Ultra-advanced Materials

Ultra-accelerated Development

Special Report

Integration of Technologies in Three Areas to Realize Development of Innovative Materials

Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development Project

New Energy and Industrial Technology Development Organization

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PICK UP NEWS

Next-generation Shinkansen test train ALFA-X (left: car No. 10, right: car No. 1), operated by East Japan Railway Company (JR East)
Photos courtesy of JR East

Performance tests conducted on flooring of next-generation Shinkansen test train ALFA-X!

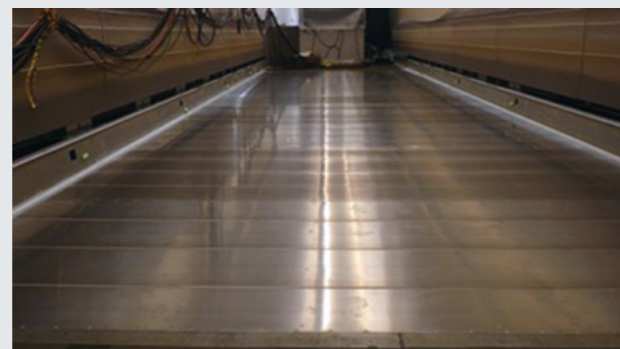## Using Flame-retardant Magnesium Alloys to Reduce Weight and Energy Consumption of Shinkansen

At present, lightweight aluminum alloys are the predominant metals used for the body and interior components of high-speed railcars such as Shinkansen. With the increasing importance of realizing higher speeds and greater levels of energy efficiency for the railways, there are growing expectations for developing even lighter railcars by using magnesium alloys, whose relative density is 30% less than that of aluminum. However, because of their relatively low levels of flame retardance, corrosion resistance, and formability, magnesium alloy wrought metals* have been used mostly in the manufacturing of small components such as electronic housing and machine parts but are rarely used for constructing large-scale structures.

Since FY2014, NEDO has been carrying out the Research and Development of Innovative Structural Materials project to improve the performance of structural materials used in manufacturing such as steel and non-ferrous metals (e.g., aluminum and magnesium). The project's primary aim is to reduce the weight of transportation-related vehicles such as automobiles and railcars, which consume considerable amounts of energy and emit CO_2 gas. NEDO has been working with the Innovative Structural Materials Association (ISMA) to develop flame-retardant magnesium alloys for use in high-speed railcars. Flooring for Shinkansen made from flame-retardant magnesium alloys that offers both high performance and low cost was used on next-generation Shinkansen test train ALFA-X, and performance test was conducted according to actual operating conditions up until March 2022.

As a result of five performance tests related to "flammability",

"adhesive strength", "indentation load capacity", "vertical load capacity" and "noise levels", weight reduction of about 23%, or correspond to 50kg/car, was realized while maintaining high levels of sound-insulation and strength. The performance test demonstrated that large-scale structures such as train flooring can be manufactured by using flame-retardant magnesium alloys. In the future, NEDO will work toward realizing full-scale application of flame-retardant magnesium alloys on high-speed railcars and explore new products for which flame-retardant magnesium alloys might be utilized, thereby contributing to energy saving and carbon neutral through the use of lighter vehicles in the transportation.

* Refers to use of rolling, extrusion, and forging processes to form metallic materials into desired shapes.

Flame-retardant magnesium alloy flooring approximately 9m in length and 3m in width used in ALFA-X passenger compartment, one of the world's largest applications, where magnesium alloys are utilized.

Performance tests of magnesium flooring

1. Flammability test
Rating of "non-flammability" was obtained for flame-retardant magnesium alloy flooring

2. Adhesion test
Optimal conditions for surface treatments and adhesive film thickness were confirmed for assembly of magnesium alloy flooring

3. Indentation load capacity test
Loads causing penetration or denting by a high heel required for magnesium alloy flooring were equal or greater than that of conventional aluminum alloy flooring

4. Vertical load test
Sufficient strength was confirmed for passenger loads

5. Noise test
- In lab tests, sound insulation performance for underfloor noise was confirmed to be equivalent to conventional aluminum alloy flooring
- There was no increase in interior noise detected on ALFA-X compared to conventional aluminum alloy flooring

NEDO news release

https://www.nedo.go.jp/news/press/AA5_101528.html

Only available in Japanese

ALFA-X is short for Advanced Labs for Frontline Activity in rail eXperimentation

CONTENTS

Reporting on Today and Tomorrow's Energy, Environmental, and Industrial Technologies

"Focus NEDO" is the public relations magazine of the New Energy and Industry Technology Development Organization (NEDO), introducing the public to NEDO's various projects and technology development activities related to energy, environmental, and industrial technologies.

Note: To prevent the spread of COVID-19, persons appearing in photos wore facial coverings except during the time photos were taken.

A Few Words from the Editor

The Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development project featured in this issue has upended the conventional wisdom that the development of materials is a long-term proposition. The project has brought about major changes in thinking about how materials are developed, which until now has been guided by the experience and intuition of engineering experts and has produced results expected to enhance the level of materials technology in Japan. In the featured news section, we also report on demonstration testing to enable the use of flame-retardant magnesium in the flooring of next-generation Shinkansen test train ALFA-X.
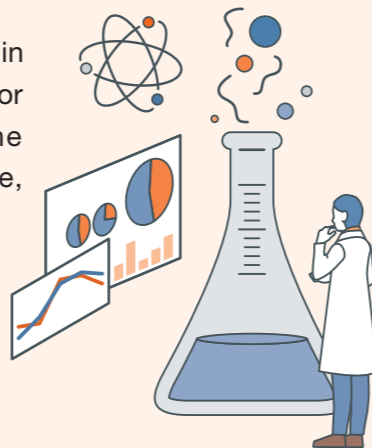
Integration of Technologies in Three Areas to Realize Development of Innovative Materials

Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development Project

To enhance the international competitiveness of the materials sector in Japan, NEDO has been pursuing the realization of core technologies for the development of innovative functional materials through the integration of technologies in three areas: computational science, manufacturing processes, and advanced measurement.

