7.4 Construction of revolutional material development methods through fusion among experiments and theory/data science

Overview

The research and development of materials is undergoing innovation based on advancements in informatics technology. In the search for new substances based on materials informatics, several achievements have been made in the acceleration phase. However, in materials processes such as substance synthesis and material structure control, theories, modeling tools, and other informatics are insufficient for expressing the behaviors of actual substances, which obstructs innovation. The development of studies in the efficient search for optimum materials processes, the construction of new processes for creating materials, and the like is necessary, recognized as similarly essential in industrial fields.

With established strategic objectives, the period of development from the search for substances to the creation of materials will be significantly shortened via collaboration between experiments and computational or data science etc. (referred to henceforth as data science etc.), studies contributing to the creation of various materials will be advanced, and industrial competitiveness will be enhanced. Furthermore, contributions will be made to nurture human resources that understand both experiments and data science.

Targets to Achieve

In these strategic objectives, the purposes are to establish collaboration with data science etc. based on experiments in substance synthesis and material structure control, regarding various materials regardless of organic or inorganic origins. Thereby, a method can be constructed that leads to the development of renovative materials.

Specifically, the following goals are set.

(1) To construct a behavioral prediction model of existing materials and to synthesize materials by using it.

(2) To construct a structure control model of materials and to develop materials by using it.

Future Vision of a Society to be looked at during the research promotion

Through the achievements of the items stated in section 3, *Goals and Objectives,* not only materials development based on intuition and experience, but also the quick and efficient development combining material data and theoretical modeling and/or actual behavior modeling will become mainstream. This will contribute to the embodiment of the society described below:

- A society in which new functional materials, structural materials, and others are created based on high-level data science etc.
- A society in which research and development efficiency is highly enhanced, for example, with research phases shortened to 2 to 3 years from the conventional span of 10 years.
- A society in which the limitless pursuit of enhanced productivity and reduced cost is supported by high-level data science etc., permitting industrial advancement.
- A society in which the relation between desired performance and materials is clarified and end users, designers, and developers may select possible new functional materials for creation.

Specific Research Examples

(1) To construct a behavioral prediction model of existing materials and to synthesize materials by using it

Efforts will be made to construct a method enabling the prediction of substance behaviors in experiments and the synthesis of substances. For instance, the conditions of a reaction and data on the variance of the substance are translated into data through synthesis experiments, which are analyzed using methods of data science etc. to construct the optimum synthesis and reaction paths that will embody the desired substance composition and characteristics. The synthesis of new substances and the optimization of existing processes are among the objects of these efforts.

(2) To construct a structure control model of materials and to develop materials by using it

Efforts will be made to construct a method that enables the prediction of variance in the organization structure in the material control processes and to develop materials with controlled organization. For instance, analyses using data science etc. in experiments on the organizational control of inorganic and organic substances can be applied to construct a technology that presents the treatment process necessary to create a desired material organization and organization structure. Furthermore, the development of organization control and materials and/or the optimization of an existing organization control method are among the objects of these efforts.

Domestic and Foreign Research Trends

(Trends in Japan)

Our country is ranked highly internationally in fields relating to trial-manufacturing processes and/or the production of object materials. The fields of synthesis optimization for materials and the control of material organization are strong in terms of the total number of papers published in and since 2006, providing an advantage in materials research and experiments. In addition, although object materials are limited, the studies on the search for and discovery of unknown substances based on calculation and/or theory have been advanced in the "Materials Research by Information Integration" Initiative (Mi^2i). The regions from material processing to material production, life-expectancy prediction, and so forth are focuses in the "Innovative Structural Material" of the Cross-ministerial Strategic Innovation Promotion Program (SIP). The Project of the Super Rapid Development Platform Technology for Super Advanced Materials focuses on multi-scale simulations; these were formed as projects earlier than others. Furthermore, studies concerning material informatics and integration, such as the Artificial Intelligence, Big Data, IoT, and Cyber Security Integration Project at AIP (Advanced Integrated Intelligence Platform Project) and efforts at specific corporations, have been increasing the momentum of progress. However, studies of the actual creation of unknown materials are regarded as problems; the advancement and development of further study is recognized as necessary.

(Trends overseas)

The number of papers related to materials and informatics increased with the average annual growth rate of 9.8 percent* from 2006 to 2015; it can be said that this is regarded as an important and developing research area. Regarding particular countries, the US, a leader in the Materials Genome Initiative, invested 500 million dollars in the five years since 2011, which far exceeded others in the scale of investment. EU invested a small amount in each of the various projects advanced by Germany, Switzerland, Spain, and others. In China, Shanghai University has established the Shanghai Materials Genome Institute on campus. Each country has promoted endeavors in various phases, including the cultivation of human resources and researches.

*This figure was obtained using keywords such as "material," "data," and "informatics" based on the data available on the Web of Science.

Background of Consideration

The following surveys were conducted according to the *Guideline for the Preparation of Strategic Objectives and the Like'*(Resolution by Strategic Basic Research Subcommittee, Science and Technology Science Council, June 8, 2015)

(Preparation of analysis to examine domestic and overseas research trends by a scientometric method using the Grant-in-Aid for Scientific Research (KAKENHI) Database and similar information)

We prepared analytical materials regarding research trends in Japan and overseas by using scientometric techniques for analyzing research papers of co-citation relations or direct quotation relations in the Grant-in-Aid for Scientific Research Database, etc.

