



The integration of “materials” and “information” will innovate the development of materials

Development of internationally competitive materials in a short period using ‘Materials Integration (MI) for inverse design.’

The western countries and China have been investing intensively in material development using Artificial Intelligence (AI). Japan, once regarded as a materials-intensive nation, shouldn't turn a blind eye to this development. We asked Prof. Yoshinao Mishima, Director of a program that integrates materials engineering and information engineering, about the detail of materials development methods covered by the program.

Q: Please could you tell us about the outline of ‘Materials Integration for Revolutionary Design System of Structural Materials’?

PD: The point is that if you integrate materials engineering with information engineering, materials development will become much more efficient.

We expect that some issues which we haven't realized or understood may be clarified by using AI. This program aims to create a system that facilitates such a realization, and a system that creates materials using that system is called an ‘integrated materials development system.’

This development will bring about a materials revolution, enabling Japan to produce and supply various internationally competitive materials to the world.

"To propose required structures and properties of materials based on desired performances."

Q: The program outline states that an ‘MI system for inverse design’, where materials and processes are designed based on desired performances, will be developed. Does this mean that the MI system for inverse design is needs-driven and not seeds-driven?

PD: That's right. In summary, if we want materials with property A, we perform a ‘back-calculation’, tracing back from the desired outcomes in order to determine the raw materials and processes that must be applied to them. This process is called ‘inverse design’ and dramatically accelerates the process of materials development.

Q: Could you explain about domain A (Inverse Design MI)?

PD: In this domain, we are working on the MI for inverse design, which was mentioned earlier. We are developing a database by collecting reliable data to account for the specific properties of materials in current use. The key here is to unambiguously solve ‘forward problems’ using various information science-based

calculation techniques so that we can address ‘inverse design.’ The aim is to develop a system capable of proposing necessary structures and the properties of materials based on desired performance as well as the processes for realizing them. That's the role of domain A. *See figure.

"It's important that this MI is widely shared."

PD: As I have already told you, structural materials would be efficiently developed by utilizing the minimum time and R&D cost by establishing the MI system. The goal of this program is to install this system at the National Institute for Materials Science (NIMS) and to share it. University and corporate researchers can engage in development by accessing the system via the Internet. It is vital to implement this MI in society.

This social implementation could be achieved if this MI is widely shared with people. Our goal is that this system enables materials and heavy industries in Japan to sequentially produce new materials - this is the exit strategy.

Q: What should be overcome for this social implementation?

PD: First of all, we need to develop many programs that support ‘inverse design’, then we have to improve accuracy and also collect vast amounts of data.

Given that these data do not necessarily have the same format, we need to check and correct such inconsistencies. This is system development in a real sense, and this is a difficult aspect.

Let's assume we have an MI system in place. In cooperative fields, all parties can engage in materials development while sharing data to some extent. However, in competitive fields, we must solve intellectual property problems in advance to facilitate use by corporate individuals.



"Great expectations of CFRP and 3D powder processing"

Q: Next, can you explain about the concept of Carbon Fiber Reinforced Plastics (CFRP) in domain B?

PD: CFRP are carbon fibers embedded in plastics and are used in the body and wings of aircraft. Japan has a competitive edge in this field, and Japan-made CFRP are used in Boeing's airplanes. In the aviation industry, there are demands for lighter aircraft to reduce CO₂ emissions and for fire retardant materials in case of lightning strikes; we hope to apply this MI to the process of fabricating sophisticated materials. This is what domain B entails.

Q: Would you explain the concept of '3D powder processing' in domain C?

PD: I'm simply going to describe it. If you spread a metal powder over a specific area and illuminate it with a laser or electron beam, that part of the powder will melt and form a plate. By spreading the powder over that plate and repeating the same process while accurately controlling the laser, you can create, for example, a cylinder.

Making complex parts normally involves the melting of material, solidifying it in a mold, followed by breaking of the mold. However, this technique is limited in terms of accuracy. By controlling a laser on the order of microns or even sub-microns, materials with very complex forms can be fabricated. This is called 3D layered-molding.

In addition, there is a technique called 'powder metallurgy' in which compact metal powder is subjected to high temperature and high pressure. This is also a very effective technique. We believe we can compete in the global aviation industry using these parts-manufacturing techniques.

"To make Japan a materials-intensive country once again."

Q: Finally, what are the prospects for materials research and development in Japan?

PD: Once this integrated materials development system is developed, we will be able to produce superior materials in a relatively short period. In addition to the production of steel materials, we can also expand the system to include titanium and nickel alloys using this system. Among high polymer materials, it may be possible to produce innovative CFRP.

As a result, the world will start to view Japan as a materials-producing nation, and our country will be able to introduce new and high-quality materials for the rest of society. Japan used to be regarded as a materials-intensive

country so we have underlying strengths and basic technology. I think that the development of a novel system for creating new materials utilizing these strengths could be a significant global impact.

マテリアルズインテグレーション Materials Integration

- ・計算機上でプロセス・構造・特性・パフォーマンスの連関をつける
In-Silico Linking among processing, structure, properties, and performance
- ・実験、データベース、理論、経験則、数値シミュレーションをデータ科学で融合
Data-scientific approach to integrate experimental data, database, theoretical & empirical rule, numerical simulation with data science

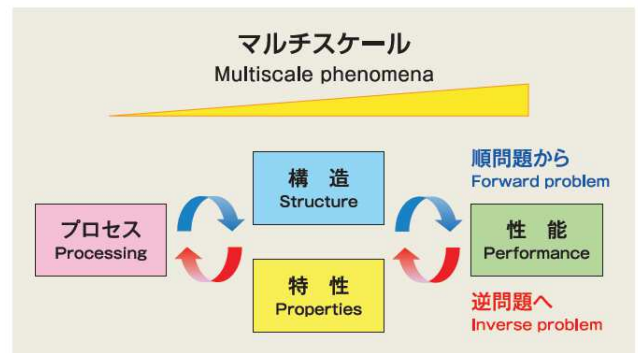


Figure: Materials integration