Cross-ministerial Strategic Innovation Promotion Program (SIP)

Research and Development Plan for "Materials Integration" for Revolutionary Design System of Structural Materials

August 22, 2019

Director-General for Science, Technology, and Innovation

Cabinet Office

Outline of the R&D Plan

1. Significance and Objectives

While Japan has been highly competitive in the field of materials, manufacturing in this field is undergoing dramatic changes as many other countries are investing heavily in the innovation of AI-driven methods of materials development. If these methods become established overseas first, Japan may be relegated to a role of materials provision and runs the risk of rapidly losing its presence in the field. In order to remain competitive with other countries, it is critical that Japan accelerates its R&D efforts through industry-academia-government collaboration.

By leveraging the groundwork of materials integration (MI) established in Japan, we will work to develop the world's first next-generation MI system capable of solving inverse problems for designing materials and processes to achieve a desired performance. Utilizing MI, we will strive to develop innovative materials that are competitive and highly reliable and to establish technologies for their design, manufacture, and evaluation with the aim of commercializing advanced structural materials and processes for producing materials used in power plants and aircraft. By utilizing a materials database storing Japan's accumulated knowledge on materials and working to augment a database for process and evaluation technologies, we will accelerate the "materials revolution" through new materials development that merges the cyber world with the physical world.

2. Content of the Research

In order to establish basic MI technologies for solving inverse problems and to demonstrate their effectiveness in the development of practical materials, we will apply MI to the development of cutting-edge structural materials and processes that are in increasingly higher demand internationally and that are one of Japan's strengths.

Domain A: Inverse Design MI
To establish a new integrated materials development system that combines materials science and engineering with data science with the goal of realizing Society 5.0. The system will be able to propose required structures and properties of materials based on a desired performance and the processes needed to achieve them. The goal is for businesses in Japan to use this system as a means of social implementation, and particularly those companies that work with advanced structural materials and processes, which will be the subject of increasingly fierce international competition.

Domain B: CFRP
To utilize an integrated materials development system to develop technologies for improving the properties and productivity of carbon fiber reinforced plastics (CFRP) that are becoming increasingly popular for use in lightweight structures. The results of these efforts will help us lead the world in the development of aircraft and other transportation equipment.

Domain C: 3D Powder Processing
To utilize an integrated materials development system to realize innovative materials and processes for 3D powder processes on heat-resistant alloys, for which competition in development is intense, and ceramic matrix composites (CMCs), which are ultra-high-temperature heat-resistant materials for next-generation transportation and energy equipment in an effort to bolster Japan's industrial competitiveness.

3. Implementation Structure

Program Director (hereinafter "PD") Yoshinao Mishima will be in charge of the establishment and promotion of the research and development plan, while Deputy Program Director (hereinafter "Deputy PD") Tetsuo Mohri will assist the PD. A Promotion Committee composed of related ministries and agencies and specialists will perform general coordination, with the PD serving as chair and the Cabinet Office as secretariat. A call for research proposals will be conducted through funding by the Japan Science and Technology Agency (JST). A Selection Committee established at the same agency will, after adequate evaluation, select the best-suited research subjects as required in the research and development plan while coordinating with the Promotion Committee, and will organize research teams comprising universities, national research and development agencies, and private companies to carry out the research tasks. The progress of each research topic will be controlled under the management of JST. Overall, the research subject shall be managed under a coherent structure in which inverse design MI is developed in Domain A while being applied to advanced structural materials and processes in Domains B and C, with the aim of demonstrating the effectiveness of inverse design MI to the industrial world in the hope that it will lead to social implementation.

4. Management of Intellectual Properties

R&D for each theme will be tackled under an intellectual property strategy emphasizing commercialization. An Intellectual Property Committee will be established under JST for the purpose of learning and managing trends in intellectual properties applied for by each contract research organization and coordinating with the contract research organizations to make their intellectual properties more adaptable to industrial use.

5. Evaluation

Prior to the Governing Board conducting each end-of-year evaluation, the PD and research bodies will conduct self-inspections. Technology readiness levels (TRLs) will be utilized to thoroughly manage the progress of research, and research tasks will be evaluated after three years, with research topics being reorganized or adjusted as needed to maintain research and development at a high level. Additionally, peer reviews are to be conducted by domestic and foreign experts while taking meticulous care to avoid information leaks.

6. Exit Strategies

(1) Use of MI systems in corporate R&D (Domain A)

The starting point of the inverse problem is set to numerical values of a target performance required by participating companies, i.e., potential users, and the effectiveness of the MI system is confirmed through solutions in cyberspace and demonstrations in physical space. We will develop a distributed computation and control technology for seamlessly linking a system operated by a centrally located MI center with calculations in a local corporate environment over the Internet. In order to use and apply company-held data, a standard data description format will be designed and widely shared (even if the actual data cannot be). These efforts are hoped to encourage the use and application of data that lies dormant in companies.

(2) Practical application and commercialization of materials developed with MI systems (Domains B and C)

Cutting-edge materials and processes for aircraft fuselages and engines and industrial power plants are envisioned as applications for MI, and practical applications and commercial products for research achievements will be found through collaboration with material and heavy industry manufacturers. While our long-term goal is to commercialize private aircraft on the global market, we will work to promote applications for our own products at an earlier stage as a form of social implementation.

1. Significance and Goals

(1) Background and circumstances at home and abroad

While Japan has been highly competitive in the field of materials, manufacturing in this field is undergoing dramatic changes as many other countries are investing heavily in the innovation of artificial intelligence (AI)-driven methods of materials development. If these methods are established overseas first, Japan may be relegated to a role of materials provision and runs the risk of rapidly losing its presence in the field. In order to remain competitive with other countries, it is critical that Japan accelerates R&D through industry-academia-government collaboration.

Europe and America are also working on methods of materials development that incorporate AI. For example, Northwestern University in the U.S. (QuesTek) and VTT Technical Research Centre of Finland Ltd are in the forefront of developing multiscale multiphysics computational techniques for designing actual materials as a consulting tool for companies in the West. However, these techniques are not sufficiently versatile for general businesses in the private sector to use and, hence, the businesses themselves cannot employ them in materials development.

Japan has worked with domestic manufacturing companies on materials integration (hereinafter "MI") in order to develop a support tool for general-purpose development that manufacturers having strength and expertise in the field of materials can use themselves according to need, and has established the world's first system for consistently predicting performance from processes. Based on this groundwork, we will develop the first MI system that supports inverse problems for designing actual materials and processes to meet a desired performance and will apply this system to actual advanced materials and processes to realize more efficient development.

Specifically, we will develop and implement an inverse design MI system to be used in industry and will utilize the system for developing advanced structural materials and processes that play to Japan's strengths. In addition to such metal-based materials as steels, aluminum alloys, and heat-resistant alloys and intermetallic compounds, examples of advanced structural materials may include ceramics, polymers, and particularly their composites, which are increasing in use as structural materials. Advanced processes may be process technologies that are currently undergoing reform in target fields, such as powder metallurgy (PM) processes focusing on additive manufacturing (AM), and injection molding of composites.

(2) Significance and strategic importance

MI must be utilized to develop advanced materials and processes capable of maximizing Japan's potential in materials science and technology and the raw materials industry, which is at a higher level internationally than in the past. Figure 1 shows the overall concept of this research subject. The aircraft industry is one example of a field that requires the highest level of qualities possessed by structural materials, including specific strength, heat-resistance, and reliability, and may have a large ripple effect on other industries in the fields of environment and energy, such as gas turbines for power generators. These days in particular, there is demand internationally to provide new added value in carbon fiber reinforced plastics (hereinafter CFRP) used to achieve lighter fuselages, such as flame-retardancy and other new features or greater freedom of design, with a focus on expanding future demand for small and medium aircraft and developing next-generation aircraft. Additionally, AM and other new powder processing technologies are expected to spread to the manufacture of intricately shaped components used in industrial power plants, for example, further expanding applications for these technologies.

Introducing MI into the development of such diverse advanced structural materials and processes will contribute further to Japan's international competitiveness in the raw materials industry by greatly reducing the time required for development and manufacturing and dramatically reducing manufacturing costs.

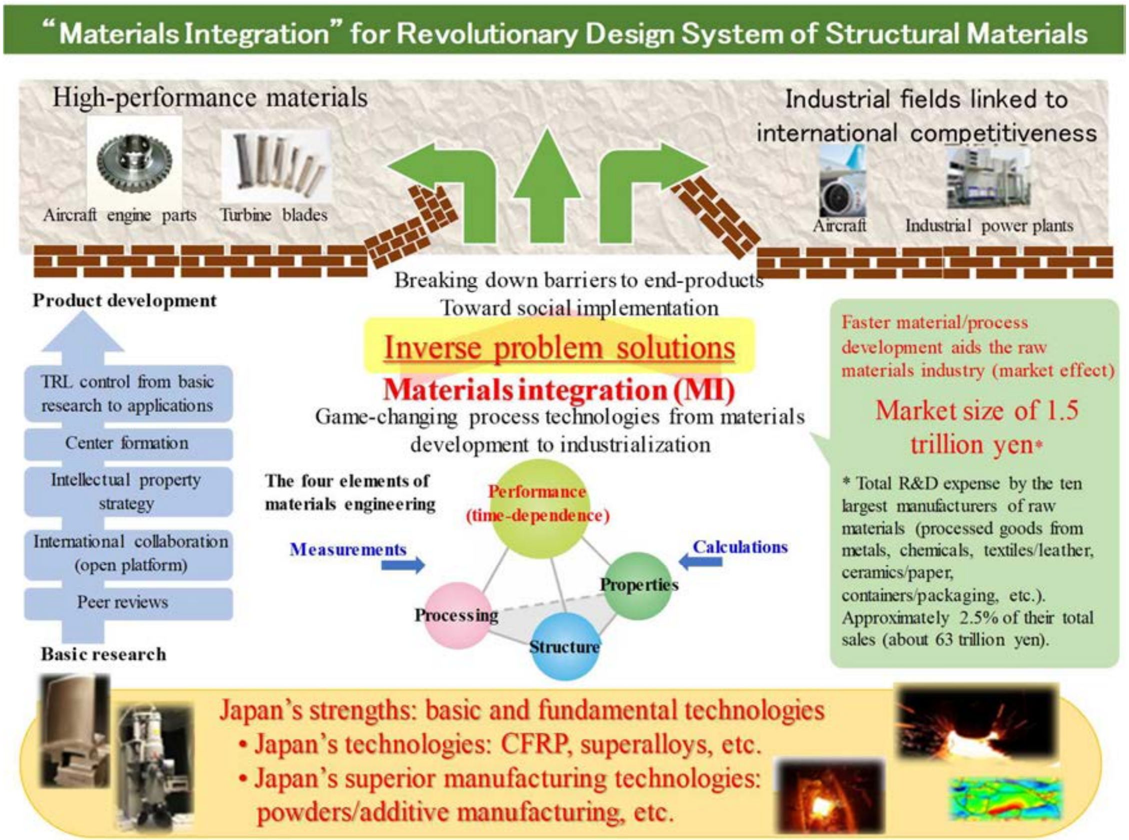


Figure 1 Overall concept of our research subject

(3) Objectives/Aims

(i) Toward realization of Society 5.0

- The "integrated materials development system" established as one of eleven systems for realizing Society 5.0 in the 5th Science and Technology Basic Plan is in fact the MI system. The achievements in MI established to date will be used to integrate materials science (physical space) with information science (cyberspace) to a high degree.
- Our aim is to develop an inverse design MI that lowers material development costs by at least 50% and the development period by at least 50% and that elicits new functions of materials. The effectiveness of the MI will be demonstrated by solving inverse problems to attain desired performance in the eleven subjects, and we will create a platform through which the MI system can be utilized broadly by private companies and research institutes.
- Inverse design MI will be utilized to develop cutting-edge processes for manufacturing composites and heat-resistant alloys with a high degree of freedom. These materials will be used in actual parts for power plants and other applications in the environment and energy industries, as well as the aircraft industry.

(ii) Social objectives

- Research centers and networks will be constructed for the development of advanced materials and molding processes utilizing MI and efforts will be made to promote international collaboration and human resources development for innovation.
- The use of high specific strength and heat-resistant materials developed through MI systems promoted to improve fuel efficiency in energy and transportation equipment and to reduce greenhouse gas emissions.

(iii) Industrial objectives

- Our aim is to establish centers available to industries for utilizing inverse design MI and to optimize materials development by dramatically reducing the development period and costs.
- We hope to expand Japan’s order share and industrial scale of aircraft parts and industrial power plants by supplying parts produced domestically using new materials and processes developed with MI.

(iv) Technical objectives

- An objective of this plan is to establish an integrated materials development system for realizing Society 5.0, which will be able to propose required structures and properties of materials based on a desired performance and present feasible processes for developing those materials.
- Technologies for improving the properties and productivity of CFRPs, which are becoming widely used as materials for lightweight structures, will be developed utilizing an integrated materials development system.
- Innovative materials and processes utilizing an integrated materials development system will be realized for powder processing of heat-resistant alloys, for which competition in development is intense, and ceramic matrix composites, which are ultra-high-temperature heat-resistant materials for next-generation transportation and energy equipment.

(v) Objectives pertaining to institutional systems

- Our aim is to establish and standardize new testing and evaluation methods using MI for materials and process development.
- We will promote an institutional system for utilization and security of a shared database platform.
- Recommendations on MI-related intellectual properties will be offered.

(vi) Global benchmarks

- It is remarkable how major countries overseas, and particularly Asian nations, have dramatically closed the gap in materials technology, which has been one of Japan’s strengths. America, Europe, and other regions have been investing heavily in AI-driven methods of materials development.
- Utilizing its massive accumulation of high-quality materials data, Japan has worked with domestic manufacturing companies to develop a support tool incorporating MI

for general-purpose development. Manufacturers with strength and expertise in materials development can use the tool as needed. With this tool, Japan has established the world's first system for consistently predicting performance from processes. Based on this groundwork, we will develop the first MI system that supports inverse problems for designing actual materials and processes to meet a desired performance and will apply this system to actual advanced materials and processes to realize more efficient development.

- We will integrate MI with Japan's strength in materials technology to develop advanced materials and processes for which Japan is known. However, to continue carrying out strategic R&D we must conduct a more detailed survey of global benchmarks in the future.

(vii) Collaboration with local government bodies

- Advanced materials development utilizing MI will be promoted in a unified national effort by assembling cutting-edge technologies from regional universities, whose strengths lie in specific technologies, and public research institutes that have amassed sophisticated technologies.
- We will publish research results in coordination with local and regional governing bodies and assist in promoting industry and developing human resources.

2. Description of R&D Activities

In order to establish basic MI technologies for solving inverse problems and to demonstrate their effectiveness in the development of practical materials, we will apply MI to the development of cutting-edge structural materials and processes that are in increasingly higher demand internationally and that are one of Japan's strengths. Program Director (hereinafter "PD") Yoshinao Mishima and Deputy Program Director (hereinafter "Deputy PD") Tetsuo Mohri will establish three domains under the direction of the PD, and specifically Domain A (Inverse Design MI), Domain B (CFRP), and Domain C (3D Powder Processing). The objectives of these domains are as follows.

Domain A: Inverse Design MI
To establish a new integrated materials development system that combines materials science and engineering with data science with the goal of realizing Society 5.0. The system will be able to propose required structures and properties of materials based on a desired performance and the processes needed to achieve them. The goal is for businesses in Japan to use this system as a means of social implementation, and particularly those companies that work with advanced structural materials and processes, which will be the subject of increasingly fierce international competition.

Domain B: CFRP
To utilize an integrated materials development system to develop technologies for improving the properties and productivity of carbon fiber reinforced plastics (CFRP) that are becoming increasingly popular for use in lightweight structures. The results of these

efforts will help us lead the world in the development of aircraft and other transportation equipment.

Domain C: 3D Powder Processing
To utilize an integrated materials development system to realize innovative materials and processes for powder processes of heat-resistant alloys, for which competition in development is intense, and ceramic matrix composites (CMCs), which are ultra-high-temperature heat-resistant materials for next-generation transportation and energy equipment in an effort to bolster Japan's industrial competitiveness.

The domains are configured of five teams in Domain A, three teams in Domain B, and five teams in Domain C (see Fig. 2). Collaboration between Domains A and B is promoted through Team A3 (Atomic (Molecular) Structure Design), and collaboration between Domains A and C is promoted through Team A2 (Process Design) (see Fig. 3). Researchers that belong to Domains B and C are also placed in these two collaboration teams to facilitate the utilization in Domains B and C of technologies developed in Domain A.

