

Science and Engineering



Title of Project : New Materials Science on Nanoscale Structures and Functions of Crystal Defect Cores

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【Purpose of the Research Project】

In this project, specific electronic and atomic structures of grain boundaries, interfaces and dislocations that can realize novel and distinct materials properties are defined and referred to as “crystal defect cores”. Researchers specializing in theoretical calculations, nanoscale characterization and advanced materials processing conduct collaborative studies, aiming at creating a new area in materials science named “crystal defect core”. Through establishing new scientific principles based on the concepts of “crystal defect core”, we will further explore novel properties and materials due to crystal defects.

Conventional studies have focused on average bulk structures and macroscopic properties of materials in general, and thus understanding of crystal defects is often limited to their static and averaged atomic pictures. Recent technological progresses in methods and approaches of nanoscale characterization and computational science are so remarkable that we have been enabled to acquire quantitative information on nanoscale structures of crystal defects. These advanced approaches and methods have facilitated our more in-depth understanding about the crucial roles that the crystal defects play for realizing various materials properties. For future materials design and development, it is essential to reveal relationships between nanoscale structures of crystal defects and materials properties. Thus, in this project, we aim at discovering or creating new materials functions and new exploratory materials based on “crystal defect cores”, including those emerging under external stimulus including thermal, electric, magnetic, optical or stress fields.

【Content of the Research Project】

This research project has three major Research items as follows:

- A01: Modeling and design of crystal defect cores
- A02: Nanoscale characterization of crystal defect cores
- A03: Materials development based on crystal defect cores

In Research items A01 and A02, we focus on basic science of crystal defects. We do collaborative and systematic researches of grain boundaries, interfaces and dislocations so as to establish new scientific principles based on in-depth understanding of a structure-property relationship of the crystal defects, by means of theoretical calculations, materials informatics and nanoscale characterization at the world-class highest level.

Researches in the Research item A03 of materials processing come from diverse materials fields, and try to develop novel materials and their properties by controlling crystal defects at the nanometer scale. Throughout the research area, it is expected for our intensive and extensive collaborations to prove that “crystal defect core” is a universal concept to realize novel materials development in the next generation.

【Expected Research Achievements and Scientific Significance】

- To establish new scientific principles to make it possible to explore novel and distinct materials properties originating from crystal defects
- To discover or create new materials with remarkable properties in diverse fields of materials science
- To facilitate considerable technical development of theoretical calculations, nanoscale characterization, and materials processing.

Our concept of “crystal defect core” will provide a scientific impact when we succeed in developing materials and their properties through precisely controlling crystal defect cores. This is because crystal defects have been thought to play a negative role for materials properties. This research area can find out a new strategy for controlling crystal defect cores so that they play positive roles for better properties, paving a new avenue for future materials developments.

【Key Words】

Crystal defects: Irregular atomic arrangements in crystalline materials.
Crystal defect cores: Specific electronic and atomic structures that can realize novel and distinct materials properties

【Term of Project】 FY2019-2023

【Budget Allocation】 1,098,000 Thousand Yen

【Homepage Address and Other Contact Information】

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