R&D methodologies for this project

Search for new materials
Reduction in development time
Reduction in amount of testing
Reduction in personnel costs

Ultra High-throughput Design and Prototyping Technology for **Ultra Advanced Material** Development Project

See p.08 — Development of highly active butadiene synthesis catalysts using high-throughput systems and data science.

See p.09 — Development of actuator materials using electric-field-responsive polymers

AI

Computational science technology development

Multiscale computing
Simulator technologies

See p.10 — R&D on using CO_2 in synthesis technology for useful chemicals

Development of functional materials

Development of manufacturing process technology

Technology that enables high-speed and flexible manufacturing processes

Development of advanced measurement technology

Technology that enables precise analysis of relationship between function and structure

Moving from traditional experience and intuition-based materials development to data-driven R&D

Japan's materials sector maintains a high share in international markets and is expected to continue playing a leading role in the global industry. On the other hand, as needs for materials have become more diverse and international competition has intensified, it has become difficult to develop innovative materials by relying solely on the conventional approach of repeated testing based on intuition and experience.

In recent years, with rapid advances in computing, R&D employing simulations and informatics has been actively conducted both in Japan and overseas. Although still in its early stages, materials informatics (MI) is attracting attention as a new method that does not depend on conventional R&D approaches. In Japan, the need to improve efficiency and accelerate materials development through computational science and data-driven R&D, as well as develop human resources in these areas, is an urgent issue.

Against this backdrop, NEDO launched the Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development project in FY2016, aiming to establish core technologies for materials development based on advanced computational science and rapidly develop functional materials in an integrated fashion.

The project's key point was establishing an integrated system that links not only computational science, but also flexible manufacturing process technology to rapidly produce diverse prototypes and advanced measurement technology to enable observation of previously invisible objects and places where material properties are manifested.
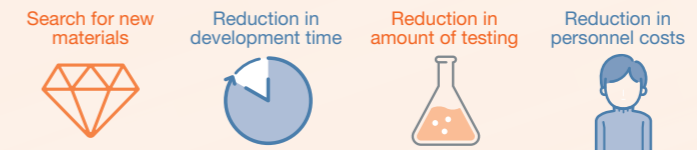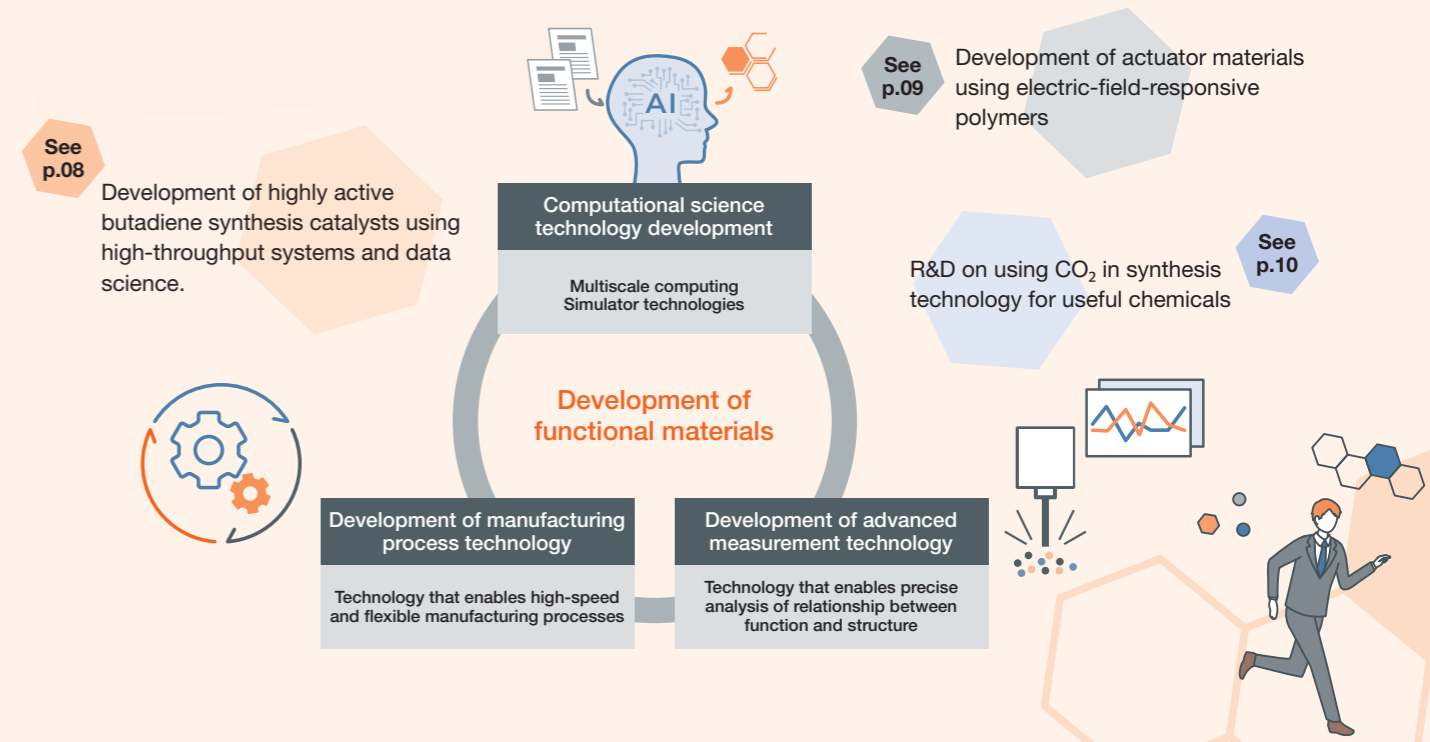
Using an inverse problem-solving approach, the project aimed to reduce the number of prototypes and development time by a factor of twenty compared with conventional materials development by having artificial intelligence (AI) learn from high-quality data generated by the integrated system and predict materials to be produced based on requirements for functions and performance.

