリーダーを務め、高磁場MRIを用いた機能性およびナノ造影剤の研究開発および病態応用研究を進める。2016年4月より組織統合により、国立研究開発法人量子科学技術研究開発機構・放射線医学総合研究所・分子イメージング診断治療研究部・機能分子計測チームのグループリーダー、2019年から量子科学技術研究開発機構・量子生命科学領域・統括グループリーダーおよび量子制御MRI研究グループ・グループリーダーを務める。主な研究テーマは、MRIの生体・病態応用で、特にナノ粒子によるDDSイメージングと腫瘍への標的化治療（セラノスティクス）、マンガン造影MRIによる神経賦活画像法などへの応用、機能性造影剤の開発と生体適用など。

一般社団法人日本磁気共鳴医学会・理事、日本分子イメージング学会・理事・事務局長、日本DDS学会・評議員、ISMRM JPC・Chair、MRIアライアンス・Chair、PLOS ONE誌学術エディター他。

Session 2
【nanotech 2019 award lecture / nano tech 大賞2019講演】

“Prospects for Digital Print Manufacturing of Lithium-ion Batteries”

「リチウムイオン電池のデジタル印刷を目指して」

Toru Ushirogochi (Ricoh)
後河内 透（株式会社リコー）

Prospects for Digital Print Manufacturing of Lithium-ion Batteries
リチウムイオン電池のデジタル印刷を目指して

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Abstract

A new approach has been developed to produce lithium-ion batteries (LIB) using inkjet printing. Newly developed nanodispersants have been found to successfully disperse relatively large and heavy particles such as ceramics and graphite used in lithium-ion battery electrodes. Additional materials for “inkjet printable nanopore paper” have also been developed and all three major LIB components (cathode, anode, separator) can be applied to roll-to-roll LIB manufacturing using digital inkjet printing. These technologies are suitable for the production of IoT devices and wearables that require batteries of various shapes. This technology is expected to allow device designers to choose battery placement in the final design phase. Meanwhile, hybrid inkjet printing methods that integrate inkjet printing with existing electrode coating lines are also being developed. This method can be expected to improve both LIB safety and yield in lithium-ion battery manufacturing. By taking advantage of these printing technologies, the prospects for future manufacturing technologies that use digital printing methods to generate LIBs have been explained.

I. Introduction

This year is a memorable year when Dr. Yoshino et.al., who invented modern LIBs won the Nobel Prize[1)2)]. We would like to express our gratitude and congratulations as one of the researchers in this field.

This may be the result of pursuing mass production for the spread of lithium-ion batteries, but in recent years, the flexibility of lithium-ion battery manufacturing has declined. In response, several attempts[3)] have been made to enable digital printing of lithium-ion batteries, but there have been few reports of practical application. This time, the authors have developed a technology for inkjet printing of lithium-ion batteries into more free shapes using nanotechnology.

Fig. 1 Typical application of IJ printed battery.
Figure above: Postcard blinking with printed battery.
Figure below: Running an IoT wireless device with a battery printed in an R shape.

II. Developing Inkjet Printable Battery Materials

Major approaches of Inkjet Printable Battery Materials are how does it convert the high-viscosity slurries typically used in the battery die-coating to low viscosity inks. Conventional LIB cathode and anode slurries both containing several mixtures of material and polymer dispersant, so the viscosity of them are usually very high (c.f. thousand mPa.s.), and total solids amount in them is for the range of 50–60%. Therefore, new nanodispersant technologies are developed for inkjet printable battery inks. This technology was applicable to most types of electrode materials used in existing LIBs, not only acheving relatively higher concentration up to 40wt%, but also typically low viscosity as several tens of mPa.s. We have developed high printing speeds using these inks and in-house printer that are acceptable for production performance. In addition to the electrode material, we have succeeded in develop a printable separator called “ink-jet printable nanopore paper” with high lithium ion mobility. These LIB component inks can be printed using RICOH MH / GH series industrial printheads. Using these inks, heads, and prototype printer systems, a freely shaped unique LIB sample is shown in Figure 1. Inkjet printable LIB has also fined to have high output performance of 30C higher. these type LIBs are thought to be suitable for a power source in IoT devices, that usually implemented process to supply higher power for transmission, such as Bluetooth. Our goal is to supply power to a myriad of IoT edge devices equipped with batteries by flexible printer system (Fig.2).

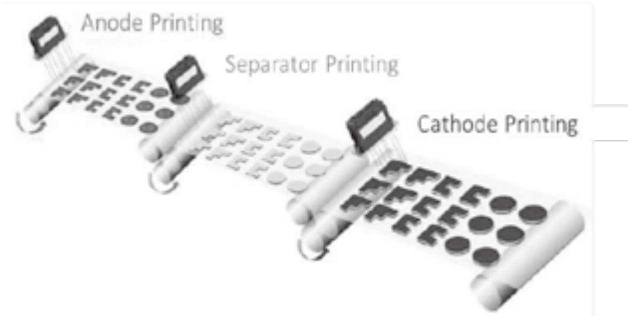

Fig. 2 Prototype Printer System (Left) and image of Flexible Printer System (Right) of LIBs.