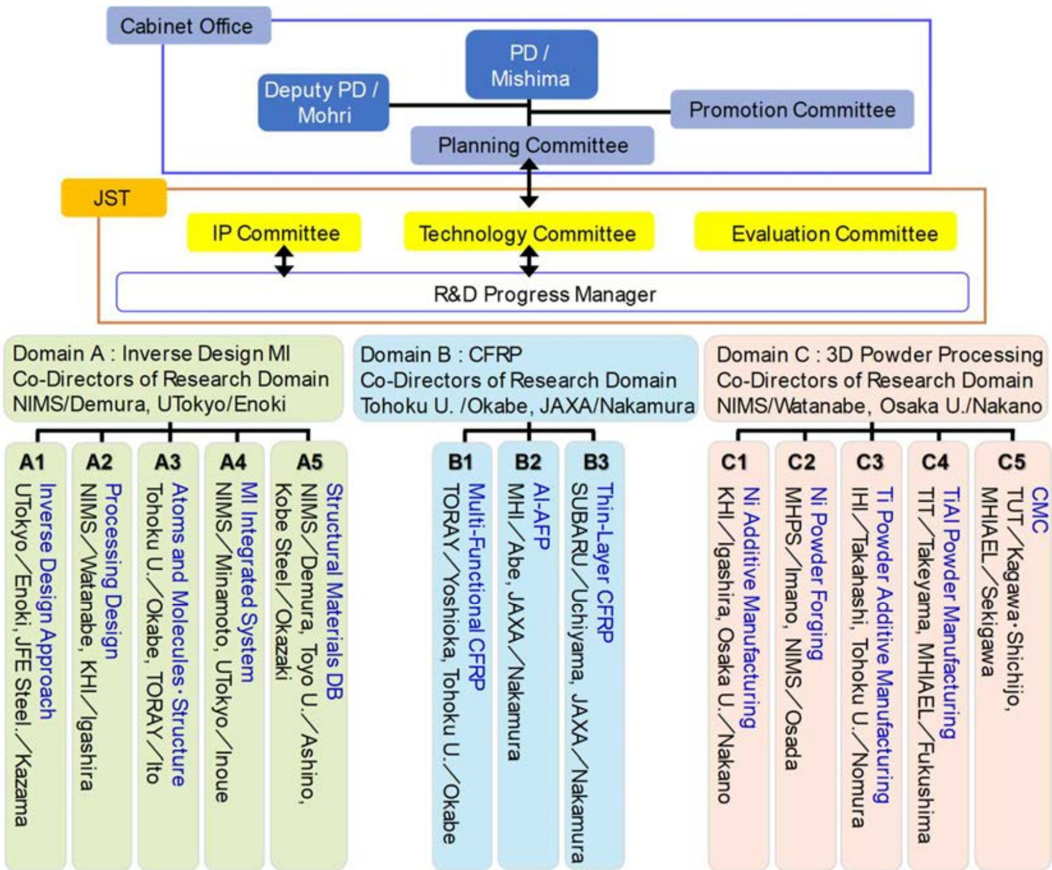


Figure 2 Organization of R&D

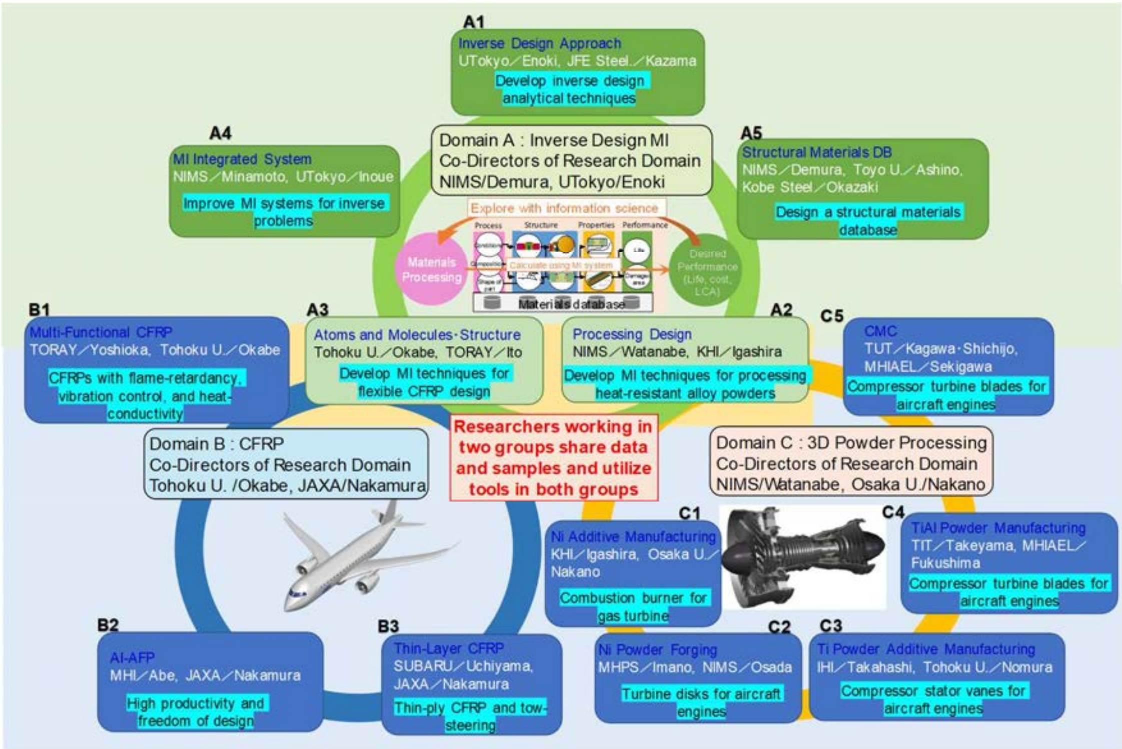


Figure 3 Overview of the R&D domains

(A) Fundamental Technological Development for Inverse Design MI

Co-directors
Masahiko Demura (National Institute for Materials Science (NIMS))
Manabu Enoki (the University of Tokyo)

Outline

Materials Integration (MI) is defined as integrated materials engineering that can lead to innovation in efficient materials development and processing. In MI, theory and empirical law of materials science are combined with experimental data and various databases by integrating computational science with data science. This enables us to implement a system for predicting in silico correlations among the structures, properties, and performances of materials. In the first phase of SIP, Structural Materials for Innovation, Japan succeeded in developing MI System ver. 1.0 using weld joints of steel materials as an exercise. This effort to realize the world's first MI system involved developing 162 modules and 101 workflows linking those modules. Thus, we are achieving success in developing calculation modules of various types and workflows that link these modules through materials engineering, as well as an integrated system to execute computational sequences according to the workflows. This system will enable us to predict performance aspects essential to structural materials, such as fatigue, creep, hydrogen embrittlement, and brittle fracture, from welding processes.

Making advances in MI and developing applications for important areas of materials are vital to the materials revolution in which new materials will lead to innovation in society. Innovative materials for supporting Society 5.0 must be developed and implemented as soon as possible, and the framework of materials development itself must be made dramatically more efficient through our approach to Society 5.0, and specifically the merging of cyberspace (MI) and physical space (manufacturing).

Globally, we are seeing accelerated investment in AI-driven materials development. There is some debate over whether AI can be used to develop materials with complex structures, and particularly whether materials developed with AI will find acceptance for use as structural materials that require long-term reliability. However, if realized, this achievement is expected to give rise to disruptive technological innovation in areas of materials wherein Japan's strength lies.

With the considerable advances being made in computer and information science, it has recently become important to incorporate computer and information science in conventional materials engineering. Japan holds a prominent place internationally in areas of materials owing to its accumulation of materials engineering knowledge, manufacturing technologies, and high-quality data. We must work to maximize these accumulations and to further expand these accumulations efficiently using computer and information science.

Taking this into account, we intend to revamp our methods of materials development by integrating materials engineering with computer and information science using the groundwork of MI developed thus far in basic MI areas. Japan will lead the world in disruptive innovation by making use of its strengths in areas of materials. Specifically, we must make advances in MI, and particularly must establish a new MI foundation addressing inverse problems for optimizing materials and processes to achieve desired performance, while bearing in mind its application in important materials areas.

This foundation for inverse design MI signifies computer programs such as MI systems and tools for solving inverse problems, hardware for executing the programs (hereinafter called an "inverse design MI system"), and a framework/structure for the use and continuous maintenance and development of these elements by companies. These systems will enable the design of optimal materials and processes in much vaster space while requiring fewer expensive experiments and trial manufacturing than conventional methods of R&D. That is, trial-and-error, conventionally performed through experiments and trial manufacturing, can be conducted efficiently and comprehensively in the inverse design MI system. As a specific method of use, the user connects to the inverse design MI system over the Internet and performs analyses for solving issues in materials development. A framework will be constructed to seamlessly connect to and utilize calculations in the user's local environment to allow for analyses that include in-house data.

Specific Approaches to Inverse Design MI

Approaches to inverse design MI differ according to the issue, but typically involve developing forward calculation techniques (modules and workflows) for predicting performance from materials and processes and attempting to optimize materials and processes efficiently in silico using these techniques. Utilizing the results of the first phase of SIP and special technologies and materials possessed by participating organizations, we will develop inverse design MI by applying design and analysis techniques for required forward problems, incorporating AI technology, and soliciting the participation of specialists in computer and information science needed to solve inverse problems efficiently. Products of this development will include modules and workflows developed and accumulated while solving various inverse problems, data science methods for analyzing inverse problems, and MI systems that integrally incorporate these products. For development to proceed efficiently, we must make advances in forward calculation techniques while simultaneously analyzing inverse problems from any point possible.

Collecting data is important for computing valid solutions with the use of AI and other technologies. Companies that establish inverse design issues possess a considerable amount of base data that can be utilized to tackle these issues. We will also conduct development based on data and expertise accumulated through many years of research at universities and national research institutes where modules are created. Experimental data needed for complementing this knowledge will be efficiently collected using such technologies as process monitoring and 3D structure analysis. This will allow us to secure enough necessary data (and expertise) to solve the established inverse problems.

The aim of Domain A is to establish an inverse design MI foundation through the combined efforts of (A-1) pioneering development in analytical techniques for inverse design, (A-2) developing new calculation modules for applying inverse problems to various advanced processes, (A-3) developing techniques for designing structures from atoms, (A-4) developing a system that integrates the aforementioned technologies to tackle inverse design, and (A-5) developing a database as a basic tool for developing structural materials.

First, for (A-1) pioneering development in analytical techniques for inverse design, R&D will be conducted on methods of analyzing inverse problems in conjunction with AI technology that target materials and processes directly utilizing calculation modules and workflows developed in the first phase. Additional studies will be conducted on efficient inverse problem analytical techniques for processes that are not always compatible with calculation modules.

Concurrently, the (A-2) team will be developing a set of calculation modules capable of supporting various processes in order to apply inverse problems to the advanced materials and processes addressed in Domain C. Utilizing the modules developed here, the team will work on streamlining development with the inverse design approach for specific application cases of advanced materials and processes while incorporating analytical techniques for inverse problems developed in (A-1).

In order to apply inverse problems at the structural level, as is addressed in Domain B, the (A-3) team will develop analytical techniques necessary for designing structures from the atomic level. The required performance for airframe and engine parts at the structural level must satisfy multiple properties. These properties are dependent on internal structures at various scales from the atomic and molecular level to the structural level. Here, an advanced technology must be developed to address multiple physical phenomena simultaneously while linking the different scales of these phenomena.

In the development of an MI integrated system for inverse problems aimed at integrating the aforementioned core technologies (A4), significant functional enhancements to the integrated system are needed; namely, the implementation of newly developed calculation modules for inverse problem techniques and advanced materials and processes that can find solutions to inverse problems.

The team must work simultaneously on improvements required for the social implementation of MI, such as enhanced user-friendliness and strengthened security.

Finally, in (A-5) the development of a structural materials database to be the foundation for developing structural materials, the team will research and develop a database structure specific to structural materials and construct a structural materials database that can efficiently accumulate experimental and computational data suitable for application to inverse problems.

The MI integrated system and structural materials database will be closely linked so that calculation tools including materials data calculation modules and workflows can be utilized organically to develop structural materials by inverse design.

These efforts are aimed at establishing a next-generation MI foundation that covers everything from metals and ceramics to polymers and composites using these materials as a matrix for the purpose of optimizing materials and processes based on the desired performance.

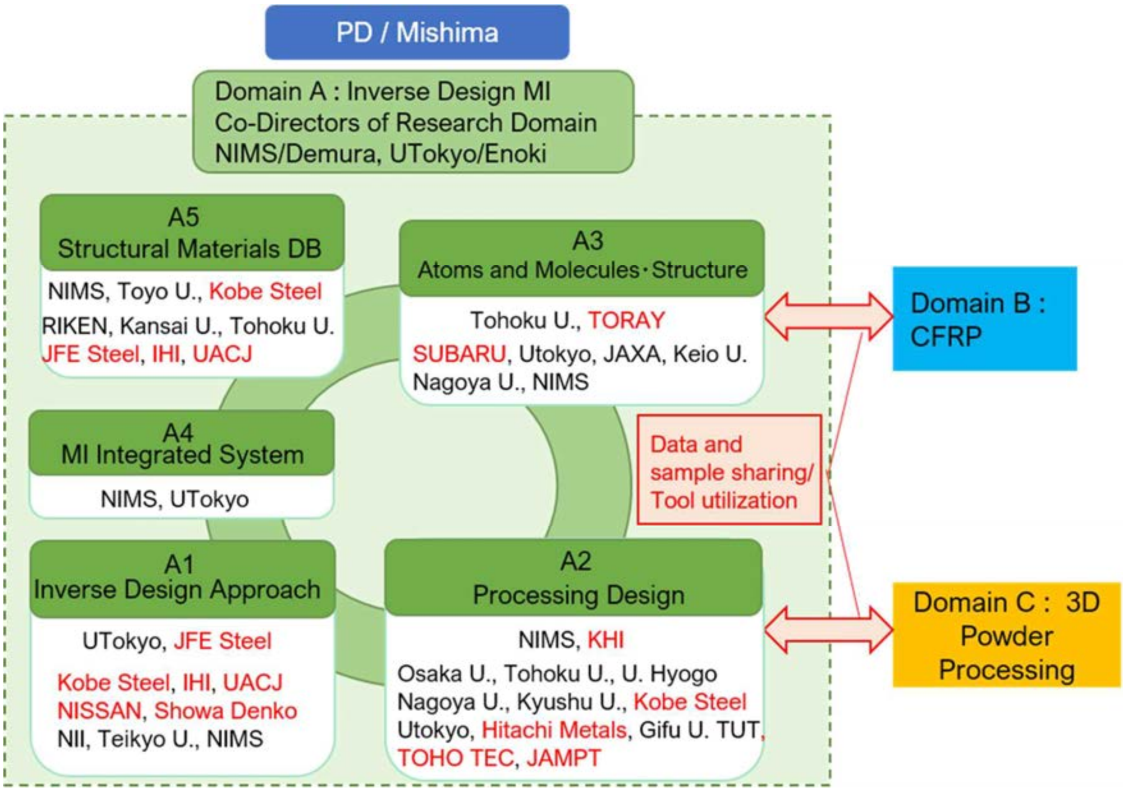


Figure 4 Domain A: research organization for an inverse design MI foundation (private companies are in red)

(A-1) Inverse Design Approach

Co-leaders:
Manabu Enoki (the University of Tokyo)
Akira Kazama (JFE Steel Corporation)

Participating organizations: the University of Tokyo; JFE Steel Corporation; Teikyo University; the National Institute of Informatics; the National Institute for Materials Science; UACJ Corporation; Kobe Steel, Ltd.; Nissan Motor Corporation; and Showa Denko K.K.

By integrating the theory, empirical law, numerical calculations, and databases accumulated in Japan thus far, we have developed a system comprising modules and databases for predicting the structure and performance of structural materials using welded joints of steel as an exercise. Since welding is a complex process involving the simultaneously occurrence of numerous phenomena that determine the structures of steel materials, including solidification, transformation, grain growth, and precipitation, the structural prediction modules cultivated in this exercise are highly versatile and can be extended to processes other than welding such as the manufacture of metal materials. Performance prediction modules targeting such performance aspects as fatigue, creep, hydrogen embrittlement, and fracture toughness were also developed for determining what time-dependent performance is exhibited by materials and structures at welded joints possessing complex microstructures in response to applied stress, temperature, and other working conditions. Developing a system for flexibly linking these calculation modules has enabled us to predict performance consistently. In addition, methods of data assimilation enable us to estimate material parameters that are difficult to measure.

However, the prediction systems developed thus far fundamentally deal with forward problems that predict performance from such processing conditions as composition and other material conditions, and processing conditions for manufacturing and use In the meantime, development has been conducted on 1.5 GPa-grade next-generation ultra-high-strength steel for use in steel materials and 750 MPa-grade high-strength materials for aluminum alloys. However, since strength has a tradeoff with environmental resistance and weldability, finding an optimal balance in performance is essential in developing materials for practical use. Consequently, to reduce the development time for materials, a new approach to optimization that links prediction modules individually developed for each aspect of performance will be needed. Further, the difficult issue of constructing a physical model for each individual process, such as a manufacturing technology for powder used in advanced AM, will require a drastic reduction in the number of R&D trials and a more efficient technique for searching processes.

Hence, we are conducting R&D on a framework (see Fig. 5) capable of finding an optimal performance balance and analyzing inverse problems. The framework will be based on the system developed thus far that primarily targets steel materials and aluminum alloys and uses forward problems for predicting performance. Our approach will effectively utilize sparse modeling and data-driven information science and data science. By applying this inverse design approach, we intend to further accelerate materials development of high-performance steels, aluminum alloys, and heat-resistant alloys that will be increasingly needed for automobiles, aircraft, and other transportation equipment.

