"Materials Integration" for Revolutionary Design System of Structural Materials

Significant reduction of cost and period for structural materials development by Materials Integration (MI)

Manufacturing industries are dramatically changing because Western countries, China, and other foreign countries are intensively investing in materials development that fully uses artificial intelligence (AI). In order for Japan to maintain and develop strength in the materials development field, it is necessary to significantly reduce cost and dramatically shorten the development period. We aim to develop an MI (Materials Integration) system for the inverse design, which designs materials and processing from required performance, for the first time globally, utilizing the MI system to develop competitive and innovative highly reliable materials and establishment of design, manufacturing and evaluation technologies. And then this can be lead to commercialization of advanced structural materials/processing while setting development of materials for power generation plants and aviation as exit strategy.

**Program Director**

MISHIMA Yoshinao

President, Japan Agency for Medical Research and Development
Professor Emeritus and Former President, Tokyo Institute of Technology

Profile

1975: Master's degree in Metallurgical Engineering at Tokyo Institute of Technology (TIT); 1979: Ph.D. at U.C. Berkeley, Assistant Research Engineer; 1981: Assistant Professor at the Precision and Intelligence Laboratory (P&I), TIT; 1997: Professor, Department of Materials Science & Engineering, TIT Interdisciplinary Graduate School of Science and Engineering and Dean in 2006; 2010: Director, the Frontier Research Center; 2011: Director and Executive Vice President for Education and International Affairs, TIT; 2012-2018: President, TIT; 2019: PD, "Materials Integration" for Revolutionary Design System of Structural Materials in SIP; 2020: President, Japan Agency for Medical Research and Development. Prof. Mishima has served in several government committees, including the Council for Science and Technology of the Ministry of Education, Culture, Sports, Science and Technology and the Industrial Structure Council of the Ministry of Economy, Trade and Industry.

Research and Development Topics

In order to strengthen competitiveness, we focus on development of an MI system that accelerates materials development by connecting processing, structure, properties and performance on a computer by utilizing data science based on experiments and theoretical calculations in material engineering methods to achieve significant speedup of material development and cost reduction. The goal of social implementation shall be to accelerate materials development by effectively utilizing the MI system in the research and development of companies, universities and national institutes. Furthermore, the program aims to put into practical use and commercialize the products and technologies developed by utilizing the MI system.

Materials Integration
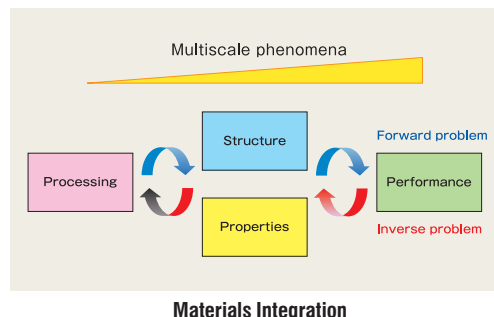
Implementation Structure

The project consists of the following three domains:

### Domain A: Inverse Design MI Basis

Aiming to establish Inverse Design MI Basis by the development of a new calculation module to apply it to the inverse design analysis technology and advanced manufacturing processing, and building a database to become the basis for the development of structural materials, and an integrated system of these.

Domain B: CFRP

The technology related to functionality/productivity improvements of carbon fiber reinforced plastic (CFRP), which is becoming popular as a lightweight structural material will be developed by utilizing the MI system. We aim to lead the world in the development of transportation equipment such as aircraft based on the results achieved.

Domain C: 3D Powder Processing

Aiming to realize innovative materials and processes utilizing the MI system for the heat-resistant alloy additive manufacturing process, which is highly competitive in development, and CMC, which is a next-generation heat-resistant material, and to put it into practical use as a material for the transportation equipment and energy industries.
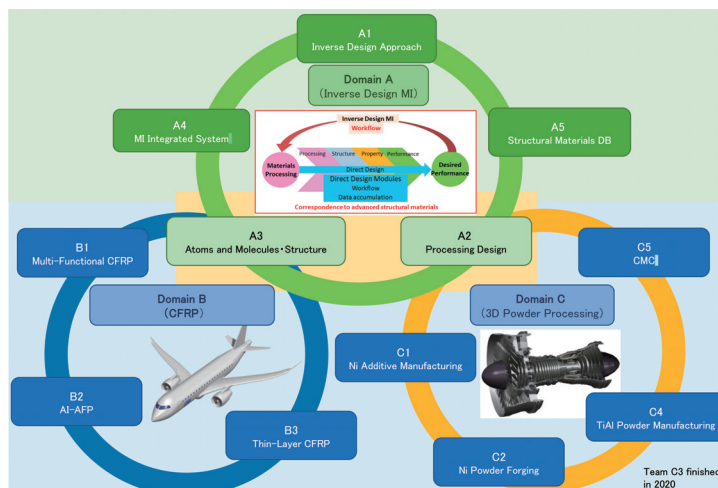

R&D Overview (Domains/Teams)

Exit Strategies

Based at the National Institute for Materials Science, we are developing MInt (Materials Integration by network technology) for general-purpose structural metallic materials. For challenges related to metallic structural materials, by creating a workflow that connects computational tools called modules based on AI and material science theory/heuristics, we can predict processing, structure, property and performance all at once. As an example, an experiment of heat treatment, observation and evaluation that normally takes half a month can be replaced half a day computational one in cyberspace. Furthermore, we can combine MInt with other kinds of optimization methods in AI in order to propose the optimal processing and chemical composition considering the desired performance. In addition, the MI consortium, an operating organization for the wide use of MInt in industry, academia and government, was established in December 2020 with the aim of promoting material innovation.