(Implementation of a questionnaire for specialists using analytical materials and preparation of notable research trends)

We implemented a questionnaire on noteworthy research trends based on the analytical materials that we had prepared for respective field units of the Center for Research and Development Strategy (CRDS) for Japan Science and

Technology Agency (JST), for the program directors etc., of the Japan Agency for Medical Research and Development (AMED), and for the experts participating in the expert network operated by the Science and Technology Foresight Center of the National Institute of Science and Technology Policy (NISTEP). We then analyzed the responses to the questionnaire and identified "Innovation of the Informatics Technology by Stage Fusion" as a noteworthy research trend.

(Holding of workshops and preparation of Strategic Objectives)

We held a workshop to bring together experts from industry and academia involved in the "Innovation of the Informatics Technology by Stage Fusion," which was identified as a noteworthy research trend. At the workshop, we focused on notable trends in Japan and overseas, social and economic impacts of progress in research and technological developments, visions of society arising from these advances, and the objectives to be met during the research period. We then prepared the Strategic Objectives based on the discussions in the workshop.

Relevant Matters in Cabinet Decisions, etc.

5th Science and Technology Basic Plan (approved by the Cabinet on January 22, 2016)

Chapter 2, (3), <1> It is necessary to further enforce the technology as a core of creating new value in which our country has advantage.

Chapter 2, (3), <2>, 2)

- The "material and nanotechnology" to lead to the differentiation of the system by the enhancement of various components such as innovative structural materials and new functional materials.

Chapter 3, (1), <3>

The creation of innovative functional materials, structural materials, etc. by making full use of computational science and data science is to be advanced, and, at the same time with this, an extreme reduction of their development period is to be realized.

General Innovation Strategies for Science and Technology 2016 (approved by the Cabinet on May 24, 2016)

Chapter 2, (1), 3, 2), [A]

In order to secure superiority against other countries, it is important that, not only the material informatics with a substance search as the main body, but also, by expanding the above-mentioned, all science technologies including theories, experiment, analyses, simulations, and databases are to be fused to construct a material development system capable of predicting the performance of materials (durability, safety, etc.). (Omitted) This system is capable of realizing the reduction of the periods of the creation of innovative substances and materials and of the research and development that anticipate needs, and thus is capable of realize the strengthening of the competitiveness of material industries. Furthermore, as new materials are early implemented in the society as energy-saving members, weight-reducing members, and so forth, they bring solutions to social problems such as energy and global environmental problems.

Japan Revitalization Strategy 2016—to the Fourth Industrial Revolution (approved by the Cabinet on June 2, 2016)

II, 3-1, (2)-2)-3

in the fields where Japan's strengths can be utilized, such as nanotechnology and materials, the Government will establish a global research center that will enable strategic sharing, application and use of big data, and construct human and research networks.

Other

- Researchers from the fields of experimental measurement, theoretical calculation, and information and mathematics are acting in the "Construction of Platform Technology for Advanced Materials Informatics Linking and Fusing Theory, Experiment, Computational Science, and Data Science" (established in 2015) by the Japan Science and Technology Agency (JST) Presto. With this objective, fusion among the experiments of substance synthesis, organization control, etc., data science, and so forth is promoted, as is the use and development of informatics technology in material development.
- In Mi^2i, efforts for advancing material development by the fusion of the construction of databases and data science are

implemented, where the search for new substances using the construction of a data platform and informatics is conducted. Consortium activities, in which 40 corporations or more participate, have begun.
- As for SIP-Innovative Structural Material, the development of structural and functional materials has been implemented regarding aviation materials; in the field of materials integration, a study integrating materials and anticipation has been implemented. The construction of software to integrate results is also advancing.
- Between the desired substance found in research at each location and the actual developed materials, a large technological gap separates the virtual substance and the real substance. With this objective, the creation of research results that mend this gap is also expected. In other words, the research is expected to link the studies on both sides for each project; an efficient and effective material development platform can be realized by bridging this gap.

7.5 Advanced interaction technologies within networked intelligent information environment

Overview

A recent global goal is to realize a "super smart society" in which everyone has access to optimized high-quality services in natural forms through endeavors to fuse cyber space and society at a high level based on widespread use of artificial intelligence technologies, big data analysis technologies, and so forth. For this purpose, research and development in relation to "human to human" and "human to machine" interactions have been managed in a variety of ways as essential technologies; a great leap in the development of such research fields is expected to be made for the realization of a super smart society.

For this purpose, the research field of interaction is widely recognized as focusing on "mutual actions with the whole environment connected to a network." In this field, interactions in a variety of forms such as "human to human," "human to machine," and "human to the whole environment" are supported at a high level, and behaviors are understood and controlled to lead to the design of innovative systems that promote the optimization of social structures and human behaviors. Thus, interaction research aims to realize a highly optimized society in which everyone can enjoy the benefits of fast-growing artificial technologies.

Targets to Achieve

In these strategic objective, the purposes are to create new technologies for the enhancement of interactions and to attempt to further deepen the understanding of interactions for use in a variety of situations in society. Specifically, research engages in cooperation with other academic fields such as cognitive science, psychology, neuroscience, and primarily information science and technology to realize the following goals:
(1) The development of technology in relation to interfaces and the expansion of human abilities to support interactions.
(2) The solution of the principles and structures for understanding interactions and the development of the technology in relation to collection and analysis of the information to contribute to the above-mentioned goal.
(3) The development of technology to design the social structure and the environment that prompts the optimization of human behaviors using interactive technologies.

Future Vision of a Society to be looked at during the research promotion

Through the achievements of the items stated in paragraph 3, *Goals and Objectives,* contributions are made to the realization of the society described below.

- The society in which the enhancement of interaction contributes to realizing a super smart society and is spreading to various fields as a platform technology to support industrialization and a wide range of implementation of artificial intelligence technologies, big data analysis technologies, IoT technologies, and the like, the development of which has been advancing.
- The society in which mutual interaction data of "humans to humans," "humans to machines," and "humans to the whole