EMS39

Session Th1 (9:00-9:30)

Invited

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

JST-CRDS「未来材料探索イニシアティブ―多様な安定層のエンジニアリング」へのお誘い

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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 and interviews, from the perspective of creating highly functional materials from diverse stable phases.
- Based on the analysis of them, a strategy proposal called “Future Materials Exploration Initiative - Engineering of Diverse Stable Phases-” was compiled in July 2019, .
- In this presentation, the strategic proposal for Creation of Future Materials is briefly introduced.

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 this purpose, coexistence of multiple functions or conflicting functions is important.
- Although various trials have been conducted in each application field and many high-performance materials were discovered as shown in the next viewgraph, each is approaching its limits.
- Recent progress in materials informatics (MI) has lead candidate materials with complex compositions with unknown possibilities. However, it is not known whether the proposed candidate can be stably realized.

Examples of requirements for high-performance material development

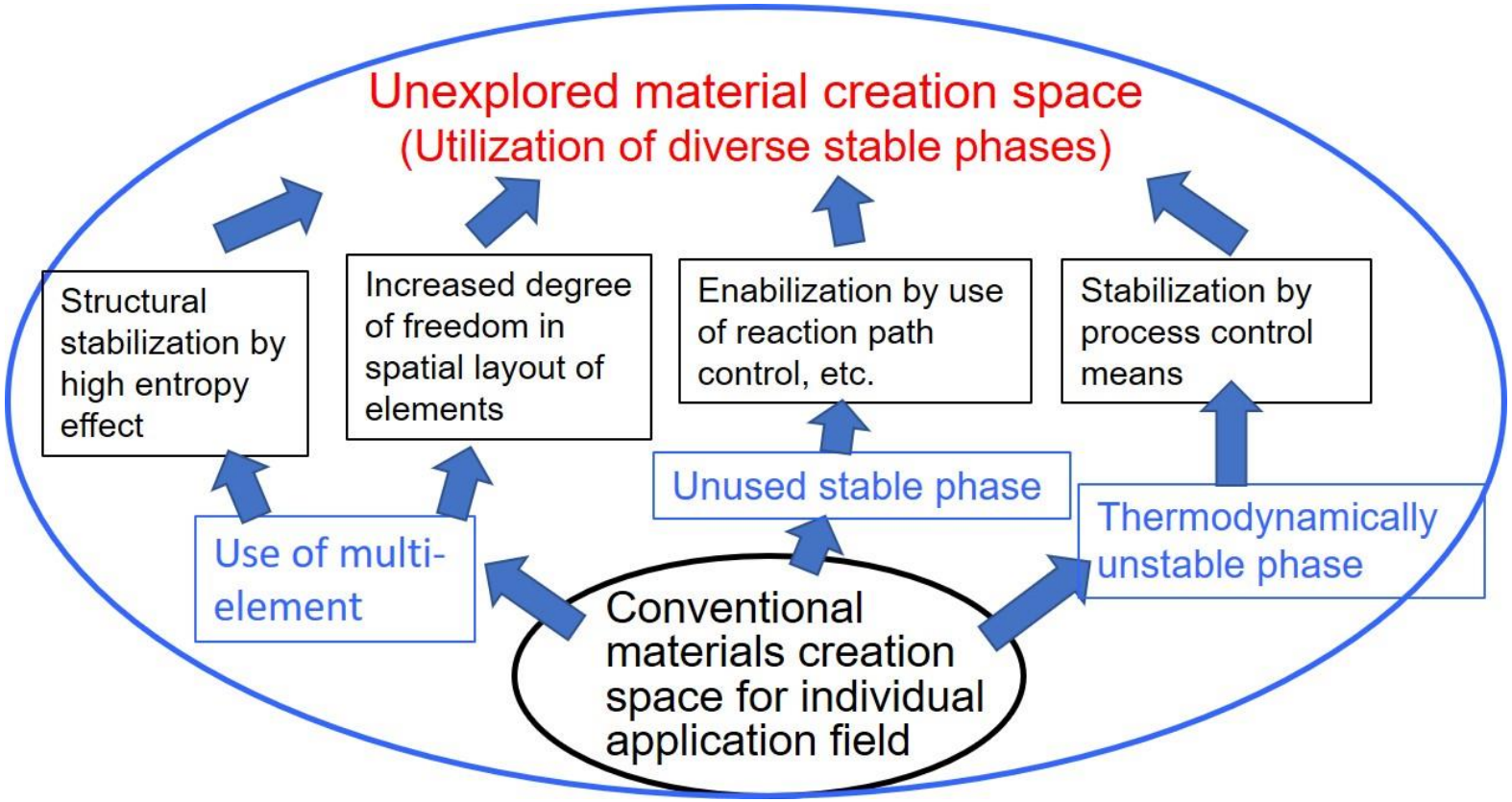
Functional Materials	Feature requirement	Examples of conventional materials	Examples of Materials currently under developed
Electrolyte	Fast Li^+-ion conduction and wide potential window	LiPS	LiSnSiPS
Cathode materials	High Li-absorption/release performance with safety	LiCoO	LiMnNiCoO
Solar cells	High conversion efficiency and long-term reliability	Si, GaAs	CIGS, MA-PVK
Structural materials	Low weight and high strength /high strength and toughness	HTSS	CoCrFeMnNi
Thermoelectric materials	High electrical conductivity and low thermal conductivity	BiTe, PbTe	PbNaGeTe
Permanent magnet	High saturation magnetization and large coercivity	NdFeB:Dy	NdLaCeFeB
Wide-gap semiconductors	High breakdown voltage and high- speed operation	SiC, GaN	α-Ga_2O_3
Phosphors	Diverse emission wavelengths and high brightness	YAG	α-SiAlON:Eu
Catalysts	High catalytic function, heat resistance and low cost	Pt Rh	PdRu< PdRuMn
Separation membrane	High material selectivity and high throughput	Cellulose acetate	Zeolite, MOF
Organic semiconductor	High mobility and large-area application	Pentacene	PBTTT