III. Hybrid Printing System Removing the Risk of Battery

Prior to the realization of fully printed LIBs, we found that using a hybrid printing concept that combines inkjet printing with existing electrode coating systems effectively improves LIB performance. The main advantages of inkjet printing are non-contact and thin printing properties, the ability to form layers on an electrode, or arbitrarily positioned printing capabilities. Promising applications having advantage of these are the realization of ceramic and / or separator layers those are either directly coated or partially printed at the hazardous location of the electrode. This has been shown to reduce the risk of ignition in abuse tests such as the nail penetration test[4)] and the heat-resistant oven test. Similar approaches using gravure coating or small gap die coating found to have productivity disadvantages such as electrode layer damage and final electrode breakage.

On the other hand, the inspection system installed in the coating line also offers the possibility of detecting defects and fixing during manufacturing. At this time, an inkjet print can be used to wipe out these defects in the desired location. This system, which prevents defects with real-time feedback, will become a future application of inkjet battery printing that is attracting attention.

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After joined Toshiba Corp. in 1985, he worked in nanotechnology applications and served as the leader of the Functional Materials. After joining Ricoh Institute for Future Technology in 2016, He is currently working as an executive engineer in the Ricoh Innovation / R & D division. He is also engaged in the development leader of battery manufacturing technology using inkjet printing.

Session 3
【Overseas Nanotechnology User Facility Programs / 海外ナノテク共用施設・研究成果紹介】

“The National Nanotechnology Coordinated Infrastructure (NNCI) and Selected Convergent Technologies.”

「NNCIとコンバージェントテクノロジー」

Daniel J. C. Herr (Joint School of Nanoscience and Nanoengineering, USA)

THE NATIONAL NANOTECHNOLOGY COORDINATED INFRASTRUCTURE (NNCI) AND SELECTED CONVERGENT TECHNOLOGIES
NNCIとコンバージェントテクノロジー

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Abstract

In 2015, The U.S. National Science Foundation (NSF) launched the National Nanotechnology Coordinated Infrastructure (NNCI). This network of user facilities was created to provide academic, industrial and government researchers with open access to state-of-the art nanofabrication and characterization facilities, tools, instrumentation, and expertise within all disciplines of nanoscale science, engineering and technology across the U.S. Its overarching goal is to “advance research in nanoscale science, engineering and technology”.[1] The NNCI framework builds on the National Nanotechnology Infrastructure Network (NNIN), which enabled major discoveries, innovations, and contributions to education and commerce for more than 10 years. Specifically, the NNCI broadens the scope of potential users, as it supports the infrastructure needs of traditional, convergent and emerging nanotechnologies.

This five year program builds and maintains a distributed network of sixteen academic clusters across the U.S. that leverages and engages twenty-four universities, as well as an additional thirteen non-university partners. The NNCI encourages each cluster to compose, integrate and coordinate its core facilities, so-as-to offer unique sets of resources that benefit and align with the local, regional and national needs of its user base. The distribution of the lead institutions for each of the sixteen academic clusters is shown in Figure 1 below.

Fig. 1. A site map of the lead academic institutions for each of the sixteen NNCI clusters.

The NNCI also strategically supports and shares the development and integration of best practices and resources in education and outreach programs across the network. Additionally, it assesses the impact of these programs at the local, regional, and national levels. Finally, the NNCI's social and ethical implications programs enable social scientists to interact and engage with nanoscale scientists, engineers, students and the community. Such programs foster critical thinking and a common language, so that all stakeholders can proactively consider the potential impacts and unintended consequences that new discoveries might have on society. This integrated network approach effectively makes the whole more than the sum of its parts.

This presentation provides the background and justification for the creation of the National Nanotechnology Coordinated Infrastructure. It also offers an overview of the NNCIs structure, key attributes and performance metrics. Additionally, it will briefly examine selected NNCI related convergent nanotechnologies, such as the SemiSynBio Roadmap initiative[4], as well as selected recent research highlights.

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Education

Ph.D.	1984 University of California at Santa Cruz, Physical Organic Photochemistry
B.A.	1976 Wesleyan University, Middletown, CT, Chemistry (Honors)

Appointments

2019 -	Professor, Nanoscience, UNC Greensboro
2019 -	Adjunct Associate Professor, Biomedical Engineering, NC State University
2018 -	Member, Board of Directors, Berkshire Corporation
2015 -	North American Regional Editor, The Journal of Nanoparticle Research
2013 -	Director, Nanomanufacturing Innovation Consortium, NC
2011 -	Member, Advisory Board Centre for Quantum Computation and Communication
2011 - 2019	Professor and Chair, Nanoscience, UNC Greensboro
2007 -	Senior Editor, IEEE Transactions in Nanotechnology
2006 - 2016	Founding Co-Chair, ITRS ERM Working Group
2005 -	Fellow, International Society for Optical Engineering [SPIE]
2001 – 2018	Adjunct Professor, Dept. of Materials Science and Eng., NC State University
1999 – 2005	Adjunct Professor, Dept. of Electrical and Computer Eng., NC State University
1994	Chair, ITRS MBP Working Group NTRS
1992 - 2011	Science Area Director, Semiconductor Research Corporation
1989 - 1992	Group Leader, Shipley Company/Shipley Far East, Ltd./Rohm and Haas
1984 - 1988	Principal Engineer, Honeywell, Inc.
1984	Instructor, Organic Chemistry, UC Santa Cruz

Session 4
【Topics and future perspectives of nanotechnology platforms / ナノテクノロジープラットフォームの成果と将来展望】

“Biotechnology research by using a nano, micro structural analysis with electron microscope”