Intermediate Goals (for the end of fiscal 2020)

Next-generation high-strength steel MI
Issues related to applying an inverse design MI approach to high-strength steels will be identified. The study will focus on martensitic structures, which are the base of high-strength steel, and will primarily use data obtained thus far on process conditions, microstructures, properties, and performance.

Next-generation high-strength Al alloy MI
Next-generation high-strength steel MI Through the use of MI, heat-treating processes will be searched in data collected to date on properties and microstructures in an attempt to find conditions necessary for producing new high-strength Al alloys.

Joining process optimization MI for high-strength steels
With a focus on welding processes that affect the fracture toughness of high-strength steels, an inverse design MI approach will be used to search processing conditions for

improving fracture toughness of high tensile steel. This MI approach will be used in addition to the performance prediction system developed thus far for fracture toughness.

Joining process optimization MI for heat-resistant steels
With a focus on welding processes that affect the creep performance of high-strength steels, an inverse design MI approach will be used to search processing conditions for improving creep performance of heat-resistant steel. This MI approach will be used in addition to the performance prediction system developed thus far for creep.

Product application MI
Utilizing MI, a database on manufacturing processes will be developed to turn expertise accumulated by companies into explicit knowledge.

End Goals (for the end of fiscal 2022)

Next-generation high-strength steel MI
A strategy for formulating guidelines will be established for new materials development applying an inverse design MI approach to high-strength steels. Development will be focused on martensitic structures, which are the base of high-strength steel, using primarily data obtained thus far on process conditions, microstructures, properties, and performance.

Next-generation high-strength Al alloy MI
Through the use of MI, a basis will be established for identifying conditions in data collected to date on properties and microstructures related to heat-treating processes for new high-strength aluminum alloys.

Joining process optimization MI for high-strength steels
With a focus on welding processes that affect the fracture toughness of high-strength steels, an inverse design MI approach will be used to find optimal processes for realizing good fracture toughness of high-tensile steels. This MI approach will be used in addition to the performance prediction system developed thus far for fracture toughness.

Joining process optimization MI for heat-resistant steels
With a focus on welding processes that affect the creep performance of high-strength steels, an inverse design MI approach will be used to find optimal processes for realizing good creep performance of heat-resistant steels. This MI approach will be used in addition to the performance prediction system developed thus far for creep.

Product application MI
Utilizing MI, a foundation for discovering new manufacturing processes will be established to turn expertise accumulated by companies into explicit knowledge.

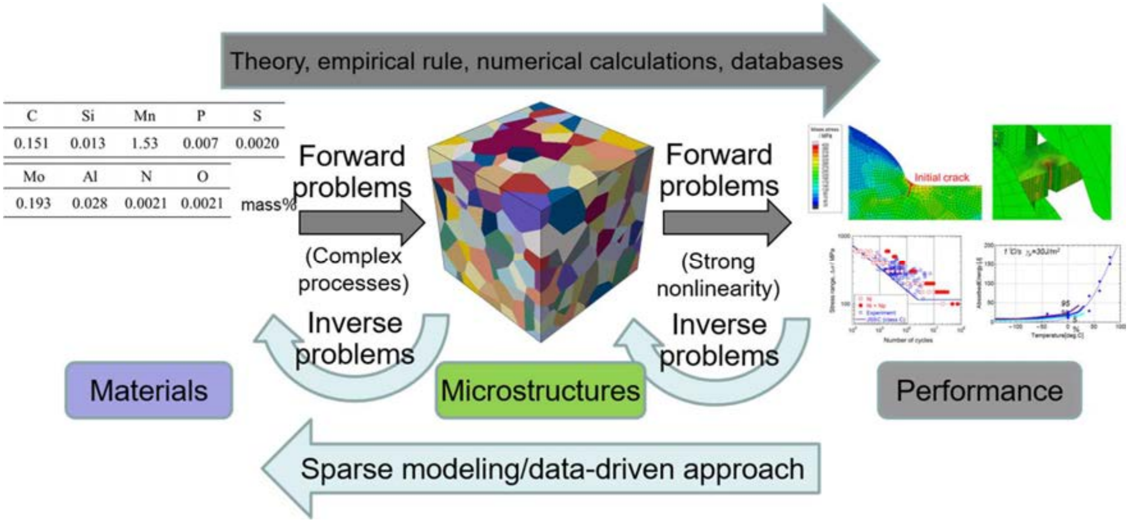


Figure 5 R&D concept for inverse problem analysis

(A-2) Process Design

Co-leaders:
Makoto Watanabe (National Institute for Materials Science (NIMS))
Kenichiroh Igashira (Kawasaki Heavy Industries, Ltd.)

Participating organizations: National Institute for Materials Science; Kawasaki Heavy Industries, Ltd.; Osaka University; Tohoku University; the University of Hyogo; Nagoya University; Kyushu University; Kobe Steel, Ltd.; Hitachi Metals, Ltd.; Gifu University; the University of Tokyo; Katayanagi Institute, Tokyo University of Technology; Toho Technical Service Co., Ltd.; and JAMPT Corporation

Processes, structures, properties, and performance are the four elements of materials engineering, and materials development essentially involves clarifying their correlations to linking these elements together. Hence, the development of calculation modules for connecting these four elements of materials engineering is essential for applying inverse problems to advanced materials and processes. Here we will take on metal powder-based molding as the advanced process in order to develop calculation modules required for applying this technology to the development of advanced heat-resistant materials (see Fig. 6). Specifically, we will construct a calculation module base in order to develop analytical modules for common physical phenomena and prediction modules for individual materials, and to apply inverse problems to advanced materials and processes.

The calculation modules for various processes developed here and analytical techniques for 3D structures will be utilized to apply inverse problems to the advanced materials and processes addressed in Domain C in order to design those materials and processes. Specific development targets are summarized below.

- Common base modules for materials development
  To develop modules for common physical phenomena, such as melting-solidifying processes and sintering processes for metal powders.
- Structural control modules for AM
  To develop techniques for designing alloys that purposely utilize nonequilibrium processes targeting AM and to establish a new technology for proposing alloys that have both heat-resistance and moldability. To perfect modules by developing and collecting data on in-line monitoring techniques and comparing and verifying prediction results.
- Analytical modules correlating structures and performance in 3D powder forging
  Near-net-shape forging and heat-treating control the three-dimensional shapes and structures of primary materials obtained by powder sintering and billet formation, and their performance is determined by such factors as creep and fatigue. Here, we will establish a technique for correlating structures and performance as a base for determining the optimal conditions of 3D powder forging from performance, and particularly from creep-fatigue, which is the superposition of two important performance aspects in heat-resistant components.
- Prediction modules for CMC performance
  To collect and organize existing knowledge on performance degradation under conditions simulating the CMC working environment and to apply this knowledge to the evaluation of CMC component reliability.

Intermediate Goals (for the end of fiscal 2020)

Powder AM
Forward analytical techniques capable of predicting structural formation and cracking in rapid cooling processes and predicting mechanical properties will be developed for AM processing of heat-resistant alloys.

Powder manufacturing
Data will be collected on manufacturing conditions and powder properties, such as particle size distribution, aimed at manufacturing processes for heat-resistant alloy powders. Machine learning algorithms will be applied to the collected data to extract issues in optimization. Studies will be conducted on bearings for heavy loads and high-speed rotation targeting the plasma rotating electrode process (PREP), and on the effect of a non-transferred arc plasma torch for achieving fine control of average particle size.

Powder forging (powder metallurgy)
Efforts will be made to improve the NIMS program for predicting superalloy properties, to clarify issues in the collection and prediction of creep and fatigue performance data, and to create a database with correlations among powder properties, initial density, load, sintering behavior, and microstructures.

Powder sintering
A database will be developed with correlations among powder properties, initial density, load, sintering behavior, and microstructures. The diffusion mechanism of additive elements will be clarified, and the effects that temperature conditions in hot plastic working have on microstructural changes will be investigated.

Advanced forging
Issues will be identified by collecting data on constant-temperature forging of solid solution strengthened and precipitation hardened alloys, and demonstrating analytical models in small-scale experiments.

CMCs
The simulation of degradation mechanisms for CMCs under high-temperature dynamic load conditions will be made possible by collecting and organizing existing knowledge on such mechanisms.

End Goals (for the end of fiscal 2022)

Powder AM
A technology aimed at AM processes for heat-resistant alloys will be developed for predicting structures and defects in rapid heating and rapid cooling processes and predicting structures and performances resulting from heat treatments. Techniques for designing alloys utilizing nonequilibrium processes will be established.

Powder manufacturing
A MI technology aimed at manufacturing processes for heat-resistant alloy powders will be developed for accelerating the optimization of manufacturing conditions, which have conventionally required many experiments and much time and expense,. A new PREP apparatus will be developed for enhancing cyber-physical affinity in 3D molding.

Powder forging (powder metallurgy)
Techniques targeting the forging of powder-based, heat-resistant alloys will be developed for analyzing metal powder sintering, forging, and heat-treating processes, and a prediction technology will be realized for structures and macro-properties.

Powder sintering
Efforts will be made to systematically measure shrinkage behavior and microstructural changes in powder compacts at high temperatures, to construct a materials database for the sintering process, and to establish a sintering analysis system employing this database. A method of predicting optimal solutions for alloy design and processing conditions will be established through inverse design MI that combines experiment analyses with computational science.

Advanced forging
A high-precision forging analysis technology and a process design technology will be developed for ingot-based advanced forging.

CMCs
A performance prediction technology will be developed for CMCs under conditions simulating their working environment, virtual tests will be conducted.

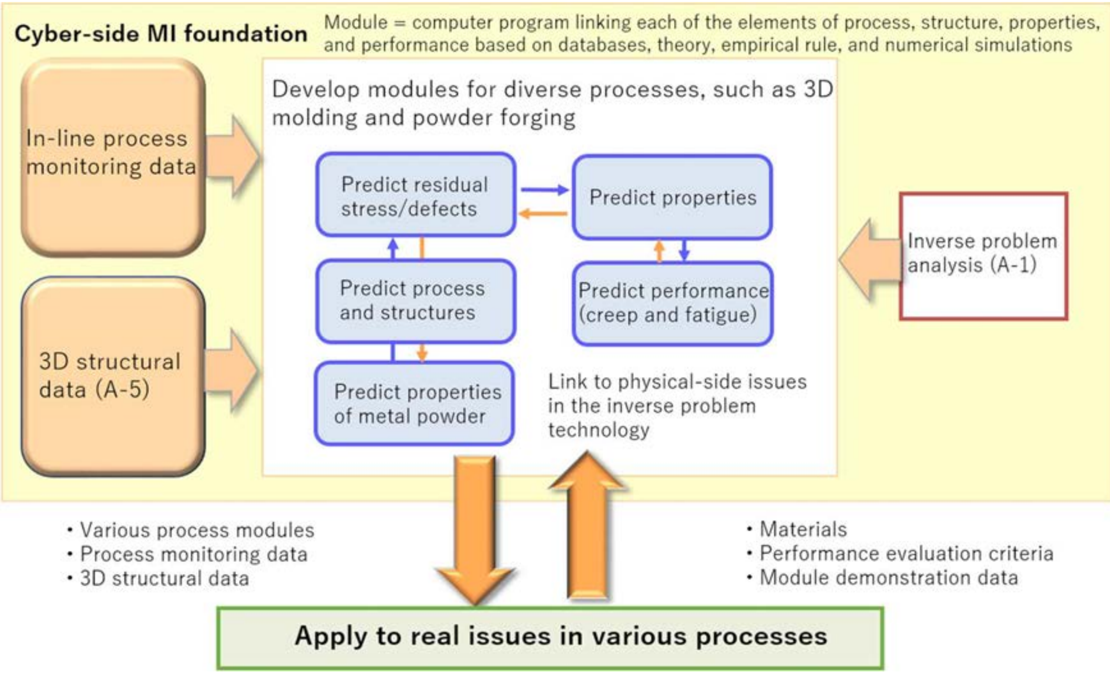


Figure 6　Concept of process design R&D

(A-3)　Structure Design of Atoms and Molecules

Co-leaders:
Tomonaga Okabe (Tohoku University)
Akihiko Ito (Toray Industries, Inc.)

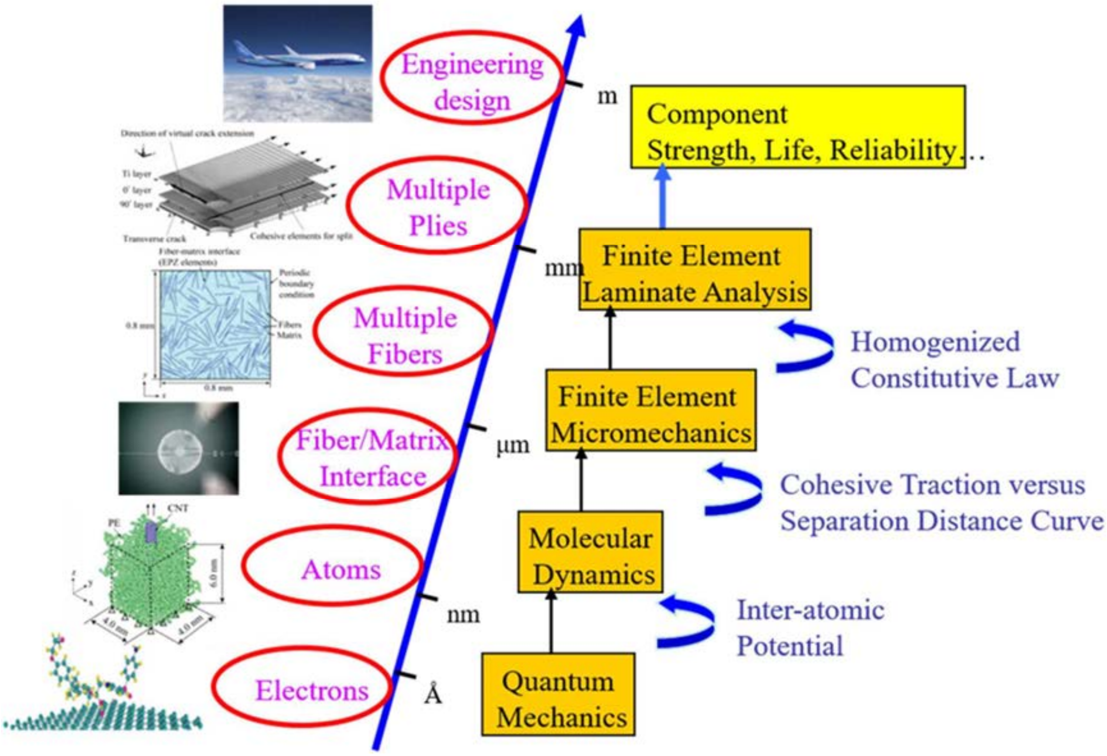
Participating organizations: Tohoku University, Toray Industries, Inc., Subaru Corporation, the University of Tokyo, the Japanese Aerospace Exploration Agency, Nagoya University, the National Institute for Materials Science, and Keio University

Utilizing inverse problems to design structures from the atomistic level will require a technology for linking different scales from atomistic and molecular to structural (multiscale) while handling multiple physical phenomena simultaneously (multiphysics). Here, using the example of polymer-based composites for aircraft, which have acute multiphysics and multiscale problems, we will address basic technologies for applying inverse problems at the airframe (structure) level. In Japan we have so far been successful in developing multiphysics, multiscale simulation techniques (see the top diagram in Figure 7) from molecular scale simulations, including crosslinking reactions based on quantum chemical calculations, to elementary airframe design. Boeing has called this initiative “atoms to aircraft.” In the first phase of SIP, Structural Materials for Innovation, the application of CFRP was possible in everything from quantum chemical calculations (three modules), molecular simulations (four modules), microscale simulations (three modules), mesoscale simulations (three modules), and macroscale simulations (six modules) to structural design (three modules). Development of a forward design tool also reached a level applicable to social implementation. The tool is already being implemented through its incorporation in general-purpose code (Materials Studio, J-OCTA, etc.) and its use in corporate materials development.

While utilizing results from the first phase of SIP, simulation tools will be further developed to make airframe applications of polymer-based composites specific application targets that are more readily adopted at development sites. We will develop a multiphysics/multiscale (MP/MS) simulator for comprehensively handling everything from R&D on multicomponent polymer networks to the design and manufacture of structural members and optimization based on inverse analysis. Based on these results, we will propose multifunctional composites or optimal structural components. Items of development required for achieving these goals are as follows.

- Establish dissipative particle dynamics (DPD) simulation techniques targeting network polymers
- Perform multiphysics analysis using DPD or all-atom molecular dynamics (MD) simulations
- Establish a self-consistent field (SCF) theory that considers fiber-fiber interactions
- Compare compositional designs and experiments for epoxy network polymers
- Propose new materials using both experiments and multiphysics analysis as training data
- Establish multiscale modeling that incorporates the continuum scale
- Propose modeling methods for automatic lamination of composite materials and modeling based on these methods
- Achieve optimum multiscale design for auto-laminated structural members to reduce stress concentration

Among the above items, efforts to characterize multicomponent network polymers aimed at composites having nano/microscale phase-separated structures, simulation modeling of phase-separated structure formation occurring during the reaction processes of epoxy resins in particular, and an attempt to scale-up this process to actual structural members will be the world's first ever, ahead of even Boeing. It is critical that Japan establish software technologies in order to maintain its dominance in such strategic resources as carbon fibers or composites.