Creating environment where ideas can be tested without concern about labor/cost constraints or risk of failure

Specifically, development of innovative material design schemes and accelerated development of functional materials has been realized by creating data sets from simulations, prototypes, and evaluations, and then integrating them utilizing MI.

Until now, researchers have been hesitant to pursue the development of new ideas because of constraints such as the high levels of labor and costs needed for developing new ideas and the risk of failure. However, if MI can be utilized and R&D outcomes become available immediately, such hurdles to developing new ideas would be greatly reduced.

At the time this project began, AI was rarely used in the development of materials, but since that time numerous studies have demonstrated AI's effectiveness, and it has now become an indispensable tool for the development of innovative materials. On the following pages, we will introduce the major outcomes of this project and feature a dialogue between Project Leader MURAYAMA Norimitsu, Senior Vice President and CTO of the National Institute of Advanced Industrial Science and Technology (AIST) and Project Manager MIYAKE Masami, formerly of the NEDO Materials Technology and Nanotechnology Department, who have been deeply involved with this project.

We hope wide range utilization of the project R&D result for growing of the material industry

MIYAKE Masami

Project Manager, Ultra
High-throughput Design and
Prototyping Technology for Ultra
Advanced Material Development
(Former) Chief Officer
NEDO Materials Technology and
Nanotechnology Department

MURAYAMA Norimitsu

Project Leader, Ultra High-throughput
Design and Prototyping Technology for Ultra
Advanced Material Development
Senior Vice President and CTO
National Institute of Advanced Industrial
Science and Technology (AIST)

PROJECT MANAGER ╳ PROJECT LEADER

Project Manager MIYAKE Masami and Project Leader MURAYAMA Norimitsu,

playing a leading role in the project from its concept creation stage

talk about the project result and its future outlook .

The common basic technology paving the way for enhancing Japanese material companies' competitiveness are now ready

Murayama: In planning this project, we interviewed a lot of company people from engineers to chief officers about what they want in order to gain and strengthen global competitiveness of their companies. We then realized that they want significant reduction of uncertain but often long period of time inevitable for new materials development, that's it. Based on this interview result, we create our project concept and plan summarizing them in an ambitious target number of 1/20 representing a reduction factor of period of time for new industrial materials development and number of trials for new prototypes compared from the present ones. Our data driven materials development scheme, which is the core achievement of this project, was checked by 18 companies joining the project and we made sure that the target number was achieved in all cases, which I am very proud of.

Miyake: Indeed, it is so amazing that the scheme is success for 19 material target examples including ones from 18 companies.

Murayama: Behind the episode that I said, I was strongly motivated that materials informatics (MI) should be introduced and developed as a novel basic common technology for materials industries. From another point of view, I also felt that we need to introduce a new idea into the framework for project management.

Miyake: You introduced getting together type of research management applied both to real life research place and IP management defined and agreed in the contract between AIST and the Research Association of High-throughput Design and Development for Advanced Functional Materials (ADMAT) to which 18 companies belong. Do you mean this?

Murayama: Sure. 'Getting together' like this scale of large amount of people: about 1 - 3 researchers from every 18 ADMAT companies and about 50 - 60 researchers from AIST, all focused for the definite research target, to my knowledge, has never been.

Introducing the model material concept activates the project

Murayama: One of the focal points in the project management was how we balance open and close nature of the foreground IP produced in the project, which is inevitable to have something to do with interests and unopen information that companies have. By virtue of building common basic technology, which this project aims, sharing all the project results would be desirable and it sounds like even more beautiful, when contributions from young expected engineers from 18 companies are to be acknowledged. On the other hand, because our target lies on the verge of industrial competitiveness, the project outcome cannot be very free from interests and unopen information from companies, which they may not want to open them up. We decided to solve this problem by introducing the concept of model materials.

Miyake: I heard that ADMAT companies spent quite a lot of time discussing how they define their contribution to the common basic technology and it's technical element setting away from their unopen information.

Murayama: To be specific, we defined five focus areas: semiconductor materials, high-performance dielectric materials, high-performance polymer materials, functional chemicals (i.e., ultra-high-performance catalysts), and nanocarbon materials (i.e., CNT and graphene) for model materials and categorized these into the five focus areas. 13 technical elements of the common basic technology including MI were developed whose performance to achieve the target reduction factor of 1/20 was checked and examined in at least one of the five focus area. In that way, research and development in our project went.

Miyake: Research progress report meetings were held once every three months. All of them were successful and nearly 100 participants joined every time.

Murayama: All the reports including those from companies were shared among the participants leading to an impressive example of 'sharing', where an MI method reported by a ADMAT member company for a model material problem were then adopted by another ADMAT company for another model material problem after the meeting, which of course was acknowledged by the company that reported.

Miyake: It is a good example of the benefit of the getting together type of research management that you introduced!