「電子顕微鏡による構造解析手法を用いたバイオ研究」

Yasutaka Matsuo (Hokkaido University)
松尾 保孝（北海道大学）

“R&D support by open collaboration based on shared facilities”

「共用設備を基盤としたオープンコラボレーションによる研究開発支援」

Kentaro Totsu (Tohoku University)
戸津 健太郎（東北大学）

“Research Support for the Interdisciplinary Research between Nanotechnology, Biotechnology, Quantum Technology, and AI, and Future Perspective for Nanotechnology Platform”

「ナノテクノロジーとバイオ・量子・AI融合領域の支援成果と
ナノテクノロジープラットフォームの将来展望」

Yoshinobu Baba (Nagoya University)
馬場 嘉信（名古屋大学）

Biotechnology research by using a nano, micro structural analysis with electron microscope
電子顕微鏡による構造解析手法を用いたバイオ研究

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Abstract

Hokkaido University provides support for the analysis of (1) surface structure, (2) internal/3D structure and (3) electronic state. The surface analysis equipment includes the latest X-ray photoelectron spectrometer, electron probe microanalyzer and UHV-SPM. The internal structure can be studied by several electron microscopes including the world's only ultrahigh-voltage electron microscope with two high-energy ion accelerators and laser, FIB-SEM and so on. The electronic states of nanomaterials can be measured using a time-resolved photoelectron microscope. We provide comprehensive care and total supports for advanced characterization and analysis of material surface and 3D structure. In this presentation, we will show you some supporting experimental of biotechnology fields.

I. INTRODUCTION

Various electron microscopes play a very important role in the biotechnology research field. In particular, it has a wide range of applications, from structural analysis of proteins for drug development to structural analysis of whole tissues in nanometer order. In addition, various kinds of nanoparticles are developed for cancer treatment and exploring in vivo structures, and it is also necessary to investigate the structure and dynamics in vivo of them. Here, applications of TEM and FIB-SEM will be reported, we talk about how our advanced characterization nanotechnology platform program should interact with your research in the future.

II. SUPPORT EXAMPLES FOR BIOTECHNOLOGY RESEARCH

Recent efforts to make effective and safe vaccines or drug delivery system (DDS) have focused on the development of various kinds of nanoparticles. In order to avoid antibody production, gold nanoparticles (AuNPs) are strong candidates. In fact, gold nanoparticles (AuNPs) have already been used as antigen carriers for subunit vaccines without the production of anti-AuNP antibodies. In this support case, binary mixtures of small and large GNPs modified with a glucose-terminated fluorinated OEG ligand (GFL) spontaneously self-assemble into a size-segregated yolk/shell structure in solution, in which clusters of large GNPs are covered with a monolayer of small GNPs due to entropy-driven size segregation was reported ([1]-[3]). The surface and internal structure of binary mixtures of GNPs were clarified by using two observation modes of a STEM. (Fig. 1)

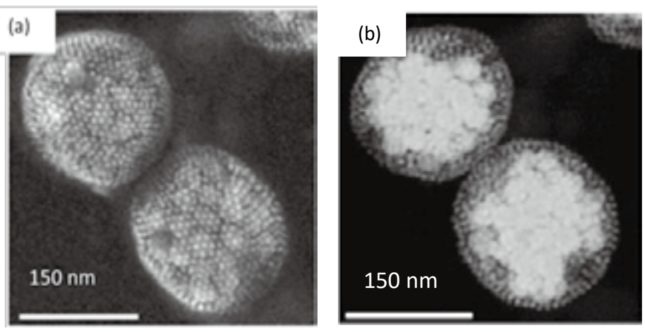

Fig. 1
(a) SE-STEM and (b) HAADF-STEM images of small and large Au NPs mixtures with a glucose-terminated fluorinated OEG ligand (GFL)

In addition, three-dimensional observation of the tissue internal structure by FIB-SEM and analysis of the tissue structure by TEM tomography were performed in our supports.

III. NEXT STEP OF ADVANCED NANO-CHARACTERIZATION SUPPORT

In biotechnology research, electron microscopes are used in various objective. Recently, it has become possible to observe chemical reaction dynamics in a solution through the development of a high-speed camera, a liquid MEMS cell holder, and it is also possible to observe the dynamics of living tissue with an electron microscope. On the other hand, in life science, optical microscopes, including super-resolution microscopes, have advanced one step further, and it has become possible to observe living individuals and brain tissue *in vivo*. It is important that there is a complementary relationship with each other, and it is thought to advance new research field through seamless the sample transfer and data interpolation and the development of new technology.

Another important issues in the microscope observation, especially in the field of biological research, are problems of how to prepare the sample, how to find the best condition of observation and how to analyze the captured image. Numerous data (sample preparation, measurement conditions) have been accumulated in the nanotechnology platform program. By processing these many support contents with AI technology, it is thought that we will be able to extract the optimal experimental conditions and the optimal measurement method. We would like to accelerate user's research in this way.

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He received B.S. and M.S of Department of Applied Physics in Osaka University. And he received Ph. D (Engineering) from Hokkaido University in 2001. After receiving his Ph. D, he started research carrier as a research fellow in RIES, Hokkaido University. In 2004, he was Postdoctoral Fellow (PD) of Japan Society for the Promotion of Science (JSPS) and assistant professor at RIES Hokkaido University. He moved to Nanotechnology Research Center of RIES as an associate professor in 2010. He was promoted to a professor at the same institute in 2018. He is now managing the Promotion Office for Nanotechnology Collaboration.
His main research is the creation of functional surface by Nanofabrication method and analysis of it.