3. Research and development issues to tackle

3.1 Expansion of material search space

from conventional research space of individual materials

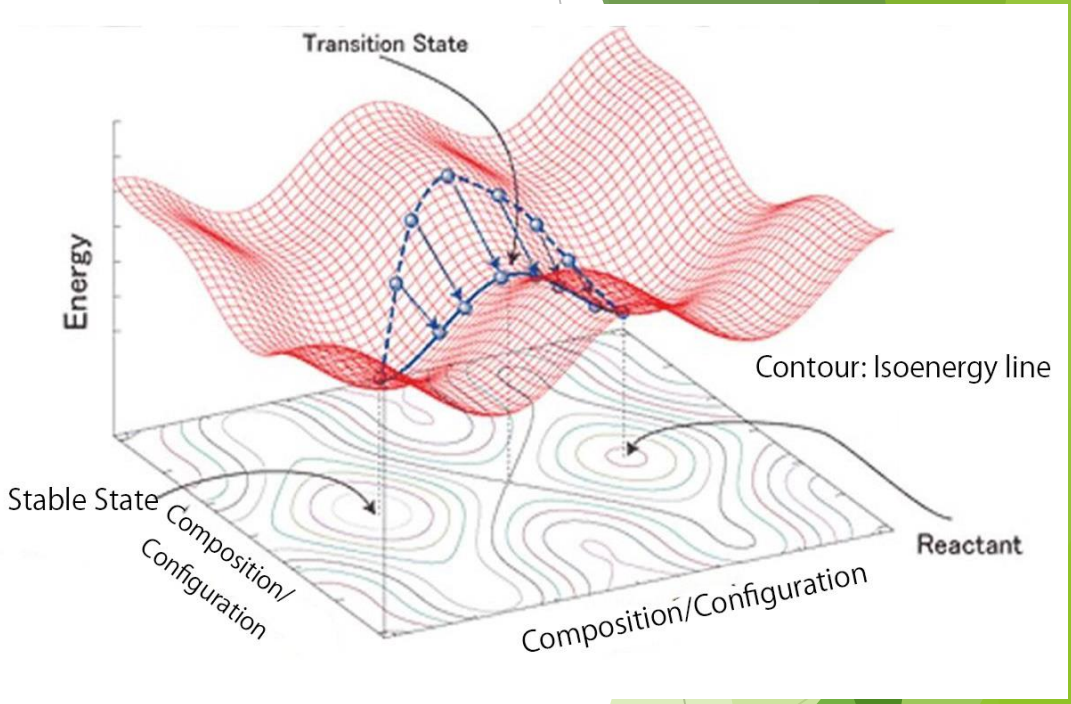
to Unexplored material creation space by utilization of diverse stable phases



- Use of multi-elements:
  Increased degree of freedom in spatial layout.
  Structural stabilization by high entropy effect.
- Unused metastable phases:
  Use of reaction path control
- Utilization of unstable phases:
  Stabilization by process control