Murayama: Young engineers with strong MI and AI backgrounds joined our project from ADMAT companies. This helps us a quick start of our project creating the synergy effect example like I said from an early stage of the project. Besides the main project achievement, I believe our project provided important opportunities and seeds that should become more useful in the future of materials industries over next 20 or 30 years.

Miyake: In 2015, AIST established its Research Center for Computational Design of Advanced Functional Materials. How do you make of the impact of this on the research progress of this project?

Murayama: At that time, I was Director General of the Department of Materials and Chemistry, and was in charge of establishing the Research Center where 30 computational science experts were deployed. It was one year in prior to the date when the project starts, which was fortunate.

Take advantage of Consortium for Data-Driven Materials Design!

Miyake: NEDO made a unique decision on how it defines the key performance concept: 'putting to practical use'. The definition says utilizing the project result among companies for their industrial material developments. You may notice another appearance of the NEDO decision like the word of 'prototyping technology' in the English name of the project.
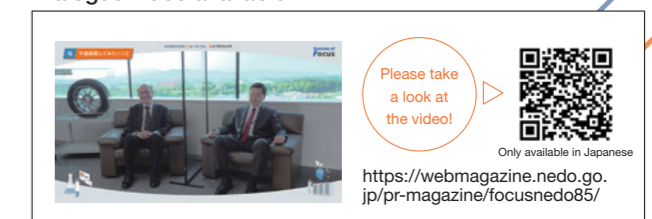
Murayama: As a major premise, we have a clear objective that the innovative MI technology has to be brought into practical use for industrial material development under the getting together type of research management with companies, which is designed on the verge of companies' competitiveness. Also, we are very clear that really strong competitiveness leading us to win originates back to the most fundamental science, which cannot be disregarded.

Miyake: AIST established Consortium for Data-Driven Materials Design for this purpose.

Murayama: Not limited to materials data mining scheme, we bring data creation scheme into the consortium like high-throughput synthesis and high-speed-prototyping facilities combined with nanoscale measurement facilities. The consortium can be a gateway for data-driven development of materials intended for commercial applications and also it can be a community for exchanging common basic technology information of data-driven materials design.

Miyake: I have heard that some project member researchers made joint research proposals. I would like to expect more to come: more companies utilize the common basic technology of MI established in this project for their industrial material developments, which hopefully leads to further prosperity of materials industry in this country.

Dialogue video available!

Please take a look at the video!

Only available in Japanese

https://webmagazine.nedo.go.jp/pr-magazine/focusnedo85/

01

Development of highly active butadiene synthesis catalysts using high-throughput systems and data science

Dramatically Reducing Development Time for Highly Active Catalysts

Rapid development of world's most productive catalyst system which realized prototype tire made from biomass-derived butadiene rubber

Dr. SHINKE Yu

The Yokohama Rubber Co., Ltd.
Group 1 Raw Materials for Compound
Tire Materials Development Department No. 1
Research & Advanced Development Division

BluEarth-GT AE51 prototype tire made from biomass-derived butadiene rubber

Contributing to sustainable society by developing products not dependent on use of fossil resources

Under this project, AIST, ADMAT, and The Yokohama Rubber Co., Ltd. have been collaborating on the use of bioethanol in the production of butadiene rubber, one of the main raw materials for manufacturing tires. Dr. SHINKE Yu of Yokohama Rubber says, "There have been few systematic studies on this topic, and the detailed catalytic reaction mechanism has not yet been elucidated. However, it was not practical for researchers to verify complex reactions one by one during experiments."

The project successfully developed a catalytic system with the world's highest yield of butadiene by utilizing technologies in three areas: computational science to elucidate the mechanism of multi-step reactions, a highly automated high-throughput system capable of performing many experiments in a brief period of time, and catalytic informatics. As a result, the time required for the development of catalysts was reduced by a factor of 22.

Subsequently, a large catalytic reactor with about 500 times the bioethanol throughput was built that produced approximately 20 kg of butadiene. This butadiene was highly purified and used in butadiene rubber obtained by a polymerization reaction. The butadiene rubber was used to produce prototype automobile tires whose performance was confirmed to be equivalent to that of tires derived from conventional petroleum-based rubber.

Dr. Shinke recalls, "I think we were able to develop catalysts that realized target performance levels largely because we used the high-throughput system developed under the NEDO project. The healthy competition among the researchers in various fields at the AIST joint research site also helped encourage the development of catalysts."

Yokohama Rubber is also working on the development of more efficient technology under a NEDO Green Innovation Fund project that aims to commercialize bioethanol-derived butadiene rubber.

02

Development of polymer actuator materials responsive to electric fields

Enabling Rapid Development of Molecular Structure Predictions for Soft Actuator Materials

Using machine learning to identify molecular structures possessing target properties and accelerate development of soft actuator materials

Realization of multiscale simulations to accelerate development efforts

Devices that support the activities of senior citizens are attracting attention in today's graying society. Soft actuator devices, in particular, are expected to be applied in the rehabilitation and nursing care sectors because they are flexible, lightweight, and easy to wear in comparison with robotic devices. However, the development of liquid crystal elastomers (LCEs), which are promising candidates as soft actuator device materials, is time-consuming and costly.

Against this backdrop, R&D is being pursued under this project to develop basic technologies that realize multi-scale simulations capable of reproducing material deformation from the molecular to the device level. Computational technologies are also being developed to accelerate the development of LCEs.

During the project, a coarse-grained molecular model was developed to calculate LCE deformation behavior, and a database was compiled of simulation results together with experimental data from previous research. Machine learning was used to refine the necessary parameters and correlate them with the mechanical properties of the materials. This reduced by a factor of 19 the amount of time required to predict molecular structures that exhibit significant degrees of deformation (or soft elasticity) with no loss in output.