共用設備を基盤としたオープンコラボレーションによる研究開発支援
R&D Support by Open Collaboration Based on Shared Facilities

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概要
微細加工によるデバイス開発の特徴の一つは、様々な装置、技術を用いて加工を行っていくことである。適切な材料、加工方法、装置、評価方法を選択し、進めていく必要があり、研究開発者には一連の経験も要求される。このようなリソースを自前で構築して維持することは容易ではないが、共用設備を基盤とするオープンコラボレーションにより、これらの困難を乗り越える場が提供される。オープンコラボレーションとは、共用設備、技術情報に研究開発者がアクセスし、加工結果などの情報を他と共有しながら、デバイス開発を加速させるものである。成功に近づくように、経験豊富な技術支援スタッフが全面的にサポートする。このような拠点には設備、技術が蓄積し、それらが他の開発にも活用されるポジティブフィードバックが働く。実際の経験を有し、技術の本質を知った、その先の研究開発を切り拓く人材も育成される。ここでは、東北大学での実践例を紹介した上で、今後の展開を考える。

I. 東北大学試作コインランドリでの実践
2010年から東北大学西澤潤一記念研究センター内の1,800 m^{2}の大型クリーンルームを中心として、「試作コインランドリ」と名付けた共用設備を運営している。4/6インチウェハ用を主とする試作ラインで、30年以上前の半導体製造装置と新しい装置の計120台以上が混在している。受託開発（技術代行）は行わず、利用者が直接、装置を操作する（機器利用）。各装置を初めて利用する際には、担当の技術支援スタッフ（計8名、図1）が操作説明を行うが、2回目以降は必要とされるときにオンデマンドで技術支援を行う。各装置の原理、特徴をできるだけ理解していただくことにより、さらなる応用が検討できるなど、その先の研究開発に活かされる。技術の本質を捉え、自ら考えて進められる研究開発人材の育成につながるほか、運営側としても、限られたリソースを有効活用するために適した方法と考える。設備や技術を共有することで、研究開発を加速させるオープンコラボレーションの考えで、加工結果の情報は蓄積され、他の利用者とも共有する。蓄積した経験や参考文献の情報をもとにアドバイスを行い、すべての利用者がよい成果を得られるように、利用者に寄り添った支援を心がけている[1]。経験の浅い若手人材を積極的に派遣し、育成とデバイス開発を同時に、効果的に進めている例も多い。

この8年間で320以上の機関（企業：267、大学・高専：35、公的機関：21）が利用し、2018年度は年間1万件超の装置利用（約80 %が企業の利用）、約1.8億円の利用料収入（事業費全体の約70 %をカバー）があった（図2, 3）。増加傾向が続いており、2019年度も前年度比10 %増を見込んでいる。利用企業による製品化も続いている[2,3]。

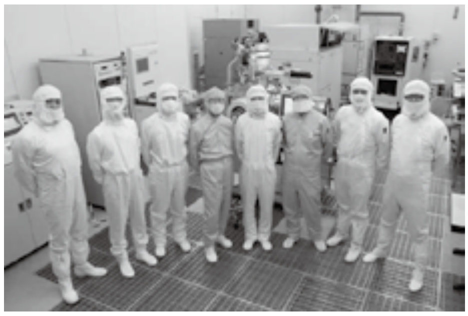

図 1.　8 名の技術支援スタッフ

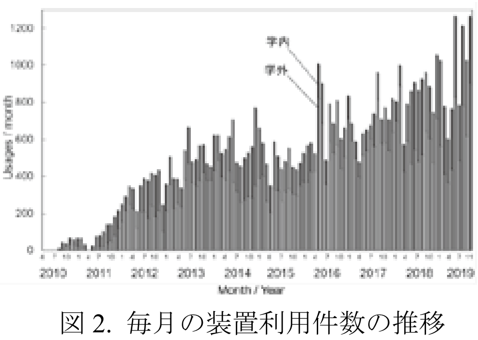

図 2. 毎月の装置利用件数の推移

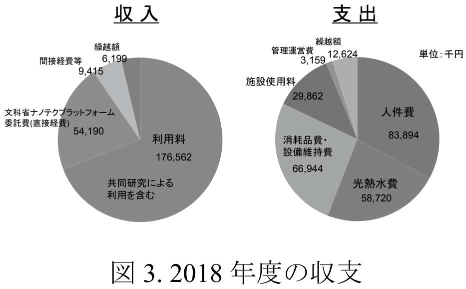

図 3. 2018 年度の収支
(事業費：約 2.6 億円)

