T. Mizoguchi LAB.
[Understanding the Role of Atoms and Electrons]

Department of Materials and Environmental Science

Nano-Materials Design Laboratory

Graduate School of Engineering
Department of Materials Engineering

http://www.edge.iis.u-tokyo.ac.jp

1 Materials Design

What kind of Structures? How to bring about the Properties

Property Structure Relationship

Paving the Way for Materials Design

Property-Structure Relationship for Materials Design

Much higher performance and higher reliability are now required to the materials to achieve further technology developments. In case of electronic ceramics, such as multi-layer ceramic capacitor and varistor, the size of grains in devices becomes smaller and smaller, and further property improvements of each grain and grain boundary are desired. To achieve this, clarification of atomic and electronic structures and finding the way to improve their properties are indispensable.

2 Seeing Atoms & Bonding

Atomic resolution analysis of glass
Analysis of energy materials
Atomic resolution analysis of liquid
Analysis of thermal expansion at grain boundaries

We are investigating electron-energy-loss near-edge structures (ELNES) and X-ray absorption near-edge structures (XANES) from experimental and theoretical viewpoints. ELNES and XANES originate from the electron transition from a core orbital to unoccupied bands. Their spectral features reflect the partial density of states of core-hole, which is introduced by electron transition from core-orbital to conduction band. Therefore, it is indispensable to calculate spectrum structures correctly.

3 Understanding the Role of Atoms and Electrons in Materials

Data-driven prediction of structure from core-loss spectra
Prediction of properties from core-loss spectra
Direct prediction of gain boundary properties
Artificial Intelligence (AI) achieve 3,000 times higher efficiency

To design materials properties, we are investigating atomic and electronic structures quantitatively by performing high-precision simulations of atomic structures such as interfaces and lattice defects, which have a great impact on the functions of materials, and core excitation spectra, which show a variety of shapes reflecting electronic states. In addition, from the viewpoint of materials informatics, where information science is applied in materials research, we are applying machine learning methods such as transfer learning, Bayesian optimization, and virtual screening to interfaces, lattice defects, and inner-shell excitation spectra to understand and predict structure-function relationships.