3.2 Visualization of reaction process and dynamic control of reaction path

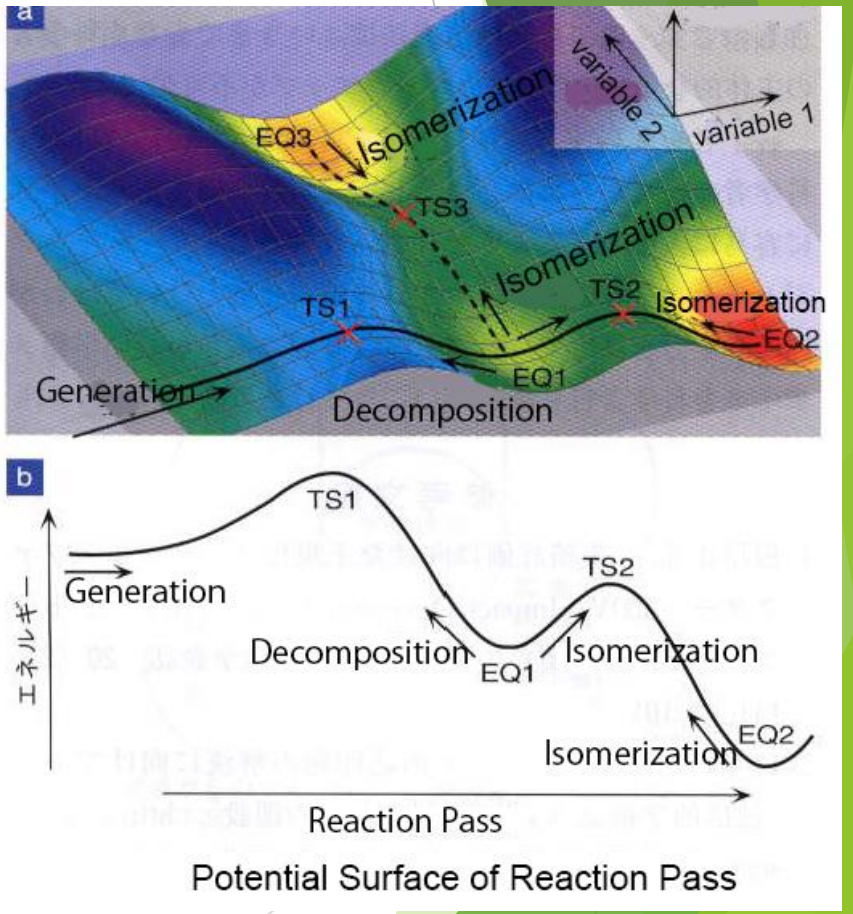
- The introduction of **multiple elements** makes the phase diagram **multi-dimensional**, and various stable phases appear. (Fig)
- Visualization of the reaction by in-situ observation /measurement (operando measurement) and grasp the situation is important to obtain desired phase materials.



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.

3.3 Prediction of the reaction mechanism

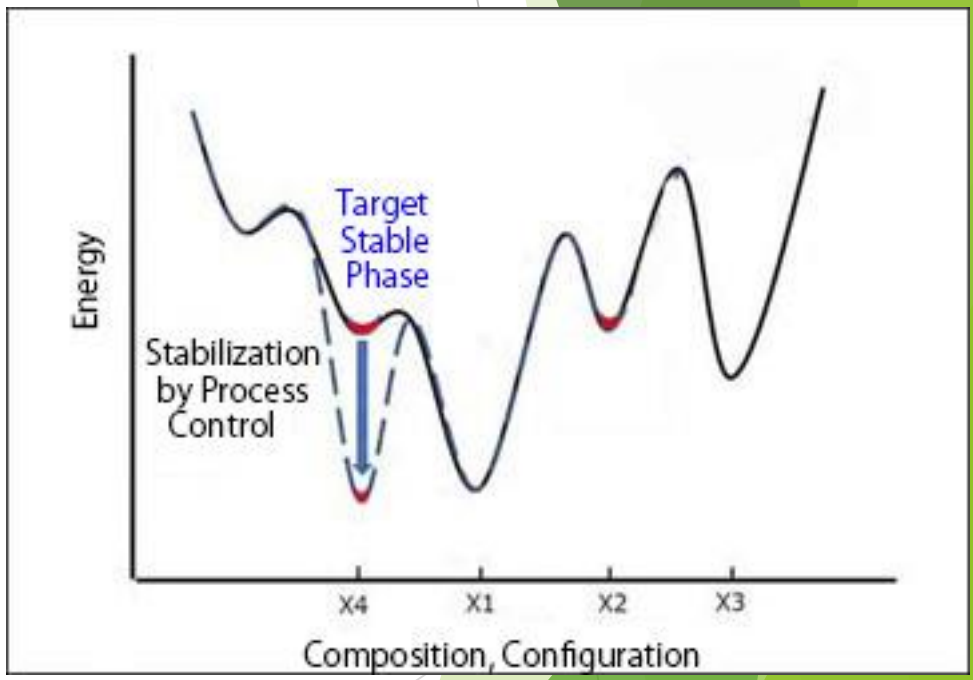
- Prediction of the reaction mechanism from the theoretical calculation of the reaction is important.
- Systematical search for unknown elementary reaction processes by quantum chemical calculation has succeeded in automatic search for unknown chemical reactions using a computer.