II. 今後の展開

これまで、Si系材料を主に用いるデバイス開発支援で実績を残してきたが、最近は例えば化合物半導体やセラミックス、金属と多岐に渡る材料について微細加工の要望が増加している。今後は、微細加工を必要とする分野全般、とくに新規材料を含めた多種材料加工の支援に力をいれる。具体的には、設備の多重化により、クロスコンタミ（汚染）を気にせずに加工できるようにする。さらに、社会実装を加速させるため、デバイスコスト低減、高機能CMOSとの集積化に必須となる8インチウェハ試作にも対応できるようにするとともに、IoT用途に代表されるモジュール化のための実装技術も提供できるようにしたい。利用増に伴い混雑が目立ってきている装置があるが、設備増強と夜間休日の有効活用によるスループット向上を図りたい。人材育成も重要であり、従来と同様に機器利用と技術支援による研究開発者の育成にも取り組み、微細加工が社会のより多くの場面で活用されるようにする。今年度から市内中学生の職場体験を受け入れているが、将来活躍する科学技術人材の育成にもつながるようにしたい（図4）。委託加工の要望については、これまでどおり、地域の企業が受託する形を基本とする。人材の交流を一層活発にするなど、地域の微細加工リソースとの連携を強化し、幅広いニーズに応えられるように開発支援体制を発展させる（図5）。東北地域の公設試の技術者が、その地元の企業の開発を支援するために、付き添って利用するケースも出てきている。このように、各県の公設試とも連携して、東北地域全体の微細加工のニーズにも応えたい。

図 4.　3 日間の職場体験の中でフォトリソグラフィに取り組む仙台市内の中学生（2019 年度は 4 校から計 11 名が参加）

図 5.　地域の微細加工リソース（設備、人材、技術）が連携したナノテク研究開発支援体制のイメージ

微細加工は、材料科学、生命科学などのサイエンスをSociety5.0やSDGsの社会で使える形に実装するための重要なツールでもある。研究基盤、産業基盤として重要な「微細加工」を必要とするときに、いつでも、だれでも、実施できる開発支援環境を構築し、社会に貢献したい。

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1999年東北大学工学部機械電子工学科卒業。2004年同大学院博士課程修了。同年東北大学大学院工学研究科ナノメカニクス専攻助手。2007年東北大学産学官連携推進本部助教。2010年東北大学マイクロシステム融合研究開発センター准教授、2017年より同副センター長。これまでMEMS、微細加工に関する研究や産学連携に従事しているほか、2010年からは東北大学試作コインランドリの長として微細加工共用設備の運営を行う。試作コインランドリの取組に対して、2013年産学官連携功労者表彰経済産業大臣賞受賞。2007年から2019年まで仙台市MEMS開発ディレクター（仙台市経済局非常勤嘱託職員）として、地域のMEMS関連産業振興にも取り組んでいる。

RESEARCH SUPPORT FOR THE INTERDISCIPLINARY RESEARCH BETWEEN NANOTECHNOLOGY, BIOTECHNOLOGY, QUANTUM TECHNOLOGY, AND AI, AND FUTURE PERSPECTIVE FOR NANOTECHNOLOGY PLATFORM
ナノテクノロジーとバイオ・量子・AI 融合領域の支援成果とナノテクノロジープラットフォームの将来展望

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Nagoya University's nanotechnology platform for molecule and material synthesis has been supporting the interdisciplinary research between nanotechnology and biotechnology and more recently we are expanding to support the AI system for nanobiodevices and quantum technology for biomolecular imaging.

We have supported to develop nanofluidic devices, in which billions of nanowire structures are fabricated. This nanofluidic devices efficiently isolate billions of extracellular vesicles in a 1-mL of body fluid sample, such as blood and urine. The performance of the isolation for extracellular vesicles is much superior to those for the conventional techniques, including ultracentrifugation and isolation kits. The nanofluidic devices also enable us to detect over two thousand miRNAs, which can extract from the billions of extracellular vesicles. This efficiency is also much higher than the conventional techniques. We can isolate extracellular vesicles and detect miRNAs from over five hundred patients and normal person. Machine learning system is applicable to this big date set to diagnose brain tumor, liver cancer, lung cancer, pancreas cancer, bladder cancer, and prostate cancer.

We have supported to prepare quantum sensor based on diamond nanoparticles, which has nitrogen-vacancy center and develop the method for transfection of nanodiamond quantum sensors into the stem cells and cancer cells. These nanodiamond quantum sensors are successfully applicable to highly sensitive measurements of temperature inside stem cells and cancer cells with higher spatial resolution less than 100 nm. The information obtained by nanodiamond quantum sensors are so useful to know the functions of stem cells and cancer cells.

Nagoya University's nanotechnology platform will expanding the research support from the interdisciplinary research between nanotechnology and biotechnology to material technology, quantum technology, AI, and bio-economy in order to support not only each research topics but also the prototyping, the process science/engineering, and clinical research to accelerate interdisciplinary research and industrial-university collaborations as the open innovation platform.

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Dr. Yoshinobu Baba received PhD degree in 1986 from Kyushu University. After Assistant Professor at Oita University and Associate Professor at Kobe Pharmaceutical University, he was promoted to the full professor at The University of Tokushima in 1997. He was moved to Nagoya University in 2004. He is now a Professor of Department of Chemistry and Biotechnology, School of Engineering, a Professor of Department of Advanced Medical Science, School of Medicine, and a Director of Institute of Nano-Life-Systems, Nagoya University. He is also a Director General of Institute of Quantum Life Science, National Institutes for Quantum and Radiological Science and Technology, and a Research Supervisor, JST (Japan Science and Technology Agency) CREST "Extracellular fine particles" Project. He is a co-initiator for microTAS meeting and the world largest Nanotech International Meeting. He is a general chair of numerous international meetings (microTAS, MSB, nanotech, ISMM). He is an Associate Editor of *Anal. Chem.* of American Chemical Society and serving to over 15 scientific journals as an editorial/advisory board member. He has been admitted as a Fellow of the Royal Society of Chemistry and received over 85 awards for his contributions in nanobiotechnology: MERCK Award in 2004, The CSJ (Chemical Society of Japan) award for creative work in 2008, The Japan Society for Analytical Chemistry Award in 2015, and The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology in 2016. Dr. Baba's research studies are directed at the development of nanobiodevices for omics, systems biology, medical diagnosis, tissue engineering, and molecular imaging. He is the author or co-author of 1,022 publications, including research papers, proceedings, reviews, and books and is also an inventor of over 100 patents. He has delivered more than 1,000 plenary and invited lectures at conferences. His work has been cited on 472 occasions by newspapers and television.