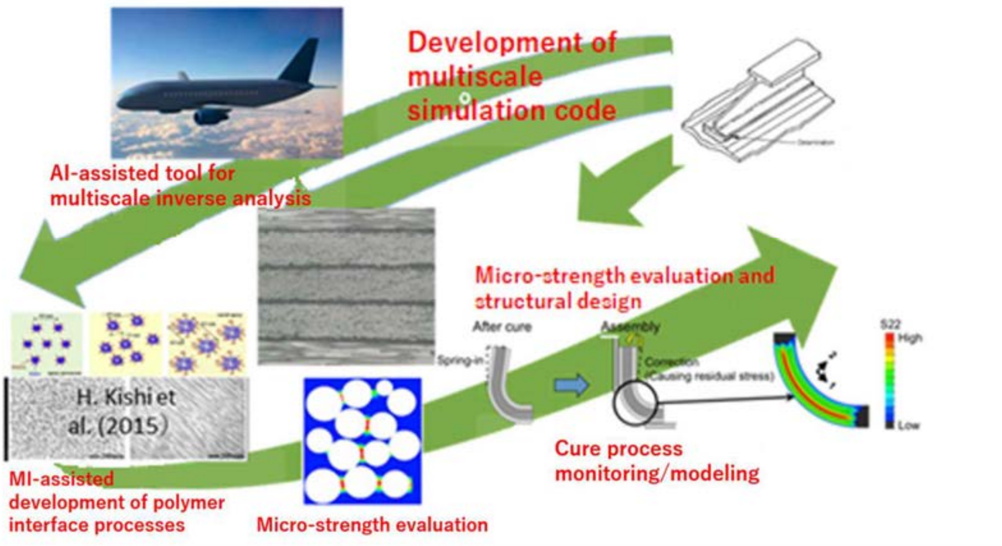


Figure 7 R&D concept of structure design for atoms and molecules

Intermediate Goals (for the end of fiscal 2020)

Modeling the crosslinking process of network polymers in advanced composites for aircraft
Quantum calculations for crosslinking of network polymers will be formulated in a Gaussian basis and incorporated in curing reactions of polymeric materials to implement DPD simulations of reactions responsible for the formation of crosslinked networks.

Meso/microscale modeling of advanced composite matrix resins for aircraft
Polymer simulations for reaction-induced phase separation will be developed using the SCF theory and the density functional theory (DFT) to obtain reproducible results in both DPD simulations and experiments on reactions.

Integrated analysis tool for multiphysics/multiscale (MP/MS) simulations
An integrated analysis tool for MP/MS simulations on advanced composites for aircraft will be developed to obtain reproducible results for experiments in Domain B.

Machine learning-assisted tool for inverse design MI
With the support of machine learning, an analytical tool will be developed for multiscale analysis and hierarchical screening of material properties.

End Goals (for the end of the fiscal 2022)

Modeling the crosslinking process of network polymers in advanced composites for aircraft
A modeling tool will be developed for the atomistic or molecular scale that targets matrix resins in advanced composites for aircraft. More particularly, quantum chemical calculations for crosslinking processes of network polymers will be formulated and incorporated in curing reactions of polymeric materials to develop DPD simulations of reactions in the formation of crosslinked networks. The results will be reproduced in experiments to enable their use at materials development sites.

Meso/microscale modeling of advanced composite matrix resins for aircraft
Coarse-grained simulations of polymers will be developed using SCP and DFT theories to reproduce phase separation around fibers, and efforts will be made to reproduce the results of both DPD simulations and experiments on reactions. We will also construct micromechanical models based on the microscopic scale to establish an analytical technique for composite materials aimed at producing practical multifunctional CFRPs, and CFRTPs or thin-ply CFRPs formed of a crystalline thermoplastic resin matrix.

Integrated analysis tool for multiphysics/multiscale (MP/MS) simulations
An integrated analysis tool will be developed for MP/MS simulations of advanced composites for aircraft. The MP/MS analysis tool will be implemented in materials development or manufacturing technologies at participating companies in collaboration with Domain B. Implementation of this analysis tool in all integration tools of MI will be promoted. Multiscale modeling of thermoplastic CFRPs with a short cycle-time will be performed to develop an AFP manufacturing technology.

Machine learning-assisted tool for inverse design MI
Techniques will be established for machine learning-assisted multiscale analysis and hierarchical screening of properties. These techniques will contribute to the multiscale design of optimal materials and the development of manufacturing technologies through inverse problem analysis.

(A-4) MI Integrated System

Co-leaders:
Satoshi Minamoto (the National Institute for Materials Science)
Junya Inoue (the University of Tokyo)

Participating organizations: the National Institute for Materials Science and the University of Tokyo

In order to employ an inverse design MI system in materials development, not only will it be essential to develop the base of an integrated system for solving inverse problems, but also usability of the system must be improved. Additionally, in order to apply this system to various actual problems, newly developed workflows and modules must be implemented in the system in coordination with teams (A-1), (A-2), and (A-3), and support will be needed to ensure calculations for materials development go smoothly.

Thus, with the aim of establishing a base for MI systems that can solve inverse problems, development of the integrated system will be focused on the following three research themes: basic development of an integrated system for inverse problems, development and improvements in usability, and applications to real problems (Fig. 8).

- Basic development of an integrated system for inverse problems

Applying inverse problems to materials having heterogeneity at various levels will require 1) that physical phenomena be described in great detail in the underlying technology for solving forward problems going from processes toward performance and 2) that calculations based on these descriptions can be executed robustly without such instabilities as divergence and termination. Also needed are workflows for integrally resolving the various scales and physical phenomena in real problems.

For this reason, the foundation of the MI system produced in the first phase must be substantially reinforced to be able to handle inverse problems. Specifically, we must first upgrade each of the programs and greatly enhance the database functions and the functionality of the various application programming interfaces (APIs) developed thus far, including the MI-API (API for connections), DB-API (API for database operations), and vocab-API (API for vocabulary information).

Inverse problems can be solved using AI to fully control robust forward calculation techniques backed by these detailed physical descriptions. Hence, in order to expand the MI system to a base system capable of handling inverse problems, it will be essential to implement algorithms for solving inverse problems and to develop new technologies using AI to control forward calculations. Expanding the base system to handle inverse problems will be achieved by developing inverse problem algorithms based on the latest AI technology and a WF-API (an API for workflow operations) and by incorporating these items in the MI system.

In materials engineering, a workflow may be regarded as the manner in which a problem is solved. Hence, by digitally accumulating and networking these workflows, expertise in areas of materials can be restructured to a form suitable for machine learning. Use of these so-called digital textbooks will help us rapidly examine methods of solving similar problems and may lead to the discovery of unexpected paths to solutions. The challenge lies in how workflows are to be networked. A workflow is essentially concepts and links connecting those concepts. Concepts are expressed with vocabulary (technical terminology). Hence, it should be possible to network workflows by structuring the connections between different vocabulary terms. Based on this idea, we will substantially enhance the functionality of vocabulary management developed in the first phase with the aim of building a network of knowledge on materials engineering. Networking knowledge will be achieved using a framework for describing the relationships among concepts in order to connect expertise possessed by engineers on different materials and different processing technologies. Doing so will require a vocabulary analysis system and a vocabulary visualization system for extracting knowledge in synchronization with human thought while referencing sets of recorded vocabulary and experimental and computational data. In short, we must develop a system to search databases on vocabulary and materials that is fast, user-friendly, and scalable.

- Developments and improvements in usability

Since it is vital to gain a clear understanding of the user layer in MI systems for a wide range of fields, user opinions must be gathered to implement a graphical user interface (hereinafter "GUI") that each user can intuitively manipulate for solving problems. Further, in light of the variety of APIs that will be developed, a framework will likely be developed to facilitate functional development and data collection for individual problems. AI-driven data analysis functions including error handling, data logging, and visualization, must be developed in order to implement an interactive GUI that can tap into the user's intuition. System expansion will also include enhanced functions for remote access and security-related technologies.

- Applications to real problems

In this phase, research achievements developed by teams (A-1), (A-2), and (A-3), such as workflows, modules, and algorithms for inverse problems, must be incorporated in the system in order to complete our tool for developing materials through inverse design. We will work together to understand and organize input/output for products being incorporated in order to enhance the program so that it is versatile, robust, and large in scale. The results of these efforts will be implemented in the system.

Intermediate Goals (for the end of fiscal 2020)

System implementation of mathematical techniques for inverse analysis
Several generalized case studies for flexibly implementing techniques developed in (A-1) aimed at mathematically analyzing inverse problems in a system will be carried out to validate system implementation of such techniques.

Flexible control for repeated calculations in inverse analysis workflows
Control techniques for repeated calculations in workflows required for inverse analysis and a flexible framework for searching similar workflows will be established by utilizing the APIs described below.

Implementation of newly developed modules for advanced materials and processes
A large number of new modules are anticipated to be developed for advanced materials and processes, and their prompt implementation will be essential. At present, recording information such as vocabulary inventories is complicated. Therefore, we will establish a technique for simplifying the operations required for implementing modules in the MI system.

User interface
Public hearings on usability will be held for users during this fiscal year and next. Priority items will be studied and implemented while ensuring security.

API set
A set of APIs will be developed for defining input/output between modules, manipulating workflows themselves, and other functions. A framework will also be established for providing users with more flexibility in designing modules that incorporate these APIs.

Remote access control
An infrastructure will be established to enable remote system access and utilization. In addition, we will create an environment for managing workflows and computational data uniformly with local systems.

End Goals (for the end of fiscal 2022)

System implementation of mathematical techniques for inverse analysis
Techniques developed in (A-1) for mathematically analyzing inverse problems will be generalized for flexible use and implemented in the system.

Flexible control for repeated calculations in inverse analysis workflows
A flexible control technology will be established for repeated calculations in workflows required for inverse analysis.

Implementation of newly developed modules for advanced materials and processes
Newly developed modules for advanced materials and processes will be implemented, while simultaneously establishing a systems approach for simplifying these operations.

User interface
The user interface will be completed with improved usability and security measures.

API set
A set of APIs will be developed for defining input/output between modules, and a framework will be developed to provide users with flexibility in designing modules that utilize these APIs.

Remote access control
Technologies for remote access control will be established to ensure consistent workflow control while effectively utilizing computer resources scattered throughout research labs and companies.

System implementation of data structures for describing structural materials
A framework will be established for reflecting the data structures that were developed in (A-5) to describe structural materials in the system and for looking up data associations.

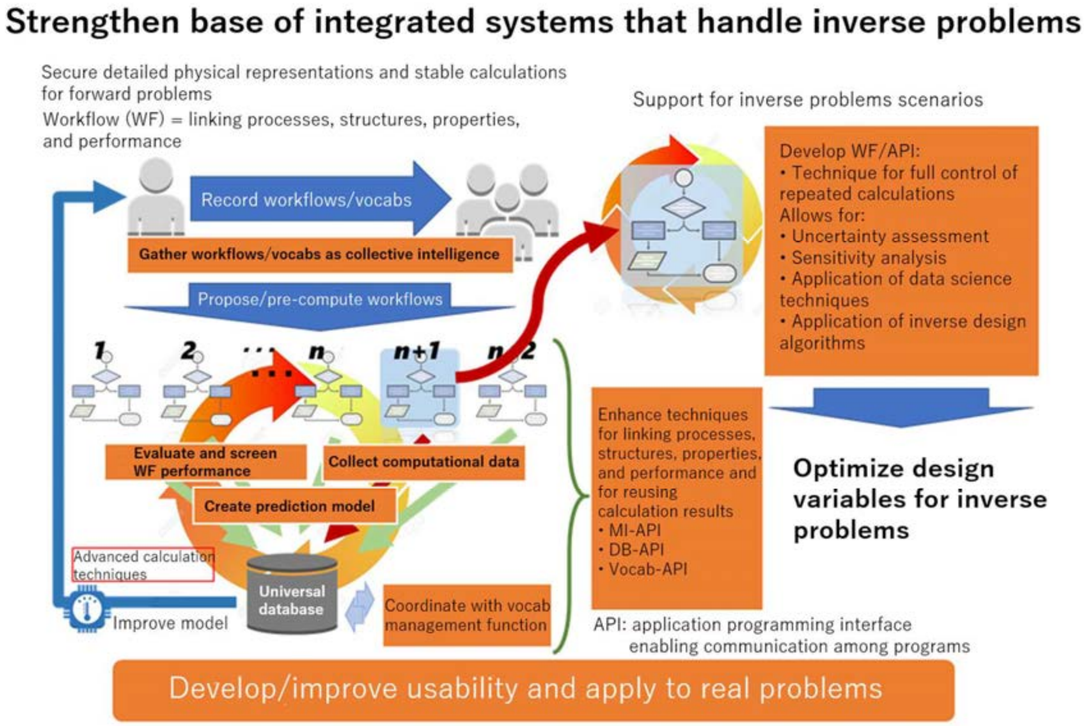


Figure 8 R&D concept of MI integrated systems

(A-5) Structural materials database

Co-leaders:
Masahiko Demura (the National Institute for Materials Science)
Toshihiro Ashino (Toyo University)
Yoshitomi Okazaki (Kobe Steel, Ltd.)

Participating organizations: the National Institute for Materials Science, Toyo University, Kobe Steel, Ltd., RIKEN, Kansai University, Tohoku University, JFE Steel Corporation, IHI Corporation, and UACJ Corporation

Structural materials have hierarchical heterogeneity, also known as structure, at different size scales ranging widely from the atomistic to the structural. Structures are located at nodes linking processes to properties, whereby the process determines the structure, and the structure determines the properties. Performance can be considered by also accounting for the application environment. The method of describing hierarchically heterogeneous structures is key for the advanced utilization of materials data in developing structural materials. In addition, there exists a major bottleneck to digitizing information on such heterogeneous structures. Material structures are collected as images using various microscopic techniques. However, the work required to sort these images by hierarchical form and to quantify them as digital information must be delegated to experts with a deep knowledge of structural images and requires a significant amount of time and cost. One must also bear in mind that models constructed in conventional materials engineering are based on two-dimensional information of structures due to technical limitations. By utilizing the original structural information of materials characterized three-dimensionally, it is expected that one can better understand the intrinsic connections between processing, structures, properties, and performance.

Based on this awareness, we will carry out R&D on a database structure designed specifically for structural materials to describe connections among structures, properties, and performance and handle inverse problems. Specifically, we will develop a method of describing the internal structures of hierarchically structured materials, from lattice defects to precipitates and crystal structures, while drawing connections between levels. The focus will be on the internal structures of materials that govern the properties and performance of structural materials. We will then construct a database linking processing with properties and performances. Among the four elements of materials science and engineering, “structure” is the element that links processing to properties. Therefore, a technique will be developed for efficiently compiling databases of 3D information on structures. The performances and properties of materials are greatly dependent on structures having 3D geometric features across a wide range of scales from the nanometer scale to a scale on the order of several hundred micrometers, and their structures vary greatly according to the processes. Hence, quantitative 3D information on material structures that link performances to processes must be compiled in a database in order to determine through inverse design the most suitable process from the desired performance. Here, a technique will be developed for efficiently collecting multiscale 3D information on structures formed under a variety of processing conditions.

- Development of a database structure for structural materials

Utilizing materials data on weld joints for steel and aluminum alloys, we will take the lead in a study on database structures for such materials in industry, academia, and government. To construct a database structure that will aid in the utilization of data for structural materials, a computer science framework will be utilized fully for describing hierarchical connections, such as a material ontology. Once data has been collected for application examples, a similar study will be initiated on advanced materials and processes applying inverse design MI. Since international cooperation will be indispensable for the investigation and implementation of such a study, we will work to promote de facto standards in collaboration with such organizations as Granta MI that are behind other projects on structural materials databases.

- Development of analytical techniques for multiscale 3D structures

Conventionally, the support of prominent experts has been essential for determining the three-dimensional shapes of materials, as the shapes are too difficult to guess from a single sectional image. The creation of a machine learning model capable of automatically determining structure from a sectional image through segmentation has been needed. Such a model would facilitate the collection of multiscale 3D information on structures. Here, we will construct a system that will be able not only to determine structures, but also to extract the structure factor in any two-dimensional image automatically. At the same time, we will develop a technology for analyzing multiscale 3D structures that eliminates the scale gap present in current techniques for observing 3D structures. One particular target is a technique for observing 3D structures in the micrometer to submillimeter range, which is the most important range for structural materials.

Intermediate Goals (for the end of fiscal 2020)

Design and publication of description methods for structural materials data
A method of designing data will be proposed for three or more types of inverse problems.

Acquisition of multiscale 3D structural information between nm and cm
Techniques will be established to enable large-area 3D observations with scanning electron microscopes and efficient 3D observations with optical microscopes.

Automatic extraction of quantitative information for material structures from 2D optical/electron microscopy images
A methodology will be established for sequentially generating supervised 2D images from labeled 3D images and creating a machine learning model for quantifying structures.

Proposal of new descriptors having strong correlations with the performance of structural materials
New descriptors will be proposed through mathematical science techniques for material structures.