Dr. TAGASHIRA Kenji of Panasonic Holdings Corporation, who participated in this project area, recalls, "The project's success can be attributed to its joint research system that allowed researchers to work together over a period of six years. I also believe that since this is a NEDO project, we have been able to realize positive results." Another Panasonic project participant, Dr. YASUOKA Haruka notes, "We were able to create the basis for simulations to determine the molecular structure based on the device's performance requirements, which should greatly reduce the number of experiments. In the future, I hope we can apply the project results not only to actuators, but also to a variety of other commercial products."

Results of analyses using finite element method
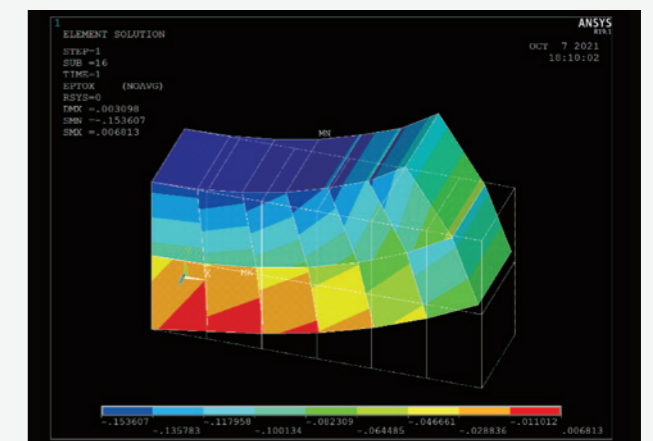
The results of finite element analyses confirm that the predicted level of deformation is attained when electric fields are applied.
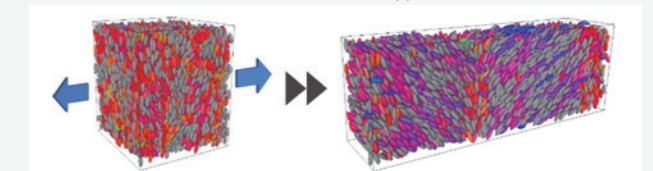
Calculation of uniaxial elongation using coarse-grained molecular dynamics

Dr. TAGASHIRA Kenji

Staff Researcher
Applied Materials Technology Center
Technology Division
Panasonic Holdings Corporation

Dr. YASUOKA Haruka

Applied Materials Technology Center
Technology Division
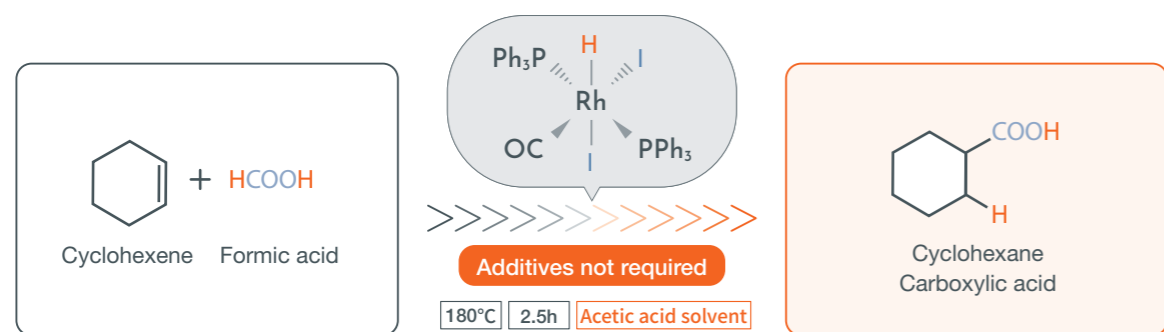Panasonic Holdings Corporation

03

R&D of synthesis technology for useful chemicals using CO_2

Development of High-performance Catalysts 20 Times Faster Than Conventional R&D Approaches

Project's tripolar approach succeeds in synthesizing carboxylic acids in an environmentally benign process without any additives.
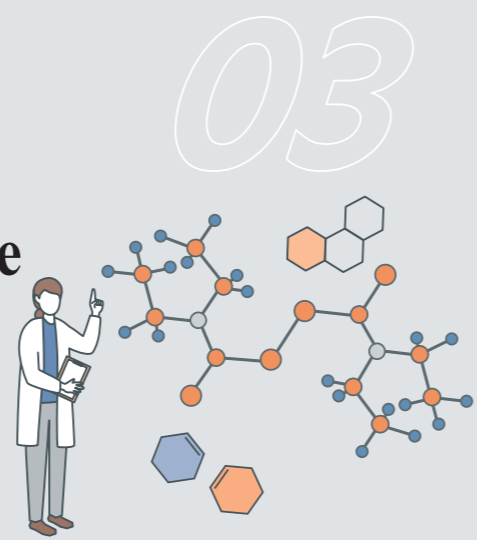
Hydroxycarbonylation of cyclohexene catalyzed by RhHI₂(CO)(PPh₃)₂ in acetic acid solvent

Cyclohexene   Formic acid

Ph₃P   H   I
Rh
OC   PPh₃

Additives not required

180°C 2.5h Acetic acid solvent

COOH
H
Cyclohexane
Carboxylic acid

Using acetic acid as solvent, carboxylic acid obtained in high yields without using additives.

Yields of nearly 80% achieved through combination of experimentation and computational science

Industrial uses of formic acid synthesized from carbon dioxide (CO_2) and hydrogen (H_2) is a research focus area relevant to the realization of a carbon-neutral society. Moreover, carboxylic acid produced from formic acid is expected to be applied as a key raw material for producing useful chemicals products such as pharmaceuticals and agrochemicals, and polymer materials such as acrylic resins and superabsorbent polymers. Until now, however, the conventional chemical reaction process has required high-pressure conditions, the use of toxic and explosive carbon monoxide gas, and large quantities of additives detrimental to the environment.

