Future Materials Exploring Initiative
-Engineering for Diverse Stable Phases-

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The strategic proposal "Future Materials Exploiting Initiative ─Engineering for Diverse Stable Phases─" aims at exploring materials to meet with contemporary requirements such as improved performance and functionality, coexistence of multiple functions, and compatibility of conflicting functions, by substantial expansion of scopes for materials search into areas that have never been explored[1].

Here, we boldly pursue novel methods for creation of materials, using diverse techniques such as an increase of number of constituent elements, high-entropy effect, utilization of diverse stable phases including metastable ones, and process control to stabilize thermo-dynamically unstable structures. We expect a large paradigm shift in materials creation by formulating guidelines and principles for design of new materials and processes through above-mentioned efforts.

1. Expanding the scope of material search

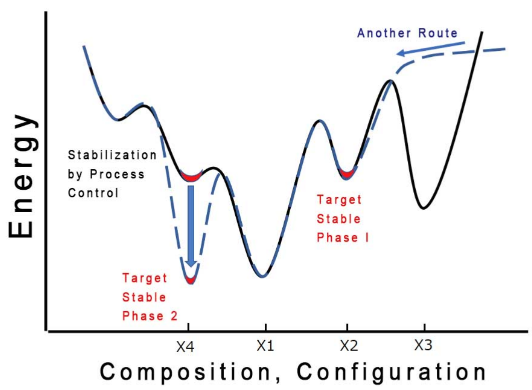
We must clarify the roles of such primary factors as constituent elements and bonding states that have a great effect on the basic properties and functions of materials, as well as the role of each element among multiple-elements structures and the complementary roles of added elements. The use of theoretical calculations and materials informatics and the application of high-throughput experiments will be essential for clarifying the roles of these factors.

2. Visualizing reaction processes and dynamically controlling reaction pathway

Visualization in in-situ observations and measurements (operando measurements) to grasp the state of the reaction product, process parameters, phase transitions, and the like is essential for producing target stable phases at will.

3. Achieving the target stable phase through use of process control means

Some materials in a stable phase may become unstable in the operating environment due to low energy barriers, so that an approach toward further stabilizing the target stable phase must be formulated. Applying process control means, such as forcibly arranging atomic configurations in an intended structure during epitaxial growth using a crystal substrate that possesses specific lattice constant and surface structure, or rapidly lowering the temperature and pressure from a high-temperature, high-pressure state, is effective in some cases for achieving the target stable phase.



Reference:
[1] Strategic Proposal of JST CRDS 2019, CRDS-FY2019-SP-02