First-Principles based Comparative Study of Oxygen Incorporation Process on Grain and Grain Boundary of Yttria-Stabilized Zirconia

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Although solid oxide fuel cell (SOFC) is a highly efficient and low polluting technology, its high operating temperature, that is, low electrolyte conductivity and electrode efficiency at lower temperature have been severe restrictions for the practical applications. Thus, many efforts have been attempted to improve SOFC's performance. Prinz et al. recently reported that nanoscale YSZ thin film promotes the exchange current density more than in the bulk at low temperature, suggesting that the enhancement is attributed to the nanogranular structure. However, these empirical observations have not suggested the detailed reaction mechanism. To provide fundamental information on each elementary step reactions, we performed first-principles calculations to quantitatively access the mechanism that may govern the fast oxygen incorporation at the GB. Our results provide not only fast oxygen incorporation mechanism on the GB of YSZ but also fundamental insight of oxygen surface kinetics at the interfaces on defected oxide materials.