【Grant-in-Aid for Scientific Research on Innovative Areas (Research in a proposed research area)】
Science and Engineering

Title of Project : 3D active site science

Hiroshi Daimon
(Nara Institute of Science and Technology,
Graduate School of Materials Science, Professor)

Research Project Number : 26105001　Researcher Number : 20126121

【Purpose of the Research Project】

Active sites, such as dopants, interfaces, and nano-structures, play an important role in many functional materials. To date, Japan has been the world leader in the research and development of 3D atomic imaging methods. The "3D active site science" project will combine advanced materials and computational sciences to develop a new generation of microscopes that focus on active sites, pushing the boundaries of conventional life sciences and green technologies, pioneering a new field of materials science. The imaging tools will be used to study how the active sites interact with the surrounding atoms in solar cells, proteins, and catalytic, spintronic, and optoelectronic materials, among others, paving the way to the development of new functional materials and devices.

【Content of the Research Project】

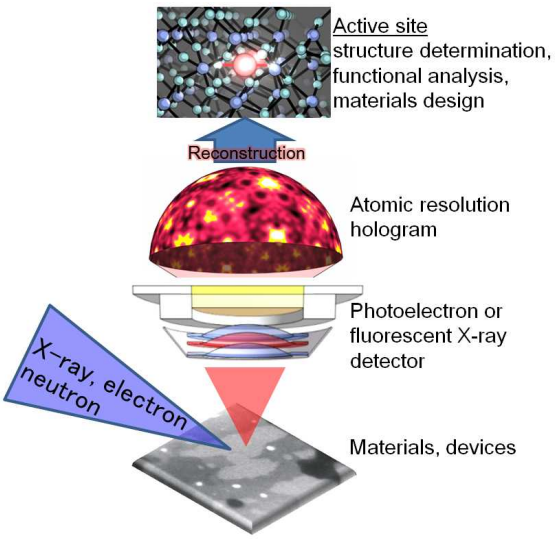

Fig.1 Research concept of the "3D active site science" project.

The "3D active site science" project has the following four branches with 13 research groups.
A01: Fabrications of materials.
A02: 3D active site imaging and analysis.
A03: Active site modeling and design.
A04: Device development and applications.

The focus will be on the following four topics:

1. Clarify the functional characteristics of active sites in proteins, organic solar cells, catalysts, optoelectronic materials, etc. by combining 3D atomic imaging methods with modeling and first-principles calculations.
2. Develop next-generation 3D imaging techniques for soft- and biomaterials, catalysts, and for time-resolved studies.
3. Construction of a 3D active site structure database.
4. Determine the relations between active site structure and materials functions. Apply the new scientific principles in novel device design.

【Expected Achievements and Significance】

"3D active site science" is a new scientific frontier that carries the potential of major advances in solid state physics and materials science. Bringing together researchers from many diverse fields is expected to provide the necessary synergy for achieving materials design breakthroughs. Since most of functional materials contain active sites, the project is expected to make a broad contribution to solid state physics and materials science, e.g., in developing a new generation of power devices and elucidating the role of metal clusters in protein molecules. Advances in this project will produce ripple effects in various related fields of device engineering and fundamental sciences, strengthening the technological and academic standing of Japan in the world.

【Keywords】

dopant, interface, nano-structured materials, atomic resolution holography, electron diffractive imaging, catalyst, soft material, inorganic material, protein molecule

【Term of Project】　FY2014-2018

【Budget Allocation】 1,145,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.3d-activesite.jp/
daimon@ms.naist.jp