【Grant-in-Aid for Transformative Research Areas（A）】

Section Ⅱ

Title of Project : Progressive condensed matter physics inspired by hyper-ordered structures

HAYASHI Koichi
(Nagoya Institute of Technology, Faculty of Engineering, Professor)

Number of Research Area : 20A206 Researcher Number : 20283632

【Purpose of the Research Project】

The functional properties of various materials is attributable to the cooperative effects between the matrix and dopants. Thus, the science of defects has significantly progressed. However, as long as the dopant is used as a point defect, there is a limit to the functional properties that can be achieved.

In this project, we will proactively use “hyper-ordered structures” to break through that limit. “Hyper-ordered structures” are nanostructures composed of different elements and vacancies. For example, the In-Nb-Ti^{3+} structure in FIG. 1(a) contributes to enhancing the dielectric constant of titanium oxide by 1000 times. Unlike ordinary single-element doping, we can pursue infinite possibilities of functionality originating from these “hyper-ordered structures” by controlling the combination of elements and their 3D arrangement.

Figure 1(b) shows the atomic arrangement of zeolite before crystallization, which forms a geometrically highly ordered vacant structure. It is known that the relationship between this vacant structure and the Al dopant correlates to the high temperature durability of zeolite catalysts. Such a relationship between the vacant structure and the dopant is also regarded as a "hyper-ordered structure", which can be described by the concept of topology.

“Hyper-ordered structures” can be regarded as a treasure trove of material functionality. The purpose of this project is to bring a new breakthrough in material science based on accurate determination, profound understanding, and effective control of “hyper-ordered structure”, which can be achieved by advanced experimental, theoretical, and synthetic techniques.

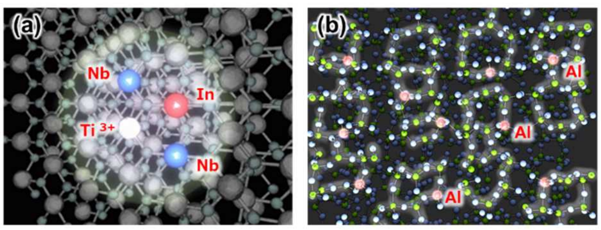

Fig. 1 Example of ”hyper-ordered structure”. (a) In-Nb-Ti^{3+} nanostructure in TiO_2. (b) Crystal-like topology in amorphous zeolite.

【Content of the Research Project】

This project sets three research targets: (A) “dopant-induced hyper-ordered structures”, (B) “hyper-ordered structures with vacancies and voids”, and (C) “hyper-ordered structures at crystal/amorphous boundary”. The organization consists of A01 sample team, A02 measurement team, and A03 theory team.

The "hyper-ordered structures" embedded in various materials will be accurately determined by site-selective quantum beam in combination with computational techniques. We will elucidate their functionality, and design a new “hyper-ordered structure” using large-scale first-principles calculations. In addition, by utilizing mathematical methods such as topology analysis, we will propose descriptors for “hyper-ordered structures”. Based on these insights, we will promote efficient exploration of “hyper-ordered structure” materials utilizing data science. We will go beyond the idea of single-site doping and pave a way to create a highly functional materials based on a topology control.

【Expected Research Achievements and Scientific Significance】

This project possesses the world's highest level of analysis techniques for determining “hyper-ordered structure”. In this project, further development of these analysis techniques can be achieved, and the international leadership of Japan can be solidified.

This project will also develop an emerging research field that connects crystalline and amorphous materials. It is expected that new academic fields will be created, which induces collaboration in fields that have few common ground. Through such collaborations, many young researchers will be cultivated.

In terms of applications, some breakthroughs are expected. For example, “Innovative dielectric with 1000 times the relative permittivity and high temperature stability”, “Super heat resistant zeolite deNOx catalyst”, “Low cost thin film transistor with $100cm^2/V \cdot s$ mobility”, “Unbreakable cover glass for smartphones”, etc., which can contribute to the development of Japanese industry.

【Key Words】

Hyper-ordered structure: a characteristic nanostructure formed by dopants and vacancy. Specifically, complex defects due to different elements and vacancies, and nanoscale atomic arrangements that show a topological order even if they are amorphous.

【Term of Project】 FY2020-2024

【Budget Allocation】 1,155,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.hyperordered.org
khayashi@nitech.ac.jp