O. Maeda, et al., Chemistry Today, No.592 pp.32-37 (2011).

3.4 Realization of target stable phase by using process control means

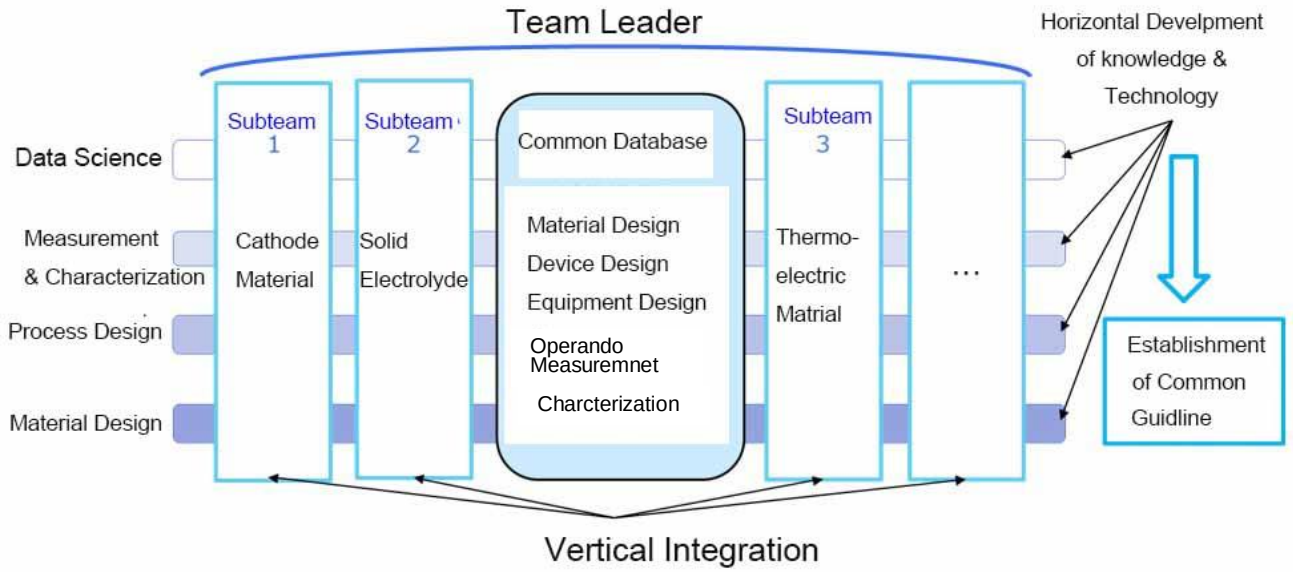
- Some stable phases have a low energy barrier to other stable phases in the thermal equilibrium state and become unstable in the usage environment, so it is necessary to construct a method to stabilize the desired stable phase.
- A crystal substrate with a specific crystal plane is used to force the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



4. R&D promotion measures

4-1 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, operando measurement, characteristics evaluation, and data science.

4-2 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.



4. R&D promotion measures (continued)

4-3. Efficient Materials Development by Sharing Equipment and Growth Method, and Establishment of a Center for Human Resource Development

- Development of In-situ or Operando Measurement Technique
- Development of Crystal Growth Apparatus with Operando Measurement
- Common Use of Equipment and Sharing of Database
- Material and Process Informaticas
- Promotion of Industry-Academia-Government Collaboration

4-3. Time Axis

○New Community Intagrating Diverse Research Fields（1～5yrs）

○Support by Projecting

- Exploration of New Stable Phases (Mext・JST, 3～5yrs)
- Process Development（5yrs、Cabinet・MITI・NEDO）
- Establishing Theory（5～10年、MEXT・JST）

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.

ACKOWLEDGEMENT

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