End Goals (for the end of fiscal 2022)

Design and publication of description methods for structural materials data
A method of describing materials data for structural materials having the following characteristics will be designed and published in a usable form for the purpose of establishing de facto standards.

- Capacity for representing hierarchies and mutual relationships of materials and being linked with techniques for analyzing 3D structural information
- Readily expandable for new measuring methods and material systems
- Capacity for integrally describing information sources of different types, such as experiments, numerical calculations, and empirical formulae, in coordination with descriptors developed for MI System ver. 1.0

- Described with standard technology on the Internet when possible with the aim of establishing de facto standards

Acquisition of multiscale 3D structural information between nm and cm
A technology for acquiring multiscale 3D structural information covering size scales from nanometers to centimeters will be established by integrating various observation methods in order to handle hierarchically heterogeneous structures for advanced materials and processes.

Automatic extraction of quantitative information for material structures from 2D optical/electron microscopy images
A technique will be established for automatically extracting quantitative information of material structures from two-dimensional images captured in optical/electron microscopy.

Proposal of new descriptors having strong correlations with the performance of structural materials
New descriptors having strong correlations with the performance of structural materials will be proposed using mathematical science techniques.

(B) Carbon Fiber Reinforced Plastic (CFRP)

Co-directors:
Tomonaga Okabe (Tohoku University)
Toshiya Nakamura (the Japan Aerospace Exploration Agency)

Domain B will apply the basic technologies for inverse design MI developed in Domain A to the development of raw materials and structures in actual CFRPs. Material structures and processes required for achieving the target performance will be derived in cyberspace (the MI system) and verified in physical space (trial manufacturing and testing). A reduction in development time and costs will also be verified. Technologies tailored to the target materials and processes will be developed based on the techniques relevant to calculation modules, workflows, and data science approaches developed with inverse design MI. Advanced structural materials and processes for practical use were selected as application targets because they are anticipated to be conducive to the application of inverse design MI, be in line with Japan's strengths, and have high global demand. One specific example is a molding technology for composite materials.

In light of the purpose of SIP, the effectiveness of inverse design MI in the development of materials and processes must be demonstrated according to a roadmap for practical application and commercialization developed by the participating raw material and heavy industry manufacturers. Specifically, we need a system involving the Japanese industry, government, and academia to give concerted support for these efforts through inverse design MI. Such a system is necessary because CRFP-related technological development is not progressing fast enough to keep up with the performances required by industry. The primary outcomes of this R&D will be used in the aircraft industry, but the current production rate is insufficient to manage future needs for small and medium-size aircraft. Further improvements are needed in production technology, and new approaches to utilizing calculation technologies and scientific foundations possessed by government and academia will be critical.

The development of structural materials has historically followed the pursuit of high specific strength and heat-resistance. This pattern will continue as long as we keep pursuing equipment with higher efficiency, lower energy use, and low environmental impact. Since materials for aircraft in particular have the strictest requirements for these two performance aspects, along with reliability, such materials are most fitting as the outcomes of R&D on structural materials.

R&D for the three teams in this domain is described below. All R&D will be carried out in collaboration with relevant sub-teams under team (A3) (see Figure 9). The calculation modules and databases developed in this domain will be collected in the inverse design MI system in a manner that will not impede commercialization, and will be utilized to improve Japan's overall competitiveness in materials development.

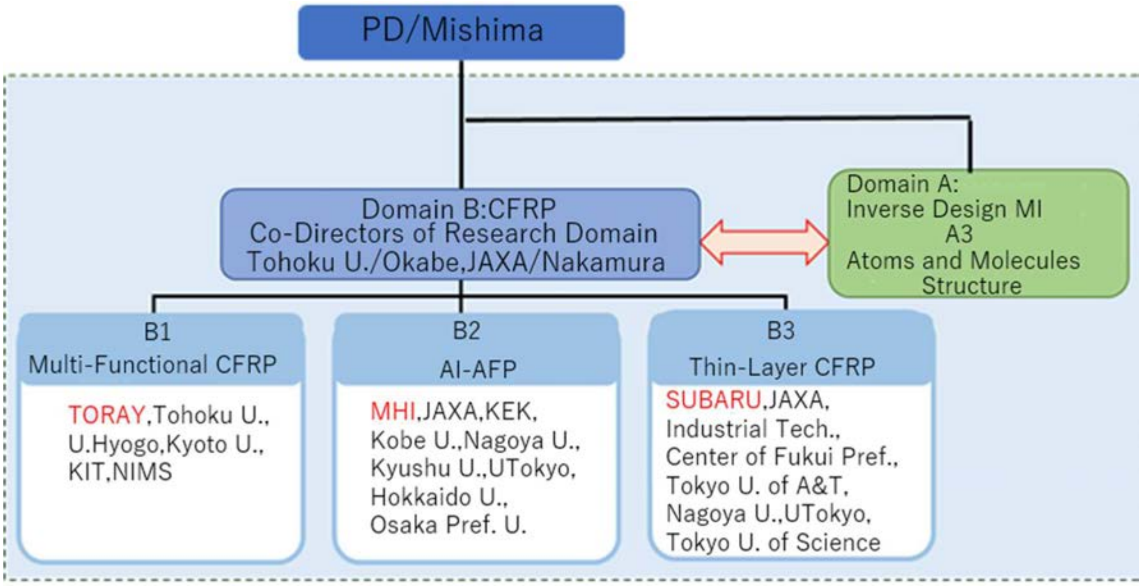


Figure 9 Domain B: research organization for CFRP (private companies are in red)

(B-1) Development of Multifunctional CFRP Providing Added Value

Co-leaders:
Kenichi Yoshioka (Toray Industries, Inc.)
Tomonaga Okabe (Tohoku University)

Participating organizations: Tohoku University, Toray Industries, Inc., the University of Hyogo, Kyoto University, the Kanazawa Institute of Technology, and the National Institute for Materials Science

Owing to their improved mechanical properties, carbon fiber composites have been adopted to produce lightweight components. With the recent focus on reducing overall weight and costs by imparting functionality to carbon fiber composites, such as flame retardancy, thermal conductivity, and damping properties, development of functionality imparting technologies that can be implemented in structural materials for aircraft has taken on importance. However, the development period for aircraft systems has more than doubled since the 1990s as the complexity of development has increased. Thus, a technical approach for reducing the development period is needed. Adding functionality to composites has also become a widespread issue in internal railway structures, automobiles, and electric appliances such as computers.

Since functionality is being added as a component of materials development, as described above, we will endeavor to utilize MI technology in the initial stages of development for providing composites with functionality from the perspective of polymer and prepreg design. The feasibility of implementing these technologies will be established at an early stage and will be verified through element tests on components.

While prepregs have conventionally been employed to achieve a target performance in mechanical properties, success has been achieved in separating stiffness and toughness functions in the design of polymers or prepregs. The current development will not only cover conventional design in the mechanical domain for pursuing improvements in mechanical properties, but will also target structures having at least one functional domain as the final composite. In this development, functional particles and polymers will be combined in prepregs in an effort to impart new functionality, such as flame retardancy, thermal conductivity, and damping properties. Prepregs will be designed with the support of MI to acquire basic mechanical and functional data for realizing this objective. Structural design will be conducted by identifying optimal structures for functional particles or polymers needed to implement a functional domain. Parameters will be acquired during reactions involved in structural formation to confirm correlations between the actual domain properties and phenomena related to flammability and thermal conductivity. Based on this experimental data and hierarchical screening for functional polymers/prepregs, a materials design tool will be constructed with the use of deep learning.

Finally, we will construct a design database for polymer systems and prepreg systems comprising multiple functional domains and a mechanical domain having mechanical properties required for structural materials, and will design materials that impart multiple functions while preserving or improving the mechanical properties. Additionally, we will utilize MI to construct a design tool based on hierarchical screening for multifunctional polymers/prepregs and will establish a method of predicting material properties with good accuracy. The effectiveness of the design prepregs will be verified through small-scale element tests simulating composite members.

By using MI technology to implement the cycle between inverse analysis based on end products, such as airframe structures, and forward analysis based on the molecular design of materials, technologies will be developed to shorten the development period and predict the properties of resins, carbon fibers, resin-fiber interfaces, and the components (products) themselves. Specifically, we will develop a multiphysics/multiscale (MP/MS) simulator to comprehensively handle everything from the development of multicomponent network polymers to the design and manufacture of structural materials, and to handle optimization based on inverse analysis. From this simulation information, we will develop a technology for proposing multifunctional composites or optimal structural members while shortening the development period.

Intermediate Goals (for the end of fiscal 2020)

Our aim is to design CFRPs having at least one functional domain. Specifically, with tensile strength and compressive strength of CRFP perforated sheets used in aircraft structures being typically 480 MPa and 310 MPa, respectively, the objective is to reduce burn length by 35% in a practical evaluation method for flammability, which will be introduced in this study as an index of flame retardancy, while preventing a drop of more than 5% in tensile and compressive strength. To realize this objective, we must first acquire fundamental mechanical and functional data on CFRP structures and the design of resin compositions and prepregs constituting the materials of these structures, thereby building this data on mechanical and functional properties in a database. The target level is TRL 3.

End Goals (for the end of fiscal 2022)

A design database will be constructed for polymer systems and prepreg systems comprising multiple functional domains and a mechanical domain having mechanical properties required for structural materials. Materials will be designed to have multiple functions (flame retardancy, thermal conductivity, damping properties, etc.) while maintaining the mechanical properties required for structural materials in particular. Specifically, assuming that the tensile strength and compressive strength of CFRP perforated sheets used for structures in aircraft are generally 480 MPa and 310 MPa, respectively, the goal is to avoid a decrease of more than 5% in these parameters, while improving thermal conductivity by 10% along the thickness direction of the CFRP and improving the damping ratio by 10% in oscillation measurements on CFRP.

At the same time, we will construct a tool for utilizing the MI described above for designing structural materials based on MP/MS modeling of multifunctional polymers and prepregs. We will establish a method of predicting material properties in the final structural materials with high precision. The effects of the designed prepregs will be verified through small-scale element tests simulating CFRP members. The target level is TRL 5.

These outcomes will be demonstrated by manufacturing prototype prepregs that exhibit the above properties and conducting evaluations similar to quality assurance tests for products (fiber content, areal weight, etc.). CFRP panels will then be molded from these prepregs to confirm whether panels of a sufficient grade can be manufactured under actual molding conditions, and a full evaluation will be conducted on not only the mechanical properties, but also the flame retardancy, thermal conductivity, and damping properties described above. The evaluation method for flammability introduced in this study will be used for evaluating flame retardancy. A common standard of measurement will be used for measuring thermal conductivity. A conventional method of measuring CFRP oscillations shown to be effective for sports equipment will be employed for evaluating damping properties.

(B-2) Development of CFRP Design/Manufacturing Automation Technology Using AI-assisted Stacking Optimization

Co-leaders:
Toshio Abe (Mitsubishi Heavy Industries, Ltd.)
Toshiya Nakamura (the Japanese Aerospace Exploration Agency)

Participating organizations: Mitsubishi Heavy Industries, Ltd., the Japanese Aerospace Exploration Agency, the High Energy Accelerator Research Organization KEK, Kobe University, Nagoya University, Kyushu University, the University of Tokyo, Hokkaido University, and the University of Osaka Prefecture

The entrance of the Boeing 787, which embraced the use of carbon fiber composites, has spurred rapid introduction and growth of automated manufacturing equipment in recent years to manufacture composite structures for aircraft. With expectations high on carbon fiber composites for producing lightweight structures, this trend is becoming manifested in wind turbines for wind power generation, as well as high-speed rail and high-speed craft. Europe in particular has made great strides in producing automated fiber placement (AFP) machines capable of high-speed, high degree of freedom fabrication of composites. The introduction of these machines has made it easy for anyone to fabricate composite structures. Consequently, Japan's international competitiveness from previous accumulated composite technologies is now rapidly declining. In order to once again lead the world in composite technologies, Japan must innovate and standardize techniques of manufacturing suitable for AFP. On the other hand, Japan has world-leading manufacturers of carbon fibers and other raw materials. We intend to take advantage of Japan's competitive edge in these materials to make improvements and modifications in coordination with MI in order to overcome problems and defects. One specific issue with these materials, shrinkage behavior when curing polymeric materials, is directly linked to shape inaccuracies produced during parts manufacturing. Such inaccuracies are a major obstacle in the assembly of aircraft structures and a factor in increased production costs. Further, while AFP improves productivity, the interior quality of products produced by AFP is inferior to products produced from hand layup by laminate experts due to the lower layup accuracy. This can result in degraded performance in the product's strength and stiffness, for example. AFP has functions for placing tape along curves rather than just straight lines and for producing optimal designs that make use of the strength of carbon fibers. However, the improved productivity is not sufficient to be considered an advantage, and the gaps and overlaps between tape layers in AFP cause numerous internal defects that have an adverse effect on structural quality, reducing strength and stiffness.

In the meantime, Europe and the United States currently have a monopoly on AFP machines. Despite the best-performing composites and intermediate base materials known as prepregs originating in Japan, Japan has been unable to acquire materials design and molding methods suitable for existing AFP machines, making it more and more difficult to comply with requests from the machine manufacturers. Emerging powers such as China have been quick to introduce AFP machines from the West and have begun to undertake research on the manufacture of relevant materials.

In light of these circumstances, our aim is to enter the next emerging aircraft business promptly by using general-purpose AFP machines for the optimal AI-assisted design of composites and by improving molding precision using prepregs already developed in Japan.

In order to overcome Japan's weaknesses in AFP and other manufacturing automation, our goal is to introduce general-purpose AFP machines being commercialized in Europe and America in order to perform optimal AI-assisted design of composites and to improve molding precision using prepregs that Japan has already developed. Through these efforts, we hope to achieve materials technology and high-precision molding techniques unique to Japan and to enter the next-generation aircraft business promptly. For this reason, we will link technologies related to the cost-competitiveness of product manufacturing or the products themselves to MI technology driven by multiphysics/multiscale (MP/MS) analysis. This will enable us to promote activities to improve and modify materials, make Japanese products competitive once again, and ultimately give a boost to Japan's aerospace industry. At the same time, we will connect research findings for composite structural optimization/automation to AI-assisted automated design and formulation of a system for curing (correcting irregularities, etc. during molding).

Future development of aircraft is expected to bring fierce competition from other countries including China, which has been rapidly increasing its market presence in technology. Seizing a commanding lead in this technological area will require an innovative technology that can improve productivity in the manufacturing of composites rivaling that of today's aluminum structures, while utilizing the virtues of composite materials. Without inhibiting productivity, we must analyze issues specific to polymeric materials, such as cure shrinkage, or issues of quality lost in exchange for dramatic improvements in productivity over traditional hand layup, such as the drop in layup precision due to the application of AFP. We must also utilize MI technology to improve and modify materials in order to take advantage of the virtues of composites, including their low weight, high strength, and high stiffness. Utilizing MI technology driven by MP/MS analysis, multiscale research for material improvement and modification will be carried out on a wide range of issues, from nanoscale observations of raw materials or crack paths to the development of new structural types applicable to the relevant materials. The aim of the new structural types is to suppress fracture phenomena appearing on the meter scale, and particularly fracture behavior specific to the relevant materials, such as separation and interlaminar crack propagation. Ultimately R&D will be carried out to transform the design and structures of products employing carbon fiber composites or the products themselves, leading to materials-based innovation that will become a force in Japan’s high-efficiency, high-productivity manufacturing industry.

Intermediate Goals (for the end of fiscal 2020)

Research results obtained to date will be incorporated in the trial manufacture of panel structures simulating aircraft structures with stress concentration around holes, and the structures will be subjected to strength tests.

Evaluation items
- Lamination speed, increase in speed
- Quality assessment of laminate interior, quality assessment with profile measuring (comparison with standard aircraft quality)
- Effects of improved strength over hand layup and general laminates determined through strength tests

Target values
- The goal for fabricating laminated structures with curved surfaces utilizing the strength and qualities of carbon fibers in epoxy composites, which are commonly used in the aviation industry, is to achieve a strength at least equivalent to that of common hand layup products and a layup speed five times or greater that of hand layup (0.5 kg/hr on average).

The following are specific targets at the midpoint of each research issue
- Confirm operation performance of the AFP machine, and adjust device-side improvement tasks aimed at materials improvement
- Adjust issues of improvement and issues for manufacturing large complex-shaped structural parts for aircraft with the AFP machine
- Clarify conditions for matching multi-composites (epoxies and thermoplastics) with an AFP machine
- Identify issues in molding and curing of carbon fiber-reinforced thermoplastics (CFRTP) such as the effects of resin crystallinity and conditions of rising/dropping temperatures
- Establish a basis of molding techniques and summarize challenges for establishing AFP and in-situ consolidation technologies
- Study materials improvement aimed at in-situ consolidation of thermoplastic composites and set policies for methods of materials improvement
- Observe fracture features, focusing on the internal structure of CFRPs, and particularly composite structures formed through automated layup, optimize layup for improving fracture strength based on these observations, and extract goals for new structural types

Target level for intermediate evaluation (end of March 2020): TRL 3

End Goals (for the end of fiscal 2022)

Demonstration tests and strength tests will be conducted to clarify outcomes and challenges for elements of this study (materials improvement, AI system development, etc.).

