Grain Boundary Atomic Structures, Segregation and Vacancies in Oxide Materials

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Grain boundary (GB) atomic structures are dependent on the GB characters such as misorientation angle and GB planes. In addition, GB structures are also influenced by the segregated dopants and vacancies to form the relaxed and stable structures. It is therefore needed to investigate the sites of vacancies and dopants segregated at GBs, depending on the GB characters, to fully understand GB atomic structures, which are related to the material's properties. In this study, various types of GBs were systematically fabricated for doped and pristine Al\textsubscript{2}O\textsubscript{3}, ZrO\textsubscript{2}, ZnO, CeO\textsubscript{2} by the bicrystal techniques, are used as the model systems, and the behavior of the GB structure reconstruction due to the vacancies and the dopants are investigated by combining aberration-corrected STEM, EELS mapping and first principles calculations. STEM observations were mainly performed using ARM-200F (200kV, JEOL) equipped with CEOS Cs-corrector and Grand ARM-300F (300kV, JEOL). EELS spectra were acquired in STEM mode by an Enfina spectrometer (Gatan Inc). For theoretical approach, static lattice and density functional theory (DFT) calculations were used to understand the GB segregation and reconstruction behavior quantitatively.