Research area in Strategic Objective *"Creating novel materials by controlling and utilizing fluctuations"*

Materials innovation through understanding and controlling fluctuations

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Overview

In this PRESTO research area, we aim to create innovative materials that contribute to solving social issues and improving human happiness by understanding and controlling spatial fluctuations, such as heterogeneity and defects, and temporal fluctuations, such as dynamics and non-equilibrium phenomena.

Recent advances in materials research include the development of measurement techniques using high-intensity synchrotron radiation, high-intensity neutron beams, high-precision electron microscopes, and scanning probe microscopes, as well as the dramatic improvement in computer performance, as typified by the supercomputer Fugaku, and advances in materials simulation methods. The development of AI and data science methods also supports these. Materials informatics, which uses experimental and simulation data to search for novel materials, is also progressing.

We will utilize these advances in measurement technology and computer science to gain a fundamental understanding and control of fluctuations. we will focus on the material properties that arise from spatial and temporal fluctuations in structure, defects, composition, ions, molecules, orientation, etc., and aim to create materials with dramatically improved performance by elucidating the principles and mechanisms involved. We will also make the fundamental technologies that will form the basis of this research, including analytical measurement technology, simulation technology, data analysis technology, and process technology.

Research Supervisor's Policy on Call for Application, Selection, and Management of the Research Area

1. Background

The creation of innovative materials not only contributes to solving social issues and improving humanity's well-being but can also be said to be the cradle of new academic principles. Recent developments in measurement technology and computational science in materials have led to significant improvements in the technology for capturing fluctuations. Alongside advances in analysis

and measurement technology, such as operando measurements using large experimental facilities (SPring-8, SACLA, J-PARC, NanoTerasu, etc.), electron microscopes, scanning probe microscopes, etc., multi-scale and multi-modal measurements have also progressed. In addition, there has been remarkable progress in computer power and simulation methods, and it is becoming possible to model and simulate materials taking fluctuations into account. As these technologies develop, innovative materials will be created by applying fluctuations in materials, which are one of the critical factors in the expression of functions and properties.

This research area aims to understand the causes and mechanisms of fluctuations, such as why they occur and why they change the properties of materials. It also aims to control fluctuations and create innovative materials with new functions and properties, as well as the fundamental technologies that will serve as a foundation for this.

By fully utilizing advanced measurement, computational science, data-driven research, etc., we aim to understand the relationship between fluctuations, material functions, and characteristics and establish a process for designing fluctuations into materials based on this knowledge. We strive to create innovative materials with dramatically improved performance. We also aim to develop fundamental materials science and technology, including measurement and analysis technology, simulation and data-driven numerical analysis, and process technology, forming the basis for creating these materials.

Through this research, we aim to create a new materials science that focuses on 'fluctuations' ahead of the world and to produce young researchers who will lead the world in this field.

2. Principle of invitation project and selection

This research area covers creating a wide range of hard and soft materials, including inorganic, metallic, organic, polymeric, and inorganic-organic composite materials. To achieve materials development through the understanding and control of fluctuations, we are seeking proposals for the following: (1) the creation of materials with innovative functions and properties; (2) process technology that controls and utilizes fluctuations; (3) analytical and measurement technology for understanding fluctuations; and (4) simulation and data-driven analysis technology for understanding and applying fluctuations.

(1) Creation of materials with innovative functions and characteristics

・Establishment of a scientific basis for fluctuation in materials science and proposal of design guidelines for materials that control and utilize fluctuations

・Creation of materials with innovative functions and characteristics that go beyond conventional concepts of materials development

(2) Process technology that controls and utilizes fluctuations

・Establishment of design guidelines and processes that introduce fluctuations into materials by highly controlling them

・Process technology that integrates advanced measurement and simulation, etc.

(3) Analytical and measurement technologies for understanding fluctuations

・Multi-scale measurement technologies that capture the entire scale, from the nanoscale of atoms and molecules to the macroscopic element size range

・Measurement technologies that capture spatial and temporal fluctuations that exist during the material formation process

・Measurement technologies that capture spatial and temporal fluctuations at interfaces and grain boundaries of different materials and phase states, etc.

(4) Simulation and data-driven numerical analysis techniques for understanding and applying fluctuations

・Computational science techniques that predict the physical properties of materials by considering spatial and temporal fluctuations based on electronic state and atomic/molecular dynamics simulations such as first-principles calculations and molecular dynamics calculations

・Computational simulations that combine multi-physics to describe the physical properties of materials at different scales, from nano to macro

・Construction of data-driven research that incorporates the concept of fluctuations

However, these are just examples, and we are looking for proposals based on free ideas that are not restricted to these. We welcome proposals for understanding and controlling fluctuations that are not an extension of conventional technology. Please clearly state what kind of novelty and originality there is to develop cutting-edge materials science.

3. Research periods and research funds

Initial research funding will be a maximum of 40 million yen (direct costs) per research topic. The research period will be within 3.5 years from the year of adoption.

4. Principle of research-area management

In this research area, the research supervisor and area advisors will support individual researchers in engaging in original research without being fixated on short-term results. In addition, we will promote cross-disciplinary research exchange through interaction with researchers in other fields, such as those involved in related CREST and PRESTO research areas and aim to create new research from different

fields of science and technology. Furthermore, by holding workshops and symposia, we will actively promote collaboration with the CREST “Creation of functional materials through introduction/control of fluctuations” research area, which is also being implemented under the same strategic goals, as well as academic exchange with overseas research institutions.