Session 5
【Beyond Nano･AI / ナノテクノロジーのシステム化と産業応用】

“Materials Discovery Using Machine Learning : Latest Trends and Future Prospects”

「機械学習を使った材料探索の最新動向と今後の展望」

Daisuke Okanohara (Preferred Networks)
岡野原 大輔（株式会社Preferred Networks）

“Nanotechnology in automobiles : Nanomaterials in parts and units”

「自動車におけるナノテクノロジー：ナノマテリアルと部品・ユニット」

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平田 裕人（トヨタ自動車株式会社）

Materials Discovery Using Machine Learning: Latest Trends and Future Prospects
機械学習を使った材料探索の最新動向と今後の展望

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Abstract

Machine learning technologies, such as logistic regression, support vector machines, and random forests. have been widely used for materials discovery. In particular, deep learning has recently been applied to the challenging problems of generative design of molecules, estimation of properties of molecules, and retro-synthesis planning. In this talk, I present a basis of deep learning and the latest works of materials discovery with deep learning and also discuss the remaining problems and prospects.

Ⅰ. Deep Learning

Machine learning technologies, such as logistic regression regressions, support vector machines, and random forests, have been widely used for materials discovery. In recent years, a new machine learning paradigm, deep learning has emerged and been applied to many challenging problems in materials discovery.
Deep learning [1] is a machine learning framework that uses large neural networks. A neural network represents a complicated function by combining many simple computation units. These units are called neurons, and parameterized connections between these neurons are called synapses. The backpropagation algorithm computes the gradient of the function and updates these synapses very efficiently. Although a neural network is one of the oldest models in machine learning research, only recently, wide and deep neural networks were found to be very effective, and they are called deep learning. Deep learning can solve many challenging problems such as image recognition, speech recognition, natural language processing. Unlike a traditional neural network with three to five layers with hundreds of neurons in each layer, deep learning uses a much larger neural network with up to hundreds of layers with 0.1~1 million neurons per layer. The success of deep learning was first examined experimentally. Recent theoretical findings support these successes and show that deep learning has much more representation power, and unlike the traditional machine learning common sense, the bigger network is easier to train and generalize better. Also deep learning can now handle structured data, like graphs, and set and utilize more data found in materials discovery. Deep learning frameworks and libraries support the rapid development of deep learning models.
The success of deep learning is based on more computational power, larger data, and new techniques, such as piecewise linear activation function (for example, ReLU), batch normalization, skip connections, attention modules, and accelerated optimization techniques.
The training of deep learning models requires huge computational resources, but inference is fast. In particular, when a deep learning model is used for approximating existing simulation results, it can approximate the result 100~1 million times faster than conventional simulators. This is because deep learning is very good at the interpolation problem and can learn a smooth function that can approximate simulation results well in an interesting region. Besides, deep learning fits well for parallel computation and can benefit from recent advances of accelerator chips such as GPUs and new AI chips.
Let me give three application examples where deep learning is effective for materials discovery.

Ⅱ. Generative Design of Molecules

A generative model is a model that can generate a set of data in the target domain. It was very difficult to design generative models for high-dimensional data such as images and speeches. Now, deep learning can generate high-dimensional data very well, and generated ones are indistinguishable from real data even by

humans. Such a generative model that uses deep learning is called a deep generative model. The representative examples of deep generative models are variational autoencoder (VAE), generative adversarial network (GAN), normalizing flow, and auto-regressive models. They have different strengths and weaknesses, and users should use appropriate generative models based on their goal.
Such real-world high-dimensional data tend to lie on low-dimensional manifolds embedded within high-dimensional space, so-called manifold hypothesis. In other words, such data can be described by a small number of parameters, and users can generate data interactively by changing these parameters. Deep generative models are good at discovering such manifolds, and by changing the latent parameters, they can smoothly change the complex data.
Such deep generative models are now used for generating molecules [2]. For generating molecules, not only structures, but also their positions, need to be generated, and new techniques are introduced to generate valid structures and positions.

Ⅲ. Estimation of Energy potential and properties

Deep learning is good at classification and regression, and it can learn to estimate the property of molecules from training data in a supervised way. Recently deep learning is used for modeling the energy potential of molecules [3][4]. Although ab initio calculation of energy potential requires very high computational cost, neural network models can approximate energy potential with a fixed cost and 1 million times faster in some cases.
Using such a very fast energy potential evaluation, we can examine the properties and reactivity more quickly and exhaustively.

IV. Retrosynthetic planning

Retrosynthetic planning is a task for searching a path backward from a target molecule to simpler starting materials through a series of reactions. Since the search space is probably too large to enumerate, researchers' heuristics are critical. Recently deep reinforcement learning (reinforcement learning with deep learning models) achieved remarkable results in planning tasks such as Game of Go (e.g., AlphaGo), and these technologies are also useful for retrosynthetic planning. Such successes are achieved by better learning algorithms, exploration strategies, and a deep learning model that can learn and approximate better.