With this in mind, AIST, ADMAT, and Nippon Shokubai Co., Ltd. have collaborated under this project to develop a safer and more environmentally benign carboxylic acid synthesis technology that does not require the use of additives or toxic gases.

Work under the project focused on elucidating the reaction mechanism and identifying catalytically active species. By using a reaction path calculation technique that automatically determines the direction of chemical reactions, the reaction mechanism for synthesizing carboxylic acid from CO_2 was clarified in about six months, with a yield of nearly 80%, a higher level than expected.

Dr. OKADA Masaki of Nippon Shokubai says, "The NEDO

project's joint research system, which brings together cutting-edge engineers from the private sector, has led to a variety of research approaches and project results that could not have been achieved by one company working alone. A network of researchers in this field has also been created, which I expect will lead to further positive outcomes."

Dr. Okada believes constructing such a simple catalytic reaction system will have a significant impact. Nippon Shokubai is looking to leverage the computational science, high-throughput experimental equipment, and basic technologies developed under the project for applications to a wide variety of fields.

Dr. OKADA Masaki

Manager
Research Center
Corporate Research Division
Nippon Shokubai Co., Ltd.

Development of AI tools for organizing materials-related data

Extracting and Organizing Data on Physical Properties of Polymer Materials
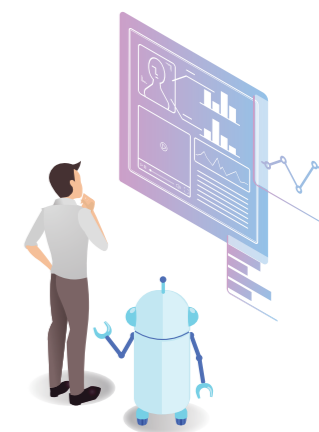
Mutual utilization of AI-organized data to accelerate development of materials and strengthen industry
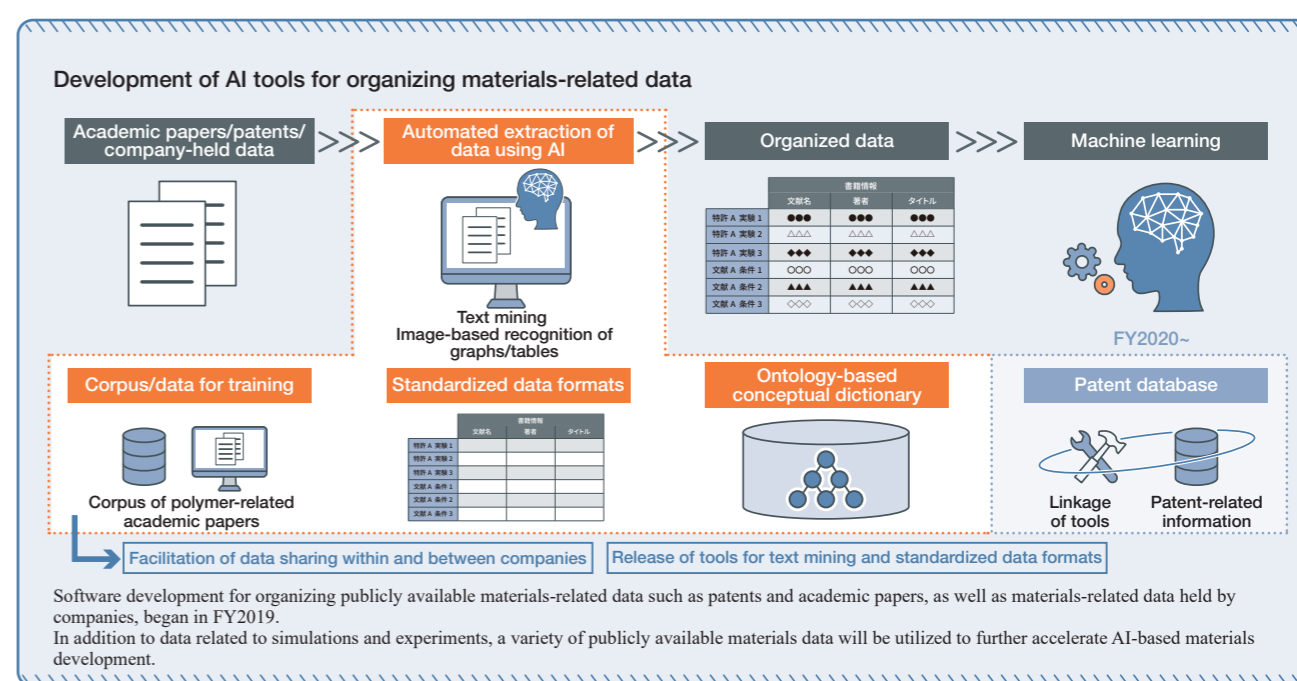
As a leader in the materials industry, Japan has accumulated a large amount of data on the development of materials. Utilizing this data as an asset is important to further strengthen the advantages enjoyed by Japan's highly competitive materials industry. To do this, it is necessary to share materials-related data held by individual institutions and companies, and to develop basic technologies that can be mutually utilized.

Since FY2019, R&D has been conducted under the NEDO project on an AI tool for organizing materials data that automatically extracts and organizes physical property information (e.g., substance names, physical property values, and their relationships) and process-related information necessary for polymer materials development contained in documents such as

patents and previously published papers/technical documents prepared by companies in the materials sector.