Evaluation items

This evaluation has essentially the same items as those in the intermediate year. However, the efficiency of manufacturing products will be comprehensively evaluated through a process of manufacturing panels having assembled structures closer to those in aircraft and assembling those panels.

Target values

Our aim is to achieve improved strength and speed five times or more that of hand layup for structural components of airfoils, which are more complex in shape than existing structures made with epoxy composites. In addition, goals will be set for out-of-autoclave layup and in-situ consolidation for thermoplastic composites.

The following are specific targets upon completion of each research issue.

- Establish a base for optimal layup design and fabrication methods, utilizing AFP machines for composites
- Clarify a strategy for materials improvement utilizing MI based on the challenges identified for the product quality and manufacturability of automated composite layup and applicable structures for composites
- Establish a basis for techniques of design and manufacturing automation that optimize multivariate parameters through the integration of multipurpose optimization techniques and data mining
- Optimize composite layup suited to AFP, establish a basis for automated design and manufacturing methods, and implement and evaluate development tests for verifying their effects
- Establish a basis of methods for AFP and in-situ consolidation of thermoplastic composites
- Calculate manufacturing costs according to improved productivity and lighter structures based on an evaluation of the demonstration tests, and study and implement a business model

Target level for the completion of SIP (the end of March 2023): TRL 4

(B-3) Development of 3D High Degree of Freedom Design Technology by Automatic Lamination of Thin-Layer CFRP

Co-leaders:
Shigekazu Uchiyama (Subaru Corporation)
Toshiya Nakamura (the Japanese Aerospace Exploration Agency)

Participating organizations: Subaru Corporation, the Japanese Aerospace Exploration Agency, the Industrial Technology Center of Fukui Prefecture, Tokyo University of Agricultural and Technology, the University of Tokyo, and Tokyo University of Science

With the global expansion of composites used in aircraft parts, the spread of general-purpose automated equipment and easy-to-use materials is bringing about an age when anyone can manufacture products with constant quality and performance. Further, as costs keep dropping due to increased sourcing from low-cost countries (LCCs), Japan is struggling to remain cost-competitive on the level playing field. Technologies for achieving high-performance, low-cost production must be established by developing materials, design, and manufacturing technologies not bound by past conventions and standards so that Japan can maintain its dominance in composite technologies. Prior composites used in aircraft parts have limitations in such aspects as materials, design, and manufacturing and have not succeeded in demonstrating their true performance. For this study, our goal is to remove these constraints, improve degree of freedom in aspects of design and production, and improve performance so that the properties of composites approach their true performance.

Specifically, while adopting an MI approach, we will establish and integrate manufacturing technologies to automate a variable fiber spreading technology for freely varying the width of composite materials, and an optimal design technology for composites having complex structures aimed at continuously varying material width and layer thickness. With unprecedented structure optimization and low-cost production, Japan will surpass other countries and maintain its superiority in composite technologies.

Our aim is to design and manufacture lightweight composites that can be competitive worldwide by promoting the three pillars of materials technology, design and analysis technology, and manufacturing technology in collaboration with industry, academia, and government. Despite the trend toward low-cost products, we aim to maintain Japan's dominance by reducing material costs through the use of lightweight materials and shorter production, including equipment development.

Since the development of composites requires equipment and designs suited to the raw materials, collaboration among materials, equipment, and airframe manufacturers is necessary. By nurturing the midstream industry (equipment) currently being dominated by overseas manufacturers in order to assume comprehensive control over the production process from the upstream sector to the downstream sector, we can improve development speed and increase Japan's competitive strength in composites.

With the aim of achieving social implementation at an early stage, we will reduce the development period and begin adopting thin-ply CFRPs in 2025. To achieve this, we must expand our laminating machines ahead of schedule to a practical scale for manufacturing parts.

Since we also need to extract the benefits of thin-ply CFRP and accelerate technological development of degree of freedom design for further reducing the weight of composite structures, we will conduct coupon tests (FY2019) for utilizing a tow-steering technique that exceeds the original estimates.

Our objective is to optimally design and fabricate composites utilizing MI technology (multiscale calculation and optimal design technologies) linking materials design with manufacturing. Material production, parts production, and parts performance evaluation will be compared between the physical space and cyberspace at the development stage to continuously improve these technologies. Algorithms for inverse design analysis will also be constructed to determine what materials, designs, and manufacturing can achieve the required parts performance.

Intermediate Goals (for the end of fiscal 2020)

Target TRL: TRL 3, complete basic development of thin-ply prepregs, equipment, and designing/manufacturing

(i) Development of thin-ply CFRP
- Establish process conditions for thin-ply prepreg sheets having improved interlaminar strength of at least 20 m/min

(ii) Development of high degree of freedom AFP (automated laminating machine)
- Install automated laminating machine in anticipation of manufacturing actual large parts, and demonstrate manufacturing
- Establish techniques of tow-steering and variable layer width and thickness using the automated laminating machine

(iii) Design and analysis technologies
- Complete basic development of a design optimization method for fiber orientation and layer thickness based on a tolerance database reflecting the strength and fracture properties of thin-ply CFRP, and begin trial use
- Verify effectiveness by conducting a comparison of conventional straight layup methods for CFRP and a layup method that considers tow-steering and variable width/thickness of CFRP for use in aircraft wing structures

End Goals (for the end of fiscal 2022)

Target TRL: TRL 4, complete core technology development using the example of structural elements for aircraft wings

(i) Development of thin-ply CFRP
- Establish process conditions for thin-ply prepreg sheets with improved interlaminar strength compatible with an AFP machine for high freedom of degree design
- Improve strength of thin-ply CFRPs even more than before for use as aircraft components, and fabricate thin-ply prepreg sheets with enhanced interlaminar strength that are compatible with AFP machines in order to realize a high degree of freedom layup design technology

(ii) Development of high degree of freedom AFP (automated laminating machine)
- Establish techniques for steering layup and variable width/thickness of multiple tape layers using the AFP machine

(iii) Design and analysis technologies
- Design test pieces using the established method of design optimization for the structural element level of aircraft wings that achieves the target 10% reduction in weight while maintaining strength and stiffness

(iv) Molded articles

- Manufacture actual large parts for structural elements of aircraft wings optimized through steering of thin tape using AFP
- Apply load to the large parts fabricated as structural elements of wings to confirm their strength and stiffness are equivalent to the analytical results

(C) 3D Powder Processing

Co-directors:
Takayoshi Nakano (Osaka University)
Makoto Watanabe (the National Institute for Materials Science)

In Domain C, basic technologies for inverse design MI developed in Domain A will be applied to the development of actual metal and ceramic-based materials and structures. Material structures and processes required for achieving the target performance will be derived in cyberspace (the MI system) and verified in physical space (trial manufacturing and testing). A reduction in development time and costs will also be verified. Technologies tailored to the target materials and processes will be developed based on the techniques relevant to calculation modules, workflows, and data science approaches developed with inverse design MI. Advanced structural materials and processes for practical use were selected as application targets because they are anticipated to be conducive to the application of inverse design MI, be in line with Japan's strengths, and have high global demand. Specific examples are powder metallurgy processes centered on additive manufacturing.

In light of the purpose of SIP, the effectiveness of inverse design MI in the development of materials and processes must be demonstrated according to a roadmap for practical application and commercialization developed by the participating raw material and heavy industry manufacturers. The primary outcomes of this R&D will be used in the aircraft industry because materials used in aircraft are subjected to the harshest conditions and, consequently, require the highest reliability. Naturally, these results will have a major ripple effect in the environment and energy industries, for example.

R&D for the five teams in this domain is described below. All R&D will be carried out in collaboration with relevant sub-teams under team (A2) (see Fig. 10). The calculation modules and databases developed in this domain will be collected in the inverse design MI system in a manner that will not impede commercialization, and will be utilized to improve Japan's overall competitiveness in materials development.

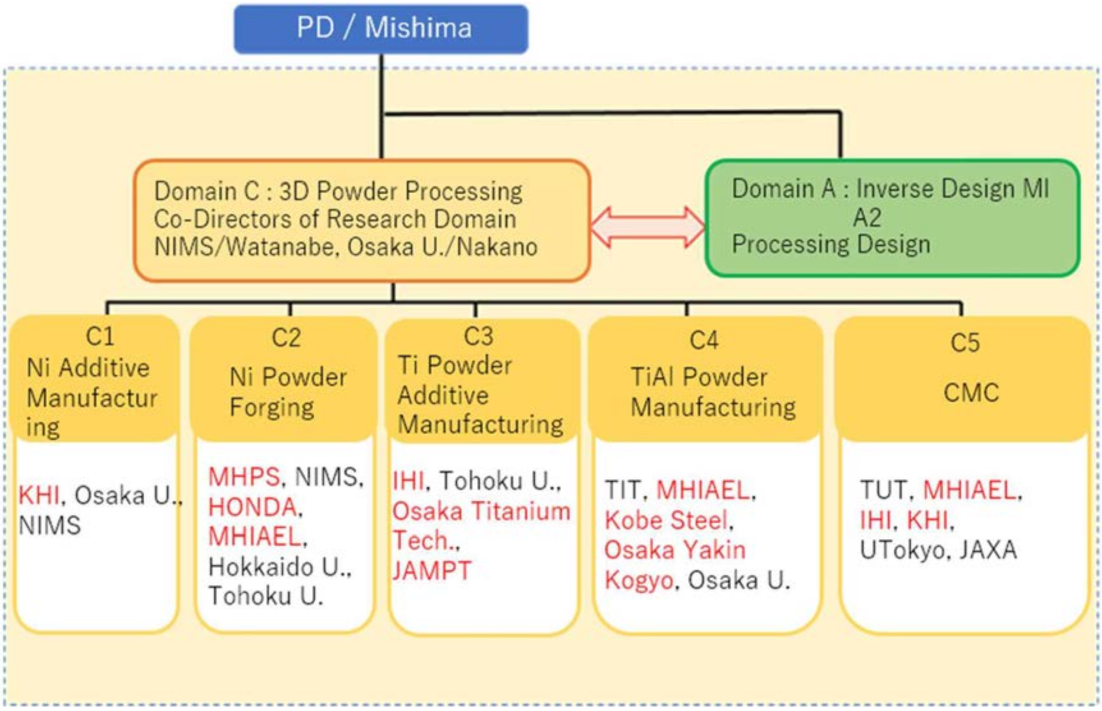


Figure 10 Domain C: research organization for 3D Powder Processing
(private companies are in red)

(C-1) Development of Additive Manufacturing Process for Ni-based Alloys

Co-leaders:
Kenichiroh Igashira (Kawasaki Heavy Industries, Ltd.)
Takayoshi Nakano (Osaka University)

Participating organizations: Kawasaki Heavy Industries, Ltd., Osaka University, and the National Institute for Materials Science

AM process technology offers advanced processes for manufacturing parts with three-dimensional, complex, and intricate designs that can not be manufactured with conventional methods. AM processes are expected not only to revolutionize design, but also to have many effective uses owing to the unique properties it imparts to materials. However, a precise means for exploring materials and processes suited to AM processes has not been established. Further, there has been increasing demand to reduce greenhouse gas emissions in order to realize Society 5.0, and studies are being conducted on expanding the variety of fuels that can be used in power plants, and particularly in gas turbines for power generation. For example, when using hydrogen gas as fuel, the combustion burner must be formed of a nickel-based heat-resistant alloy capable of supporting the high burning rate and high combustion temperatures inherent in hydrogen gas. There will also be increasing need for more complex designs and more durable materials.

An AM process using Ni-based alloy powder is the best technology for meeting these needs. Establishing MI technology for guiding the exploration of materials and processes may become a source of Japan’s competitiveness.

In view of this situation, a consistent prediction technology developed with the MI system as a common technology will be utilized in this development in order to establish a technology for predicting the material properties of Ni-based heat-resistant alloys molded in AM processes. An inverse design analysis technology developed with the MI system will be utilized with the aim of establishing a technology based on these prediction technologies for designing suitable alloys and process conditions that satisfy the required performance of the parts.

Additionally, a new technology for predicting nonequilibrium phase diagrams corresponding to the rapid solidification in AM processes will be developed while utilizing Japan’s background in Ni-based heat-resistant alloys. With this prediction technology, we will establish an MI technology for nonequilibrium alloy designs specific to AM processes that will be utilized in this study to propose alloys and determine processes. After the SIP project has ended, this MI technology may be the one that differentiates Japan from other countries in the field.

These MI prediction technologies in cyberspace will be put to use in physical space to select materials and to develop manufacturing processes. Universities and other institutes will be responsible for linking cyber to physical and will act as an intermediary with companies for parts production. We will install AM processing equipment at participating companies and select materials that match the requirements for combustion burner parts. We will also focus on establishing processes for manufacturing the parts and techniques for evaluating components. Demonstrating an improved performance in combustion burners will be an end goal of this development.

Intermediate Goals (for the end of fiscal 2020)

Overall goal and target TRL for R&D
- Mount combustion burner formed by AM for actual combustion tests
- Achieve TRL 4

Targets of individual research items

(a) Demonstrate fabrication of new Ni-based alloys utilizing MI

- Collect experimental data with existing Ni-based alloys for implementing the MI system (physical space)
- Confirm consistency between forward analysis simulation data and the above experimental data for existing Ni-based alloys (link between cyberspace and physical space)

(b) Verify improved durability of combustion burner

- Establish a manufacturing technology for combustion burners formed through AM using commercially available material (or refined versions thereof)

- Establish a technology for evaluating material properties suited to AM materials

End Goals (for the end of fiscal 2022)

Overall goal and target TRL for R&D

- Successfully conduct continuous burning of four hours or longer in combustion tests performed in an actual pressurized environment using a combustion burner manufactured by AM
- Achieve TRL 5

Targets of individual research items

(a) Demonstrate fabrication of new Ni-based alloys utilizing MI

- Collect experimental data for new Ni-based alloys (physical space)
- Confirm consistency between forward analysis simulation data and the above experimental data for the new Ni-based alloys (link between cyberspace and physical space)
- Demonstrate manufacturing of new Ni-based alloys with required mechanical properties for AM material

(b) Verify improved durability of combustion burner

- Establish a manufacturing technology for combustion burners formed through AM using the new Ni-based alloys
- Confirm improved durability of the new Ni-based alloys using a technique for evaluating materials manufactured by AM

(C-2) Development of Ni-based Powder Metallurgy Processing for High Performance Aircraft Engine Disk

Co-leaders:
Shinya Imano (Mitsubishi Hitachi Power Systems, Ltd.)
Toshio Osada (the National Institute for Materials Science)

Participating organizations: Mitsubishi Hitachi Power Systems, Ltd., the National Institute for Materials Science, Honda R&D Co., Ltd., Mitsubishi Heavy Industries Aero Engines, Ltd., Hokkaido University, and Tohoku University

Disk materials used in commercial aircraft engines have been forged of high-strength nickel-based alloys, such as Inconel 718 (IN718) and Waspaloy. Both alloys have excellent strength at elevated temperatures and good manufacturability and reliability. However, in order to handle the rising combustion temperatures, powder-processed Ni-based alloys used as disk materials (hereinafter called “PM disk superalloys”) are being adopted for high-pressure turbine disks whose operating environment is particularly severe, and applications for these superalloys are expected to continue to expand. A high-quality powder manufactured under high vacuum and inert gas is subjected to sintering under pressure or superplastic forming at high temperatures to form the PM disk superalloy into a disk shape. Members sintered using Ni-based alloy powder are also used in molds and other components. PM disk superalloys possessing excellent strength at high temperatures have become more and more indispensable in recent years for high-performance aircraft engines. However, since production requires special advanced technologies, their manufacturing costs are prohibitive outside of a limited number of manufacturers in Europe and America. This research is aimed at developing purely domestic low-cost processes surpassing those being used in Europe and America. These processes will be applied to actual aircraft parts by improving and integrating Japan's latent strengths in powder manufacturing technology and forging technology for high-strength Ni-based alloys.

The main processes required for producing PM disk superalloys are powder manufacturing, billeting forming, and near-net-shape forging. In this study, MI will be utilized to develop low-cost processes using existing facilities in Japan. In addition to reducing process costs, a study will be conducted on further lowering costs by using byproduct powders generated in the powder manufacturing process for molds and stationary components of aircraft engines and industrial gas turbines. The aim of this study is to reduce manufacturing costs to at least two-thirds the current costs, while ensuring performance is at least equal to conventional process materials.

The first three years of the study (2018–2020) will be dedicated to establishing and demonstrating technologies with simulated members through implementation items (i)–(vii) provided below. Target materials are domestically produced materials that are utilized in the latest engines for mid-size commercial aircraft. Additionally, PM disk superalloys in engines for military aircraft and castings/forgings commensurate to PM disk superalloys will be trial manufactured and evaluated as needed for comparison. In the latter two years of this research, manufacturing and evaluation aimed at commercialization will be conducted on parts formed for use on actual aircraft according to items (viii)–(xii) provided below.