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自動車におけるナノテクノロジー：ナノマテリアルと部品・ユニット
Nanotechnology in automobiles : Nanomaterials in parts and units

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1886 年のベンツによる世界初の実用的なガソリンエンジン自動車の実用化、1908 年のフォードによる世界初の大量生産方式の自動車「モデル T」の販売開始から、110 年余り経った現在、世界中で年間 9,000 万台以上の自動車が生産され、重要な移動、物流手段の一つとなっている。

近年、自動車業界は、100 年に一度の大変革の時代に入っており、「電動化」、「自動化」、「コネクティッド」、「シェアリング」などの技術革新が急速に進んでいる。

これら技術革新のうち、ナノテクノロジーが貢献する部分が多い「電動化」に関して、当社は、1997 年にエンジンとモーター動く世界初の量産型ハイブリッド車（HV）、プリウスを発表して以来、ハイブリッド技術の改良と普及を推し進めて来た。そして、この HV 技術を様々な電動車両にも共通して利用可能なコア技術と考えている。すなわち、HV の電池容量を増やして外部充電機能を追加すれば、プラグインハイブリッド車（PHV）に、PHV から、エンジンと燃料タンクを取り除くと電気自動車（EV）に、HV のエンジンと燃料タンクを、燃料電池と水素タンクに置き換えれば、燃料電池車（FCV）になる。このように、HV の要素技術は、各種の次世代車両にも共通しており、HV で培った技術、ノウハウが迅速に応用できると考えている。このイメージを図 1 に示す。

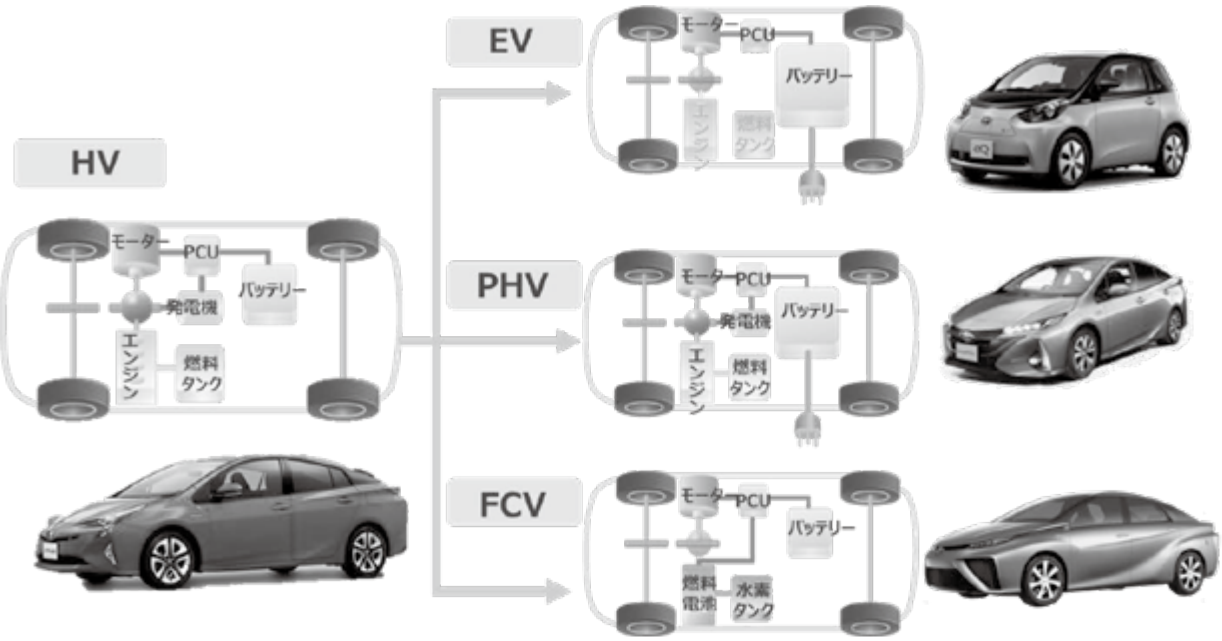

図 1　ハイブリッド技術の様々な電動車両への応用イメージ

図 2 に、電動化に必要な部品と部品を構成する材料の例を示す。トヨタでは、電動車両の性能向上に向け、ニッケル水素電池用の水素吸蔵合金、正極活物質、セパレーター、リチウムイオン電池では、活物質、電解液などの研究開発、さらにモーター用の磁石、電磁鋼板、ワイヤー、インバーターでは半導体、接着剤などの検討を行っている。FC ではそれらに加え、FC スタックに必要な触媒技術、電解質膜、カーボン、高圧タンクに使用される CFRP など研究開発に取り組んでいる。