The project involved R&D activities related to the creation of a corpus of polymer-related academic papers for AI training, the development of AI to extract data from academic papers such as information on physical properties, the creation of a tool to scan and organize information found in the graphs and tables of PDF documents, and the design of a standardized data format and an ontology-based conceptual dictionary to organize the extracted data.

After the project's completion, NEDO will proactively release newly developed tools with the aim of establishing a management/operations system for multi-scale simulators, AI, and other basic technologies. In addition to simulation and experimental data, NEDO will make effective use of a wide variety of AI-organized data in its efforts to further accelerate the use of AI in the development of materials.

Development of AI tools for organizing materials-related data

Academic papers/patents/ company-held data >>> Automated extraction of data using AI >>> Organized data >>> Machine learning

Text mining
Image-based recognition of graphs/tables

FY2020~

Corpus/data for training   Standardized data formats   Ontology-based conceptual dictionary   Patent database

Corpus of polymer-related academic papers

Linkage of tools   Patent-related information

Facilitation of data sharing within and between companies   Release of tools for text mining and standardized data formats

Software development for organizing publicly available materials-related data such as patents and academic papers, as well as materials-related data held by companies, began in FY2019.
In addition to data related to simulations and experiments, a variety of publicly available materials data will be utilized to further accelerate AI-based materials development.

Materials design platform

AIST Materials Gate data platform

Development of easy-to-use objective-based database platforms
Data security top priority
Analysis tools for data visualization/extraction of useful information

Features of analysis tools

Extraction of features from training data
Development of prediction models for unknown materials
Inverse predictions using prediction models
Adaptation via transfer learning of prediction models to predict other functions
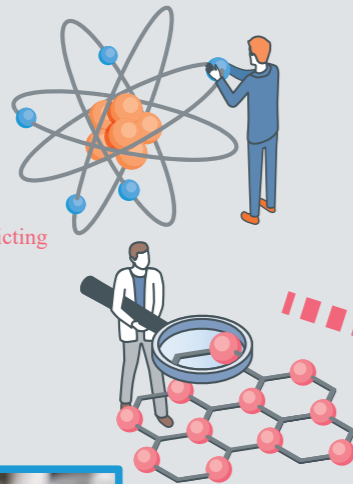
Computational Simulators

Multiscale simulations handling micro- to macro-scale
Ten kinds of simulators for predicting structure/function of materials

AI-based application technologies

Predictions using deep learning systems
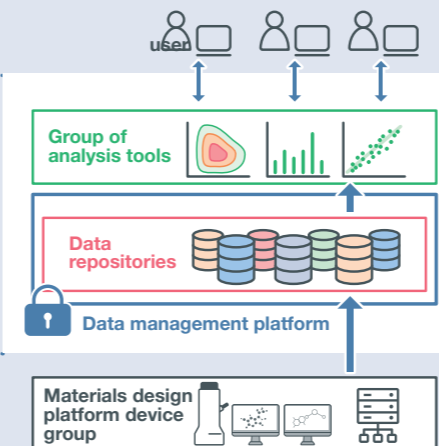Inverse problem-solving

Process-related equipment

Compatible with nanoparticle-dispersed polymers, catalysts, kneading/foaming, nanocarbons
Directly connected to various measurement instruments

Measurement instruments

Advanced instruments for multiscale analyses, in-situ measurements, and structure/function correlations.

Types of data platforms, broken down by objective

Photo-functional fine particle data platform
Light-dimming materials, inks, photosensitive materials

Wiring/semiconductor materials data platform
Wire materials, flexible devices, memory

Electronic component materials data platform
Flexible circuit board materials and capacitors

Functional polymers data platform
Rubber materials, heat dissipation/insulation materials, actuators

Catalysts data platform
Fuel cell materials, biomass-based compounds

user

Group of analysis tools

Data repositories

Data management platform

Materials design platform device group

Consortium for Data-driven Materials Design

Sharing Project Outcomes and Latest Information to Accelerate Development of Innovative Materials

Materials design platform

By creating on-demand data tailored to user needs from calculation simulators, process equipment groups, and measurement equipment groups, and linking it with AI utilization technology via the data platform, optimal solutions can be provided in the shortest amount of time.

AIST Materials Gate data platform

This data platform system consists of data repositories for generating and storing large quantities of data, a data management infrastructure for ensuring data security, and a group of tools for analyzing data. The system includes five data platforms broken down by type of material/objective: photo-functional fine particles, wiring/semiconductor materials, electronic component materials, functional polymers, and catalysts.

Creating environment for data-driven materials development using data platforms

The Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development project was launched in FY2016 and has been carried out over the past six years. With the aim of promoting the effective use and practical application of project results, NEDO and AIST established the Consortium for Data-driven Materials Design in April 2022.

The consortium has established a materials design platform that integrates the basic technologies developed in the project, including computational simulators, process-related equipment, AI-based application technologies, and measurement instruments. Consortium members can use the AIST Materials Gate data platform to share simulators and research data accumulated during the course of the project. The consortium plans to organize seminars and technical exchange meetings on data-driven materials design where up-to-date information will be shared regarding

data-driven materials development. In addition, the consortium is facilitating the provision of consulting services on individual technical issues and the conduct of joint research with AIST.

The Consortium provides a forum for information exchange between member companies aiming to develop data-driven materials and contributes to strengthening the competitiveness of Japan's materials industry by improving its technological capabilities and accelerating the needs-based development of data-driven materials. Expectations are high for the consortium to become a gateway for data-driven materials development.