Implementation items
(i) Establish powder manufacturing/classification technology, (ii) establish canning and HIP technologies, (iii) establish billet forging technology, (iv) establish near-net-shape forming technology, (v) research and examine evaluation techniques, (vi) establish techniques for developing and repairing mold materials, (vii) trial manufacture and evaluate simulated materials for actual aircraft, (viii) trial manufacture high-pressure disks for mid-size commercial aircraft, (ix) begin collecting data on acquiring certification to advance MI, (x) trial manufacture of high-pressure disks for small aircraft, (xi) begin collecting data on acquiring certification to advance MI, and (xii) study applications for next-generation commercial aircraft

In this study, physical aspects will be compiled by private companies possessing basic technologies of the relevant processing, while cyber aspects will be compiled by universities or national research institutes with a track record in studying MI technology. Many manufacturers of aircraft engines will participate in establishing development goals and evaluating development technologies for the physical side.

While this study will target a wide range of manufacturing processes, a new target will be the development of MI technology for the efficient elimination of prior particle boundaries, which are a major problem in powder processing. Here, a technology for predicting microstructural changes during high-temperature deformation in the forming of billets will be key. As before, the early stage of this study will involve the exploration of conditions for forming billets based on experimentation, and MI technology will be established based on the data obtained through this exploration. In the latter half of the study, the MI technology established early on will be utilized to further optimize conditions of billet formation by introducing inverse analysis techniques developed with the MI system. An MI technology for a billet-forming process that supports inverse problems will be established for use in post-SIP development. A common MI technology developed for the MI system will be actively applied to other methods with the aim of establishing efficient development processes. Specifically, outcomes of development with the MI system will be utilized in powder sintering processes and near-net-shape forging, and workflows will be developed to link multiple development processes. Moreover, a study will be conducted on reducing development time with MI.

Intermediate Goals (for the end of fiscal 2020)

The trial manufacture of simulated components for mid-size commercial aircraft engines will be completed using PM disk superalloys produced domestically and produced overseas. The goal is to obtain properties in a fracture study on simulated parts formed of domestically produced PM disk superalloys that meet or exceed the target mechanical properties set by manufacturers of aircraft engines.

- The target for mechanical properties is set to 95% that of process materials in Europe and America.
- TRL 4 is the target for raw materials.
- Data related to manufacturing processes for PM forged disks is provided to the MI-side as needed, and intermediate results from the MI-side are reflected in the manufacturing process for the purpose of optimization.

End Goals (for the end of fiscal 2022)

Trial manufacturing of parts for small aircraft engines using domestically produced PM disk superalloys will be completed. Once a fracture study on prototypes formed from domestically produced PM disk superalloys indicates that the target mechanical properties and costs set forth by aircraft engine manufacturers have been attained, we will begin considering applications for domestic materials formed with domestic processes in next-generation aircraft engines. Trial manufacturing of parts simulating high-pressure turbine disks for mid-size commercial aircraft produced overseas will be completed using processes developed domestically.

- The target for mechanical properties of PM disk superalloys produced domestically is at least 95% that of European and American process materials, and the target cost is no more than 66% of processing costs in Europe and America.
- TRL 5 is the target for raw materials.
- Relevant data in the fracture study will be shared with the MI system, and the consistency of predictions by tools developed with the MI system will be studied. The data from this study will be utilized to improve the precision of the prediction tools.

(C-3) Development of Powder Additive Manufacturing Process for Titanium Alloys

Co-leaders:
Satoshi Takahashi (IHI Corporation)
Naoyuki Nomura (Tohoku University)

Participating organizations: IHI Corporation, Tohoku University, Osaka Titanium Technologies Co., Ltd., and JAMPT Corporation

Below is a description of the R&D content that will be implemented with the assistance of MI. In this R&D, metal powder manufacturers, mold manufacturers, heavy industry manufacturers, and universities will collaborate to research and develop techniques for the manufacture of metal powders, additive manufacturing (AM), and the evaluation of component performance. To enable integrated production domestically, a system will be established for manufacturing AM parts from titanium alloy components with which Japan has been competitive globally. Our goal is that this system will help build a supply chain for the purpose of supplying aircraft components and medical materials, for example.

(i) Development of an economical technology for manufacturing Ti powder
In order to reduce processing costs for manufacturing materials, we aim to reduce the cost of feedstocks, which are the leading cause of increased costs in manufacturing processes for titanium alloy powders. In this research, new processes will be introduced at the feedstock production stage. We will study how to optimize the process and develop a manufacturing process for titanium alloy powders.

(ii) Development of AM processes
New powders may have different properties from existing high-cost powders. Therefore, we must conduct a study for creating a fabrication process suited to their properties in the AM process and, by reflecting the findings back to the new powders, establish a competitive AM process for titanium alloys.

(iii) Establishment of an evaluation method and guidelines for powders used in AM
Since newly developed powders have different properties from current expensive powders, their use in powder bed AM processes may yield differences in recoating behavior and conditions of the powder bed, which can affect properties of the fabricated article. In this research, we will study recoating behavior through experiments and simulations in order to identify what factors affect conditions of the powder bed and to learn what properties are required for the new powders, leading to more efficient development.

(iv) Property evaluation and application demonstration of parts manufactured by AM
AM parts differ greatly from those produced in current manufacturing methods (casting or forging) in their surface roughness, material properties, and product shape, for example. Thus, in order to adopt AM parts in actual aircraft, we must learn these differing characteristics and reflect them in their design. In this study, the mechanical

properties of AM components will be evaluated to obtain a simple database. We will also conduct microstructure observations and evaluate associations among characteristics of Ti powders, fabricating conditions, and microstructures of the metal.

Development in item (i) will be coordinated with an MI technology for new powder design to accelerate property evaluation of lower-cost powders and to reflect those evaluations in the AM process.

In this study, powder manufacturing, evaluation of powder properties, evaluation of spreading ability, and evaluations of the properties of parts manufactured by AM will be conducted in collaboration with organizations in the domestic supply chain for AM processes with the aim of improving Japan’s competitiveness in a coherent AM process from the upstream sector to the downstream sector. Establishing a recoating simulation technique (MI technology) for the AM process in particular will lead to methods and guidelines for evaluating the Ti alloy powder used in AM and will enable uniform evaluations of the powder and the entire AM process.

Intermediate Goals (for the end of fiscal 2020)

- We will conceptualize an economical fabrication process for Ti alloy powders, set up facilities, and begin trial manufacturing and provision of powders to the facilities (TRL 2).
- Fabrication conditions will be established to enable the manufacture of simulated parts having shapes proposed by IHI, using conventionally produced Ti alloy powders, and actual components will be fabricated (TRL 2).
- The properties of current and economical powders will be evaluated.
- Properties required for economical powders will be identified.
  Data on the properties of components fabricated with conventional Ti alloy powders will be acquired, evaluated, and organized.

End Goals (for the end of fiscal 2022)

- Manufacturing processes for economical Ti alloy powders will be demonstrated with the goal of reducing feedstock costs by 20% (TRL 2).
- Material and fabrication recipes will be formulated for economical Ti alloy powders and actual components will be manufactured (TRL 3).
- Design guidelines will be formulated for economical powders (TRL 3).
- Properties of components fabricated using both conventionally produced Ti alloy powders and economically produced Ti alloy powders will be evaluated, and the results will be compiled in a database (TRL 2).

(C-4) Development of Powder Manufacturing Process and Basic Technologies for High Performance TiAl-based Alloy Turbine Blades

Co-leaders:
Masao Takeyama (Tokyo Institute of Technology)
Akira Fukushima (Mitsubishi Heavy Industries Aero Engines, Ltd.)

Participating organizations: Tokyo Institute of Technology, Mitsubishi Heavy Industries Aero Engines, Ltd., Kobe Steel, Ltd., Osaka Yakin Kogyo Co., Ltd., and Osaka University

Titanium aluminide (TiAl alloy) is an intermetallic chemical compound having excellent specific strength and heat-resistance and shows promise for use as a material in low-pressure turbine (LPT) blades in aircraft engines. TiAl has reached the implementation stage in the GEnx engine of the Boeing 787 and the PW1100G engine of the Airbus A320neo. These engine parts are manufactured by machining castings or forgings, but the low yield and the inclusion of the machining process is viewed as problematic factors that increase costs of blade parts.

In the meantime, metal injection molding (MIM) has attracted attention as a low-cost manufacturing method for the mass production of small metal parts. A feature of MIM is its ability to manufacture net-shape parts. Thus, use of this technique to manufacture blade parts could reduce manufacturing costs by eliminating the machining step for the blade surface.

Hence, the MIM technique has been considered a candidate for producing low-cost titanium aluminide blades. However, TiAl is inherently a brittle material and, thus, overcoming it’s low fracture toughness will be a challenge. There is also a concern that the fracture toughness of this material may drop even further due to the increasing inclusion of oxygen and other components during the MIM process. To overcome these challenges and concerns, we must determine the chemical and phase compositions and the morphologies of materials capable of achieving high fracture toughness despite the presence of oxygen and other components. We must then set manufacturing parameters for producing high-grade, low-cost TiAl ingots for the MIM process and for reducing contamination from oxygen and other components that occurs during this process.

Unlike conventional materials development centered on experimental techniques, this R&D will address the above challenges utilizing MI technology to simulate alloy design and performance predictions with the aim of optimizing process parameters.

Actual LPT blades are large members exceeding 200 mm in length. Consequently, these blades are difficult to manufacture with conventional MIM technology. One issue in the MIM process is the control of deformation in such large structures. To resolve this issue, MI technology will be utilized to establish a process incorporating injection and sintering simulations.

The aim of materials development for TiAl is to search for material compositions having excellent heat-resisting properties aimed at improving the performance and heat-resistance of the engine. In powder-based MIM, the composition can be freely designed without the restrictions inherent in casting and forging. Taking advantage of this knowledge, we will utilize MI technology to design a TiAl alloy for MIM having excellent properties at high temperatures.

Utilization of MI technology
The following are five challenges in this R&D that will be resolved using MI.

(i) Determine the chemical/phase compositions and the morphology of a material for MIM that will improve toughness
(ii) Develop a manufacturing technology for high-grade, low-cost TiAl ingots to be used in MIM
(iii) Optimize the MIM process to improve toughness
(iv) Control deformation of large structures in MIM
(v) Determine chemical/phase compositions and morphology of materials to be used in MIM for improving properties at high temperatures

Here, alloy design and performance prediction technologies will be applied to overcome challenges (i) and (v). AI-assisted data science techniques will be used to optimize processes in (ii) and (iii). Various simulation techniques will be used to control deformation in (iv). Knowledge from universities that are global leaders in technological fields specific to TiAl alloys will be further advanced and utilized to accelerate development in alloy design and performance prediction.

The data science-based inverse analysis technology developed as a common technology with the MI system will be utilized for the MIM process in an attempt to optimize the process. We will also promote technology transfer so that MIM manufacturers themselves can master this technology. Additionally, a technique for optimizing the sintering process will be established for controlling deformation in MIM utilizing MI technology for powder sintering developed with the MI system, and this technology will be utilized to develop actual components.

Intermediate Goals (for the end of fiscal 2020)

(i) MIM: An alloy for use in powder processes aimed at achieving sufficient fracture toughness and tensile strength for application to turbine blades will be designed using the MI system (a prototype) and verified (TRL 3).
(ii) Electron-beam AM: A process map will be created using the MI system to link fabrication conditions with microstructures and mechanical properties (TRL 3).

End Goals (for the end of fiscal 2022)

(i) MIM: A process for manufacturing large blades meeting an airfoil profile that can achieve near-net shape will be designed based on the MI system, and strength feasibility of an actual blade will be confirmed using a blade prototype (TRL 4–5).
(ii) Electron-beam AM: An AM process will be optimized using the MI system and a prototype turbine blade will be manufactured (TRL 4).

(C-5) Realistic Simulation of Ceramic Matrix Composites Targeted for High Temperature Components in Jet Engines

Co-leaders:
Yutaka Kagawa (Tokyo University of Technology)
Naohiro Shichijo (Tokyo University of Technology)
Takahiro Sekigawa (Mitsubishi Heavy Industries Aero Engines, Ltd.)

Participating organizations: Tokyo University of Technology, Mitsubishi Heavy Industries Aero Engines, Ltd., IHI Corporation, Kawasaki Heavy Industries, Ltd., the University of Tokyo, and the Japan Aerospace Exploration Agency

Ceramic matrix composites (CMCs) are lightweight materials with excellent heat-resistance. CMCs are expected to replace current high-temperature structural materials (superalloys) in the near future for use as aircraft engine components. One type of CMC formed of continuous SiC fibers embedded in an SiC matrix (also known as SiC/SiC) has become the subject of active R&D worldwide owing to its particularly excellent properties.

The most important issue with regard to commercializing CMCs as aircraft engine components is to guarantee their performance and safety for long-term use at high temperatures. In recent years, simulation techniques have been used frequently in materials development, and their use is anticipated in the development of CMC components for aircraft engines. However, current simulation techniques are inadequate because CMCs have a far more complex composite structure than those of monolithic ceramics and metal materials, and their deformation and fracture phenomena is governed by factors too numerous to count. Yet, if the materials can be tested in cyberspace using MI, the ability to test components being designed using inverse problems would greatly strengthen Japan's international competitiveness.

In this study we will develop modules as a foundation for using MI in the development of CMC components. A virtual test environment will be created so that these modules can be linked in cyberspace to predict the behavior of CMCs in their operating environment, and will drive the development of CMCs as aircraft engine components. Our ultimate aim is to use virtual tests to design optimal members and to develop techniques for inspecting CMCs.

The following are four specific subjects that will be targeted in this R&D.

(i) <u>Basic technologies and an integrated platform</u>
R&D will be conducted on core technologies required for solving specific issues in the development of CMC components. Specific core technologies will include the visualization and recognition of CMC microstructures through machine learning, prediction of CMC properties, high-temperature testing for CMCs, and reliability assurance.

(ii) <u>Processing conditions for ensuring performance of CMC components</u>
A simulation system will be developed to assist in setting conditions for manufacturing processes used to fabricate CMCs.

(iii) <u>Evaluation of risk and defect distribution for ensuring CMC performance</u>
A technique will be developed for recognizing and evaluating defect distribution during the manufacturing of CMCs.

(iv) <u>Degradation prediction and risk evaluation for ensuring CMC performance</u>

A model will be constructed for predicting performance degradation under conditions simulating the CMC operating environment, and a method will be developed for evaluating risk in the deployment of CMC components.

Intermediate Goals (for the end of fiscal 2020)

(i) Basic technologies and an integrated platform
Technologies for recognition and visualization of CMC microstructures, acquisition of CMC properties, high-temperature testing of CMCs, and accelerated testing of CMCs will be provided for use in R&D on subjects (ii)–(iv).

(ii) Processing conditions for ensuring performance of CMC components
Multiphysics simulations will be implemented for CMC matrix manufacturing processes using the reactive melt infiltration (RMI) method based on an understanding of basic processes used to manufacture a CMC matrix using the RMI method.

(iii) Extraction of risk and defect distribution for ensuring CMC performance
The automatic recognition of microstructures in CMC materials based on structural data for such materials acquired with X-ray computed tomography will be achieved using machine learning.

(iv) Prediction of performance degradation and determination of risk in CMC components
A model will be constructed to predict degradation of mechanical properties for CMC materials under high temperatures, and the model will be evaluated through materials testing under similar conditions.

End Goals (for the end of fiscal 2022)

(i) Basic technologies and an integrated platform
The outcomes in research subjects (ii)–(iv) will be integrated to ensure safety in the designs of CMC components.

(ii) Processing conditions for ensuring performance of CMC components
Simulations of CMC matrix manufacturing processes using the RMI method will be made feasible for preforms having expected shapes of actual components.

(iii) Extraction of risk and defect distribution for ensuring CMC performance
Structural data will be acquired for CMCs during manufacturing and after mechanical load is applied from X-ray computed tomography, and the distribution of defects that can affect defect expansion will be automatically recognized based on structural changes identified through machine learning.

(iv) Prediction of performance degradation and determination of risk in CMC components
A model will be constructed for predicting the lifetime of CMC materials under high temperatures and mechanical load and will be made applicable to materials with realistic shapes.

3. Implementation structure

(1) Program Director, Deputy Program Director, and management agency

PD Yoshinao Mishima will be in charge of establishing and promoting the R&D plan, while Deputy PD Tetsuo Mohri will assist the PD. A promotion committee composed of related ministries and agencies and specialists will perform general coordination, with the PD serving as chair and the Cabinet Office as secretariat. This research subject will be carried out through funding provided by the Japan Science and Technology Agency (JST). JST will serve as the management agency in assisting the PD, Deputy PD, and promotion committee. In conformance with the R&D plan, JST will hold an open recruitment for Principal Researchers, execute contracts, manage funding, oversee R&D progress, implement self-inspections from a technical perspective using peer reviews, report the results of these self-inspections to the PD, etc., and conduct related studies and analyses.

(2) Selection of Principal Researchers

Based on the R&D plan, JST will conduct a call for proposals and recruitment to select research topics and the Principal Researchers that will implement these research topics. However, such selections need not be made publicly if there are sufficient grounds not to do so and if those reasons are specifically stated in the R&D plan.