Meanwhile, for the CFRP MI system, CoSMIC (Comprehensive System for Materials Integration of CFRP) has been developed based at Tohoku University. CoSMIC can consistently handle multiple scales from atom to structural scale, and will be provided to support product development not only in the aircraft but also in other industries. We have also established a committee to promote utilization so that it would be widely used by research and development institutions that are not participating in SIP.
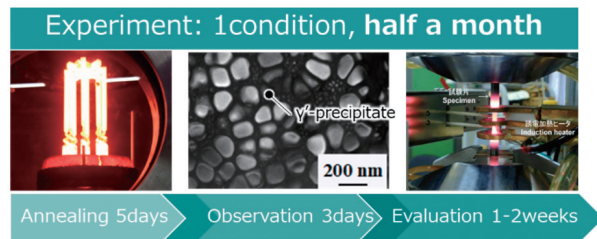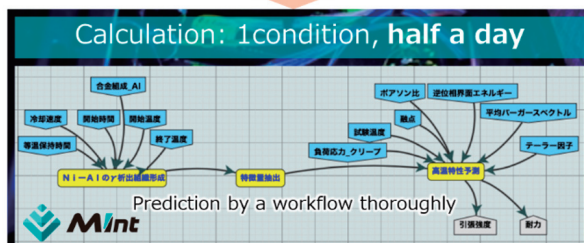

Experiment by MInt in cyber space

Past Milestones and Anticipated Outcomes

(1) Two application cases of the Inverse design MI system

　1)"Tensile strength × Elongation" for steel materials is 10-30 GPa% for high-tensile steel, and the target of the United States Department of Energy is 30 to 37.5 GPa%. By using Bayesian optimization with a target of 40 GPa%, we performed a more effective maximum value search compared to Random Search (RS).

　2) We proposed a mass production processing for high-strength/high-elongation materials that satisfy tensile strength of 750 MPa and elongation of 12%, which was not possible with the 7000 series Al alloy, and proved it through actual experimental production.
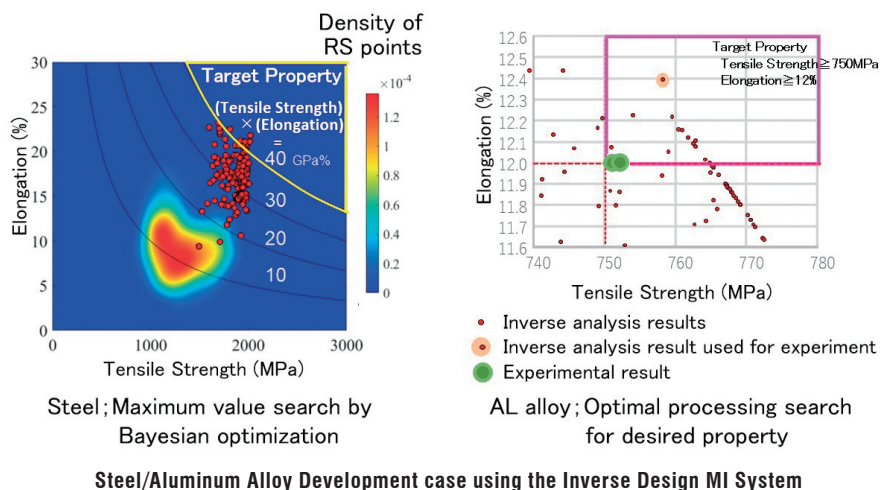
(2) Regarding CFRP, a group of modules have been developed as shown in the figure on the right, in order to carry out multiscale/multi-physics simulations for CFRP for aircraft. In parallel with that, a new system (CoSMIC) that can handle them centrally has also been built. Furthermore, large-scale high-speed calculations will be possible by integrating the supercomputer installed at Tohoku University into the system. Materials development using/utilizing CoSMIC has been advanced. For example, we succeeded in searching for the composition of resin for CFRP that has both flame retardancy and mechanical properties, and confirmed its performance by combustion tests.

Steel ; Maximum value search by Bayesian optimization

AL alloy ; Optimal processing search for desired property

- Inverse analysis results
- Inverse analysis result used for experiment
- Experimental result

Steel/Aluminum Alloy Development case using the Inverse Design MI System

CoSMIC simulation image

Cross-ministerial Strategic Innovation Promotion Program (SIP)