

First-principals study of Enhanced Oxygen Incorporation near the Grain Boundary on Yttria-Stabilized Zirconia

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Grain boundary (GB) in a solid crystalline material is the region separating two crystals (grains) of the same phase. GBs often have unusual features due to the interfacial effect. Yttria-stabilized zirconia (YSZ) has conventionally used as the electrolyte of a solid oxide fuel cell (SOFC). Using density functional theory (DFT) calculations, we mechanistically investigated oxygen incorporation kinetics near the GB in YSZ compared to grain. The elementary steps of the incorporation were investigated. Specifically, we examined the energy profiles of oxygen adsorption above the grids we divided in YSZ. In addition, the factors which induce the oxygen incorporation on GB were investigated. Our results will provide fundamental insight of the enhanced oxygen incorporation on GB in YSZ.