Introduction to “Future Materials Exploring Initiative-Engineering for Diverse Stable Phases-“

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Abstract

The strategic proposal (2019FY) “Future Materials Exploring Initiative-Engineering for Diverse Stable Phases“ compiled by JST/CRDS is briefly summarized.

1. Introduction

To pioneer future materials, the Center for Research and Development Strategy (CRDS) of Japan Science and Technology Agency (JST) has cooperated with experts, to hold workshops [1] and interviews, from the perspective of creating highly functional materials from diverse stable phases. Based on the analysis of them, in July 2019, a strategy proposal called “Future Materials Exploration Initiative-Engineering of diverse stable phases-” [2] was compiled.

2. Current situation and problems

Development of materials with new and advanced functions is expected to solve various social problems (energy, environment, mobility, IoT, etc.). For example, coexistence of multiple functions or conflicting functions such as structural materials with high strength and high toughness, thermoelectric materials with high electrical conductivity and low thermal conductivity, permanent magnet materials with high saturation magnetization and large coercive force, etc. Although various trials have been conducted in each application field and many high-performance materials were discovered as shown in Table 1, each is approaching its limits.

For this reason, it is necessary to expand the scope to untapped materials such as complex compositions with unknown possibilities and utilization of unused stable phases. In addition, due to intensifying competition in materials development, it is also required to shorten the development period, including materials design and manufacturing process design, from the search for new materials to the actual material fabrication, and it is necessary to build guidelines for creation of new materials beyond the fields of application.

Recent rapid progress in the search of new materials using materials informatics (MI) has lead materials with complex compositions with unknown possibilities as candidates [3]. However, it is not known whether the proposed candidate can be stably realized.

In this proposal it is aimed to create new materials by targeting diverse stable phases including metastable ones through control of the manufacturing process and utilizing artificial forces such as those acting at the interface between the substrate and the materials and at the interface between grain boundaries. Figure 1 outlines the research and development of this proposal.

3. Research and development issues to tackle

3.1 Expansion of material search range

It is necessary to clarify the roles of major factors such as constituent elements and bonding states that have a great influence on the basic properties and functions of materials, the individual roles of multiple elements, and the complementary roles of added elements. To clarify the role of each of these elements, it is important to use high-throughput experiments and data science as well as theoretical calculation and materials informatics. There is an experimental challenge of high-throughput discovery of materials using AI and robots [4].

One of the search directions is multi-elementization. This makes it possible to increase the degree of freedom in the spatial arrangement of elements and create a complex composition/structure. Introduction of multinary elements leads to an increase in the entropy of the configuration, and the fabrication at a relatively low temperature is possible because the Gibbs free energy is lowered. Recently, Kitagawa et al. have succeeded in synthesizing a platinum group high-entropy alloy nano-catalyst by using multi-elements and showed the effectiveness of high entropy effect by multi-elementization [5].

3.2 Visualization of reaction process and dynamic control of reaction path

The introduction of multiple elements makes the phase diagram multidimensional, and various stable phases appear as shown in Fig.2. To freely create the desired stable phase, it is important to visualize the reaction product, atmosphere, phase change, etc. by in-situ observation/measurement (operando measurement) and grasp the situation. It is necessary to develop process equipment that enables such operando measurements, in-situ observation equipment that can detect reaction products and reaction atmospheres, and measurement technology that can trace dynamic changes in stable phases.

In addition, prediction of the reaction mechanism from the theoretical calculation of the reaction is important. Maeda et al. have tried to systematically search for unknown elementary reaction processes by quantum chemical calculation and have succeeded in automatically searching for unknown chemical reactions using a computer [6].

Based on these techniques and measured data, we can understand the dynamic changes of reaction processes and stable phases under various conditions and organize them as a new theory that handles reaction processes and stable phase changes in an integrated manner.

3.3 Realization of target stable phase by using process control means

Some stable phases have a low energy barrier to other stable phases in the thermal equilibrium state and become unstable in the usage environment, so it is necessary to construct a method to stabilize the desired stable phase. A crystal substrate with a specific crystal plane is used to force the atomic arrangement of epitaxial growth to be aligned, or to rapidly reduce the temperature and pressure from high-temperature /high-pressure conditions.

For example, a diamond single crystal has a metastable structure produced only under high temperature and high-pressure conditions, but a diamond thin film can be stabilized by stress due to lattice mismatch at the interface with the substrate instead of high pressure.

In addition, an experimental example in which the metastable phase αGa_2O_3 is stabilized by using the mist CVD method is also an example of stabilization by process control [7].

4. R&D promotion measures

To promote the research and development described above, it is necessary to carry out integrated research and development from materials design to fabrication process design (reaction path design), operando measurement, characteristic evaluation, and data science. It is important to obtain a new guideline for material design and process design by looking at the application fields in a cross-cutting manner. Promotion of research under a leader who is fully aware of this and organizes the whole is desired. Although this kind of research is possible with a network system that spans related research institutes across diverse fields, it is desirable to build a research base for efficient research from the viewpoint of development,

In addition to researchers in various basic fields in universities and national research institutes, participation of researchers and engineers in industry is recommended in both academic and applicational research. The idea of expanding the search range to untapped materials and dynamically controlling various stable phases to create new functional materials is only a fragmentary activity in the world, and this research area is urgently needed in Japan. It is important to form a new community that spans materials design, process designs, measurements, and data science, as well as early implementation of equipment to accelerate this research and development.