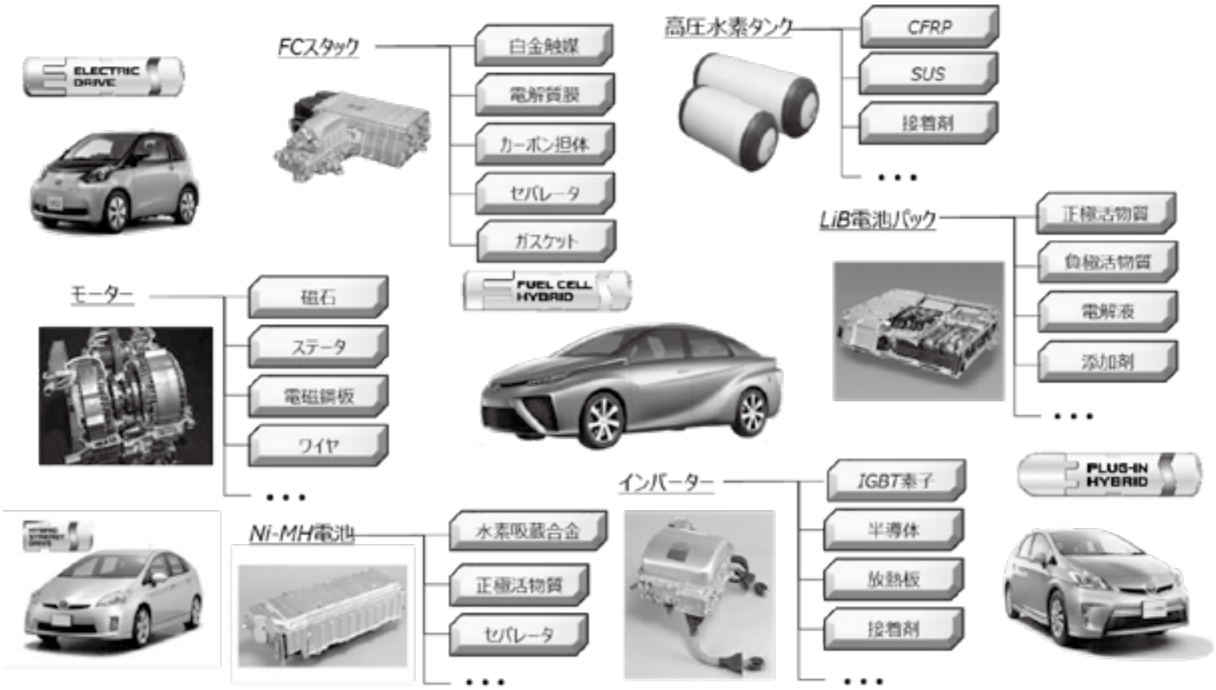

図 2 電動車両に使われているユニットと材料

ここでは、自動車におけるナノテクノロジーとして、電動化車両専用および従来型のエンジン車との共通のユニット・部品で使われる”ナノ材料そのもの”と”ナノ材料の特性を活かすための材料が部品・ユニット内部で形成する階層構造、三次元ネットワーク構造”に関する概略を紹介する。

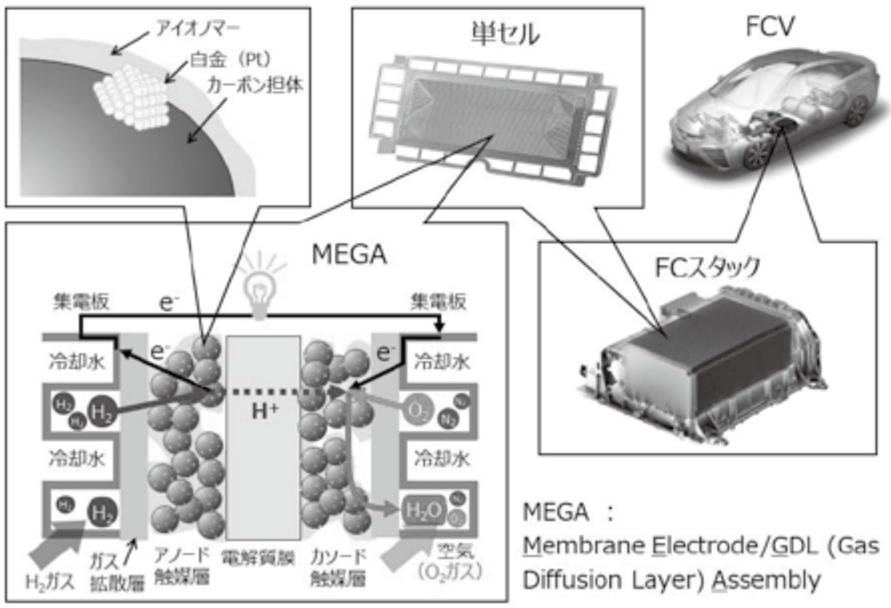

図 3　FC スタック内の階層構造

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協　賛/Cooperating Organizations

IEEE 東京支部	IEEE Tokyo Section
応用物理学会	The Japan Society of Applied Physics
高分子学会	The Society of Polymer Science, Japan
電気学会	The Institute of Electrical Engineers of Japan
電子情報通信学会	The Institute of Electronics, Information and Communication Engineers
ナノ学会	The Society of Nano Science and Technology
ナノテクノロジービジネス推進協議会	Nanotechnology Business Creation Initiative
日本ＭＲＳ	The Materials Research Society of Japan
日本化学会	The Chemical Society of Japan
日本金属学会	The Japan Institute of Metals and Materials
日本顕微鏡学会	The Japanese Society of Microscopy
日本再生医療学会	The Japanese Society for Regenerative Medicine
日本材料学会	The Society of Materials Science, Japan
日本人工臓器学会	Japanese Society for Artificial Organs
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ファインセラミックスセンター	Japan Fine Ceramics Center

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