JST will, in consultation with the PD, the Cabinet Office, and the promotion committee, determine the method of screening selections, such as screening criteria and judges. In principle, the PD, officers from the Cabinet Office, and outside experts will participate in the screening. key project personnel of researchers who have submitted a research proposal will not participate in the screening of that research topic. A definition of "stakeholders" will be clearly specified in the application guidelines established by JST. Once the research topics have been determined through selection, the topics along with their research entities and participants will be specified in this plan.

(3) Measures to optimize the research system

Companies corresponding to Tier 1 or Tier 2 suppliers of the aircraft industry and companies that supply raw materials directly to original equipment manufacturers (OEMs) will participate in teams established under this subject "Materials Integration" for Revolutionary Design System of Structural Materials, with teams configuring a vertical integration system that outputs materials for aircraft. With this system, an inverse design MI system will be developed in Domain A while being applied to advanced structural materials and processes in Domains B and C in order to accelerate the use and application of MI in companies (social implementation of MI). This will be accomplished by collecting data on cutting-edge materials for aircraft components and utilizing this data in inverse design MI to develop materials and processes that meet the required performance for social implementation, thereby achieving a vertical integration system driven by inverse design MI.

Note: Tier 1 denotes manufacturers that supply parts directly to companies manufacturing finished aircraft or aircraft engines, while Tier 2 denotes manufacturers that supply parts to Tier 1 companies.

The Cabinet Office will have flexibility to make changes to the research structure or take other measures deemed necessary by the PD, depending on the progress of the research topics, research results of technical surveys conducted by related organizations, and changes in social circumstances. Specific considerations will include changing or adding research topics and replacing or adding Principal Researchers. In order to promote more spirited personnel exchange and facility sharing, as well as the development of human resources and sustained research, R&D centers will be established to allow for collaboration among universities, national research and development agencies, and companies.

The Deputy PD will assist the PD in exit strategies and intellectual property strategies, expertise on materials science, and cross-ministerial and industry-academia-government collaboration. The Deputy PD will also be in charge of specific R&D items and domains and will assist the PD in implementing R&D in these domains.

Co-leaders established in each R&D domain will be selected from both industry and academia, and coordination within and among domains will be achieved through close cooperation between industry and academia. Activities of the domains will be conveyed through symposiums and other events. JST will support the activities of co-directors and will build a network among the participating organizations.

(4) Coordination with government ministries and agencies

Coordination among government ministries and agencies is essential for establishing a data infrastructure to support inverse design MI and for its expansion to wide-ranging materials. With SIP leading the way, MEXT is responsible for developing the materials data infrastructure and METI for expanding the outcome areas through the promotion committee and conferences for promoting the projects. All of these efforts will lead to the implementation of an integrated materials development system for supporting Society 5.0.

(5) Commitment from industry

This project anticipates contributions (both human and material) from industry. Contributions in materials development for (B) Application of inverse design MI to actual structural materials (see the Appendix) is expected to account for 20% of the total R&D expenses (including contributions from the national government and industry) for the first through third years of the project, and approximately 30% the total for the fourth and final years. Further, the matching funds will be reviewed in accordance with the Cabinet Office’s matching funds system for SIP.

4. Matters related to intellectual properties

(1) Intellectual property committee and subcommittees

- ○ An intellectual property committee will be established in the management agency, while an intellectual property subcommittee will be set up at the organization (trustee) to which the Principal Researcher belongs for each research subject or joint research item constituting the subject.
- ○ Intellectual property subcommittees will determine policies for the publication of papers and the application and maintenance of patents (hereinafter called “IP rights”) concerning the outcomes of research and development undertaken by the organization at which the relevant subcommittee was established, and will make adjustments pertaining to the licensing of IP rights as needed. Intellectual property subcommittees will submit reports concerning such paper publications and IP rights to the intellectual property committee.
- ○ The intellectual property committee will in principle be composed of the PD or an agent of the PD, key project personnel, and experts. The intellectual property subcommittees will comprise members of the participating organizations of the relevant research subjects.
- ○ Details of operating methods for the intellectual property committee and subcommittees will be determined by the management agency or the organizations establishing intellectual property subcommittee.

(2) Arrangement concerning IP rights

- ○ he management agency will determine in advance through an agreement with the trustee the handling of confidentiality, background IP rights (IP rights that Principal Researchers and the organizations to which they belong had possessed prior to participating in the program, or that they obtain without the use of SIP operating expenses after participating in the program), and foreground IP rights (IP rights generated through the use of SIP operating expenses during the program).

(3) Licensing of background IP rights

- ○ The IP rights holder can grant a license for a background IP right to another program participant under terms and conditions determined by the rights holder (or “in accordance with the agreement with the program participant”).
- ○ For cases in which measures taken by the IP rights holder, including said terms and conditions, may interfere with the promotion of SIP (including not only the research and development, but also practical use and commercialization of the outcomes), the intellectual property committee will make adjustments to obtain reasonable solutions.

(4) Handling of foreground IP rights

- ○ In principle, the provision of Article 17, Paragraph 1 of the Industrial Technology Enhancement Act will apply to foreground IP rights, which will be vested in the organization (trustee) to which the Principal Researcher who is the inventor belongs.

- In the event of an invention made by a subcontractor, etc., IP rights may be vested in the subcontractor, etc., only with the approval of the intellectual property committee. In such cases, the intellectual property committee may attach conditions to the approval.
- If the rights holder of an IP right has little intention of pursuing commercialization, the intellectual property committee may recommend that an individual who is more committed to commercialization be given possession of the IP right or granted license for the IP right.
- For any individual withdrawing from the project during the participation period, the management agency, etc., will require that the individual assign free of charge, or grant a license for, all or part of the outcomes obtained with the use of SIP operating expenses during that individual's participation period (or all of the outcomes since that individual initially participated in the project, in the event of participation over multiple years) at the time of withdrawal.
- In principle, the rights holder will be responsible for the costs of application and maintenance of the IP rights. In the case of joint application, the percentages of ownership and cost burden will be determined through discussions between the joint applicants.

(5) Licensing of foreground IP rights

- The rights holder can grant a license for a foreground IP right to another program participant under terms and conditions determined by the rights holder (or "in accordance with the agreement with the program participant").
- The rights holder can grant a license for a foreground IP right to a third party under terms and conditions determined by the rights holder, provided that such terms and conditions are not more advantageous than those for other program participants.
- For cases in which measures taken by an IP rights holder, including said terms and conditions, may interfere with the promotion of SIP (including not only the research and development, but also practical use and commercialization of the outcomes), the intellectual property committee will make adjustments to obtain reasonable solutions.

(6) Approval for transfer of, and establishment and transfer of an exclusive license for, foreground IP rights

- Under the provision of Article 17, Paragraph 1, Item 4 of the Industrial Technology Enhancement Act, any transfer of, or any establishment and transfer of an exclusive license for, foreground IP rights will require the approval of the management agency, except in cases of transfer due to a corporate merger or division, and cases of transfer of, or establishment and transfer of an exclusive license for, IP rights to a subsidiary or parent company (hereinafter collectively referred to as "cases of IP rights transfer, etc., due to mergers, etc.").
- Cases of IP rights transfer, etc., due to mergers, etc., will require the approval of the management agency, etc., under contract with the management agency, etc.
- Even after IP rights transfer, etc., due to mergers, etc., the management agency, etc., may be able to possess a license for the IP rights, including the right for sub-licensing. Unless this condition is accepted, the transfer will not be permitted.

(7) Handling of IP rights at the time of termination

- With regard to IP rights, etc., that no one wishes to possess when the research and development is terminated, the intellectual property committee will discuss a course of action (abandonment or succession by the management agency, etc.).

(8) Participation by overseas organizations, etc. (such as foreign companies, universities, and researchers)

- Participation by an overseas organization, etc., will be permitted when such participation is necessary for carrying out a research task.
- From the perspective of appropriate executive management, only an overseas organization, etc., with a point of contact or an agent in Japan capable of processing paperwork related to acceptance of the research and development will in principle be permitted to participate in the project.
- In the case of participation by an overseas organization, etc., IP rights will be shared by the management agency, etc., and the overseas organization, etc.

5. Matters related to assessment

(1) Assessing entities

The Governing Board will invite external experts to perform assessments while referencing reports of self-inspections conducted by the PD and JST based on national and international peer reviews. The Governing Board may hold assessments individually by research area or subject. Note that particular care must be taken when receiving external assessments to avoid any disclosure of information.

(2) Timing of assessments

- Assessments will include preliminary assessments, end-of-year assessments, and final assessments.
- Once a fixed period (three years, in principle) has elapsed after termination of the program, tracking assessments may be performed, as needed.
- In addition to the above, assessments may be performed in the middle of a fiscal year, if necessary.

(3) Assessment items and criteria

Based on the “General Guideline for the Evaluation of Government Research and Development (R&D) Activities” (established by the Prime Minister on December 21, 2016), assessment items and criteria are given below from the perspective of assessing necessity, efficiency, and effectiveness. Assessments are performed not merely to determine whether the goals have been attained, but will also include an analysis of the causes and factors of such attainment or nonattainment and a proposal of measures for improvement.

(i) Significance and consistency with the organizational objectives of SIP.

(ii) Appropriateness of the goals (particularly the technology outcomes) and degree of progress made in the schedule toward attaining the goals.
(iii) Whether or not proper management is being made; particularly, how effective collaboration is being demonstrated among government ministries and agencies.
(iv) Strategic relevance, and degree of achievement, toward practical use and commercialization.
(v) Expected effects or ripple effects in the final assessment. Whether or not post-program methods for follow-up have been specified clearly and adequately.
(vi) Status of meeting the requirements listed in the attachment.
(vii) Status of achieving TRLs in each research topic.

(4) Methods of reflecting assessment outcomes

- Preliminary assessments in connection with the R&D plan will be conducted annually and reflected in the plan beginning from the fiscal year following the commencement of research.
- Each end-of-year assessment will involve refining or adding to the research subject and research topics as needed.
- Final assessments will be performed in connection with actual outcomes up to the final fiscal year, and will be reflected in the post-program follow-up.
- Tracking assessments will be performed in connection with the progress of practical use and commercialization of the outcomes of each task, and measures for improvement will be proposed.

(5) Disclosure of outcomes

- In principle, assessment outcomes will be made available to the public.
- The Governing Board that performs assessments will be held privately since the assessments may involve undisclosed research and development information.

(6) Self-inspections

(i) Self-inspection by Principal Researchers

The PD will select Principal Researchers to perform self-inspections. (In principle, the primary researchers or research institutes of each research item will be selected.) The selected Principal Researchers will conduct self-inspections on the progress of R&D and efforts toward practical use and commercialization.

(ii) Self-inspection by the PD

While referencing the results of self-inspections by the Principal Researchers and, when necessary, the opinions of third parties and peer reviews by national and international experts, the PD will personally inspect the actual results of the PD, JST, and each Principal Researcher and the future plan in accordance with the assessment items and criteria provided in 5(3). The PD will summarize not only determinations of whether goals were attained, but also an analysis of the cause and factors of such attainment or nonattainment and measures for improvement. Based on the results of the inspection, the PD will determine whether each research entity should continue their research, and provide necessary advice to the Principal Researchers. In this way, the research structure can be improved autonomously. Particular care must be taken when receiving external assessments to avoid any disclosure of information. On the basis of these results, the PD will prepare materials for the Governing Board with the support of JST.

(iii) Self-inspection by the management agency

Self-inspections by JST will be conducted to determine whether paperwork procedures related to budget execution have been performed properly.

6. Exit Strategies

This research subject has two major aims for social implementation.

(1) Use of MI systems in corporate R&D (Domain A)
(2) Practical application and commercialization of materials developed with MI systems (Domains B and C)

To achieve these goals, R&D will be conducted with the following strategies.

(1) Use of MI systems in corporate R&D

- The starting point of the inverse problem is set to numerical values of a target performance required by participating companies, i.e., potential users, and the effectiveness of the MI system is confirmed through solutions in cyberspace and demonstrations in physical space. Here, indices for evaluating the obtained solutions objectively are set to define success or failure.
- We will develop a distributed computation and control technology for seamlessly linking a system operated by a centrally located MI center with calculations in a local corporate environment over the Internet. Ensuring information security is one of the most important issues. By using distributed computations and control, calculations with classified data can be performed in-house, enabling the use and application of company-held data. In order to promote such use, a standard data description format will be designed and widely shared (even if the actual data cannot be). These efforts are hoped to encourage the use and application of data that lies dormant in companies.
- In order to promote the use of MI at companies, the establishment of consortiums and venture businesses will be studied and implemented. (Since venture businesses may take on overseas institutes as clients, sufficient care must be made to ensure the businesses are consistent with improving Japan’s international competitiveness.) MI centers will serve as the core of these operations. In addition to the activities described above, the centers will work to popularize MI through development of human resources, and publicity and outreach activities.

(2) Practical application and commercialization of materials developed with MI systems

- Cutting-edge materials and processes for aircraft fuselages and engines and industrial power plants are envisioned as applications for MI, and practical applications and commercial products for research achievements will be found through collaboration with material and heavy industry manufacturers.

- While only disclosed in the non-public edition, Table 1 shows the end goals set by each participating company. If these goals are achieved, the target TRL is also expected to be attained, enabling a smooth transition to the stage of development and demonstration aimed at practical use and commercialization following the conclusion of SIP.
- For aircraft, the close relationship between participating Tier 1 and Tier 2 companies and OEMs will be utilized to formulate methods of standardization, planning, and evaluation, as well as their accreditation, and to acquire certification. For industrial power plants, the participating companies are OEMs themselves. Thus, their technologies can be applied to actual aircraft, provided they meet their own companies' standards. While our long-term goal is to commercialize private aircraft on the global market, we will work to promote applications for our own products at an earlier stage as a form of social implementation.

7. Other important matters

(1) Legal basis

This project will be implemented in accordance with "3. Basic policy concerning the expense for creation and maintenance of science, technology and innovation" (May 23, 2014, Council for Science, Technology and Innovation) of Article 4, Paragraph 3, Item 7 of the Act for Establishment of the Cabinet Office (Act No. 89 of 1991), and the Operational Guidelines for the Cross-ministerial Strategic Innovation Promotion Program (May 23, 2014, Governing Board of the Council for Science, Technology and Innovation).

(2) Flexible plan modifications

This plan may be revised according to circumstances, from the perspective of producing the earliest and maximal outcomes. The following is a history of modifications made to date (the date and main details of the modification).

December 13, 2018 The R&D plan was approved by the Governing Board of the Council for Science, Technology and Innovation and confirmed by the Director-General for Science, Technology and Innovation, Cabinet Office.

(3) Successive Generations of Project Director, Deputy Project Director, and the Manager

1. Program Director

KISHI, Teruo
(April 2018 – March 2019)

MISHIMA, Yoshinao
(May 2019 - Present)

2. Deputy Program Director

MISHIMA, Yoshinao
(April 2018 – March 2019)

MOHRI, Tetsuo
(May 2019 - Present)

3. Assigned Director

CHISHIMA, Hiroshi
(April 2018 – September 2018)

TONOUCHI, Toshio
(October 2018 – Present)

4. Assigned Personnel
HOSODA, Naoe (March 2018 – June 2018)
YANAGIDA, Masatoshi (July 2018 – June 2019)
SAHARA, Ryoji (July 2019 – Present)

Deputy Assigned Personnel
TAMAGAWA, Akiko(April 2019- Present)

Attachment

Requirements for subjects initiated through the supplementary budget for FY 2017

(1) Is aimed at the realization of Society 5.0
(2) Places emphasis on areas needing a productivity revolution
(3) Entails not mere R&D, but R&D that will transform society
(4) Is an area important for resolving problems in society and improving Japan's economic and industrial competitiveness
(5) Has clear exit strategies aimed at practical use, commercialization, and social implementation (with precise plans for commercialization in five years)
(6) Has institutional exit strategies, such as intellectual property strategies, international standardization, and regulatory reforms
(7) Involves transdisciplinary efforts requiring collaboration among government ministries and agencies
(8) Includes comprehensive R&D covering the transition from basic research to practical use and commercialization
(9) Promotes an establishment of cooperative areas and a clear distinction between competitive areas (implements an open and closed strategy)
(10) Establishes a system of industry-academia-government collaboration having a built-in matching funds component and a structure linking R&D outcomes to practical use and commercialization by participating companies

Appendix Financial planning and estimation

FY 2018 Total: 2,500 million yen

Accounting breakdown

1. R&D budget (including general and administrative expenses and overhead expenses): 2,400 million yen

   Breakdown by R&D item

   (A) Technological development for inverse design MI (participating ministries: MEXT and METI)

   (B) Application of inverse design MI to actual structural materials (participating ministries: MEXT and METI)

2. Promotional expenses (personnel, assessments, conferences, etc.): 100 million yen

   Total: 2,500 million yen

FY 2019 Total: 2,080 million yen

Accounting breakdown

1. R&D budget (including general and administrative expenses and overhead expenses): 1,953 million yen

   Breakdown by R&D item

   (A) Technological development for inverse design MI (participating ministries: MEXT and METI)

   (B) Application of inverse design MI to actual structural materials (CFRP; participating ministries: MEXT and METI)

   (C) Application of inverse design MI to actual structural materials (3D powder processing; participating ministries: MEXT and METI)

2. Promotional expenses (personnel, assessments, conferences, etc.) 127 million yen

Total: 2,080 million yen