5. Summary

The importance of exploring untapped materials with advanced functions from the viewpoint of engineering of various stable phases was described. We are innovating to dramatically expand the search space for crystal engineering. It is hoped that this will be realized as a policy such as strategic goals, with the understanding and support of all researchers involved in material search.

Acknowledgements

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References

[1] Report of the JST/CRDS Workshop on “Creation of High-Performance Mmaterials from Diverse Stable Phases”,（CRDS-FY2018-WR-11）Dec., 2018.

[2] Strategic Proposal of the JST/CRDS “Future Materials Exploring Initiative-Engineering of Diverse Stable Phases-“（CRDS-FY2019-SP-02）July, 2019.

[3] T. Chikyow, “Present status of the materials informatics and its challenge for future materials science”, Journal of Information and Knowledge Society 27 pp.297-304 (2017).

[4] T. Hitosugi, “High-throughput discovery of materials using AI and robots”, Digest for Symposium at the 67th JSAP Spring Meeting (2020)

[5] D. Wu et al., “Platinum-Group-Metal High-Entropy-Alloy Nanoparticles”, J. Am. Chem. Soc. 2020 (online)

[6] O. Maeda, et al., “Automatic search of molecular reaction paths becomes possible.”, Chemistry Today, No.592 pp.32-37 (2011).

[7] K. Kaneko et al., “Fabrication by Mist CVD Method and Evaluation of Corundum Structured Oxide Semiconductor Thin Films”, J. Soc. Mat. Sci, Jpn 59, pp.686-689 (2010)

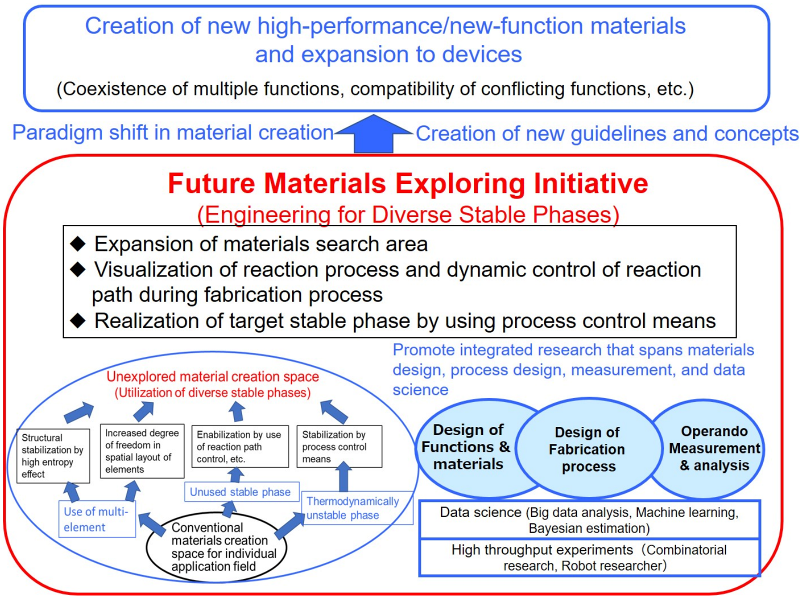

Fig.1 Outline of the proposal

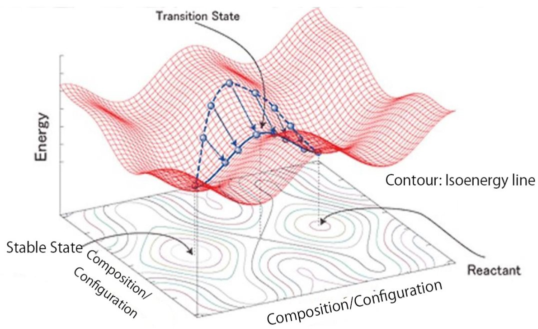

Fig.2 Appearance of new stable phases due to multi-elemettization

Table 1 Examples of requirements for high-performance material development

Functional Materials	Feature requirements	Conventional material example	Examples of materials currently under development
Storage battery solid electrolyte	Coexistence of fast Li ion conduction and wide potential window	LiPS	LiSnSiPS
Cathode materials for storage batteries	Hhigh Li-absorption /release performance with safety	LiCoO	LiMnNiCoO
Solar cells	Coexistence of high conversion efficiency and long-term reliability	Si、GaAs	CIGS、CH3NH3PbI3
Structural materials	Both weight reduction and high strength, high strength and toughness	HTSS	CoCrFeMnNi
Thermoelectric materials	Coexistence of high electrical conductivity and low thermal conductivity	BiTe、PbTe	PbNaGeTe
Permanent magnet materilas	Coexistence of high saturation magnetization and large coercive force	NdFeB:Dy	NdLaCeFeB
Wide-gap semiconductors	Coexistence of High breakdown voltage and high speed operation	SiC、GaN	α -Ga2O3
Phosphors	Coexistence of various emission wavelengths and high brightness	YAG	(Ca,Y)- α -SiAlON:Eu
Catalysts	Coexistence of high catalytic function, heat resistance, and low cost	Pt、Rh	PdRu、PdRuM
Water/gas separation membrane	High material selectivity and high throughput	Cellulose acetate	Zeolite, metal organic frameworke (MOF)
Organic semiconductors	Compatibility of high mobility and coating (large area)	) Pentacene (small molecule)	PBTTT (polymer)