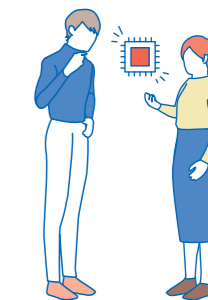Consortium for Data-driven Materials Design
(AIST website)

https://unit.aist.go.jp/cd-fmat/ja/c-dmd/index.html
Only available in Japanese

Promising NEDO Startups

Startup Support and Beyond The Future for NEDO Startups

To revitalize the economy, it is important to foster entrepreneurs that have competitive new technologies. NEDO provides startup support from a variety of perspectives to develop research and development-oriented startups and entrepreneurs. Here, we examine notable startups that are continuing to grow toward the future.

Innovator File.19

MatBrain Inc.

SHINDO Hiroyuki
CEO

Development of AI software to support data collection, organization, and knowledge creation and facilitate digital transformation in fields of chemicals and materials

https://matbrain.jp/ja/

Software for organizing materials-related literature

2019: MatBrain Inc. founded to carry out software development applying natural language and image processing technologies developed at Nara Institute of Science and Technology (NAIST).

NAIST selected to carry out R&D of AI tools to organize materials data under NEDO's Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development project.

Developed AI software to extract and organize information found in graphs and tables of academic papers.

2020: Launched sales of DeepScholar software for extracting and organizing information found in scientific and technical papers.

Q1. How have you taken advantage of NEDO's support programs?

To promote the efficient development of materials using data science, we received support for the development of AI software that extracts and organizes information on the physical properties and processes of materials found in publicly available documents such as patents and academic papers, as well as technical documents produced by companies in the materials sector. The data found in many technical documents around the world is unstructured and has therefore been difficult to fully utilize. However, in collaboration with companies in the materials sector, we have worked on the standardization of data formats and the construction of ontologies, and, by utilizing document analysis technology based on cutting-edge information science, have realized a commercial software platform to support digital transformation for the development of materials.

Q2. What is MatBrain's vision for the future?

The importance of collecting, organizing, and structuring the vast amount of data on chemicals and materials scattered around the world is increasing, for example, in data-driven materials development for a carbon-neutral society and rapid safety checks of chemical substances. In addition, if data from past experiments and technical papers held by companies can be retrieved and utilized, significant improvements can be expected in the efficiency of R&D operations. We would like to support digital transformation and materials informatics in the chemicals and materials sectors by developing software and platforms that facilitate database construction, data analysis, and data management through the use of AI and information science.

NEDO Comment

Although the Ultra High-throughput Design and Prototyping Technology for Ultra Advanced Material Development project was focused on the development of innovative materials, it was also concerned with the development of tools to enable the utilization of past R&D results. Now that its software is available on the market, we expect the company will contribute to data-driven development in the fields of chemicals and materials.

Innovator File.20

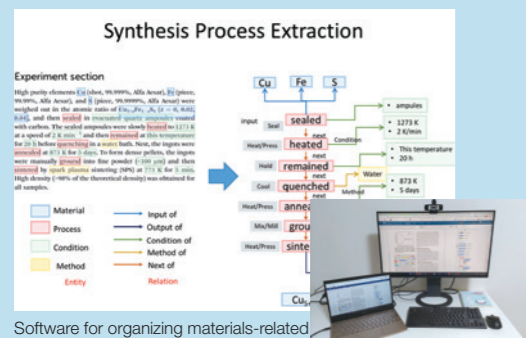### Ball Wave Inc.

AKAO Shingo
President and CEO

Development of spherical surface acoustic wave gas sensor, known as ball SAW, based on research conducted at Tohoku University and commercialization of trace moisture sensors and ultra-compact high-performance gas chromatographs

J-Startup

Japanese homepage https://www.ballwave.jp/
English homepage https://www.ballwave.jp/english/

Ball SAW trace moisture sensor and 3.3mm ball SAW element

1999: Discovery of principle leading to development of ball SAW and application for basic patent
2014: Selected under JST CREST program for "Commercialization of Compact, High-speed, High-sensitivity Trace Moisture Measurement Device Using Ball SAW Sensor"
2015: Founding of Ball Wave Inc.
2017: Release of FT-700WT high-end trace moisture analyzer
2019: Launch of full-scale sales of FT-300WT, a compact, high-speed trace moisture analyzer
Selected by JAXA Innovation Hub for "Development of Portable Gas Chromatograph Featuring High Sensitivity and Accuracy for Wide Variety of Volatile Substances"
2020: Selected for NEDO PCA Project "Ball SAW Trace Moisture Analyzer for Semiconductor Industry"
Full-scale project launched to incorporate trace moisture analyzers for advanced semiconductors
Commenced sales of Sylph palm-sized ball SAW gas chromatograph
2021: Selected for NEDO TRY Project "Development of Ball SAW Sensors to Detect Airborne Viruses in Less than One Minute"

Q1. How have you taken advantage of NEDO's support programs?

We developed and manufactured the world's first "ball SAW sensor" that applies the novel principle of surface acoustic wave propagation and have launched our first product in the Falcon Trace series, a ball SAW trace moisture analyzer. The NEDO PCA project allowed us to develop equipment for commercial-scale production of analyzers that measure impurities in gases used during the manufacturing process of next-generation semiconductors. The sensor head has now been certified as explosion-proof and is being tested at various locations.

Q2. What is Ball Wave's vision for the future?

COVID-19, the highly infectious illness that first became prevalent in early 2020, spreads when the COVID virus is exhaled by infected individuals. Currently, PCR and antigen tests are used to diagnose COVID, but these tests require considerable time and are labor-intensive. Under the NEDO TRY program, Ball Wave has started developing a sensor that employs our core SAW technology as well as bioengineering to detect airborne viruses such as COVID.

NEDO Comment

The company's ball SAW sensor technology is unique and has been steadily proven in the marketplace. We believe applications of this technology will be expanded further to help address urgent social issues.