First-principles calculations for defects and impurities in oxides and their impact on electronic devices

Minseok Choi

Advanced Characterization and Analysis Group, Korea Institute of Materials Science (KIMS), Changwon, Korea

Through first-principles calculations, we have examined the role of defects and impurities in the structural, electrical, and optical properties in oxides. For comprehensive understanding, we will present the role of defects and impurities in oxides, then their impact on electronic devices. First, our recent results for native donors in $SrTiO_3$ will be provided. $SrTiO_3$ exhibits fascinating physical properties such as very high *n*-type conductivity, visible-light emission, and ferroelectricity without doping. These properties have typically been attributed to the O vacancy or its complexes, but the roles of the O vacancy and other defects have not been well explored. Our calculations indicate that the off-centered Ti antisite significantly impacts on the properties. This defect is likely to form, even comparable with O vacancy, and introduces deep, localized states in the gap. The Ti antisite thus can be a source of the experimentally observed properties. Regarding the conventional donor, the O vacancy, we find that it induces local octahedral rotation even in the cubic phase, with the electron localization near the O vacancy. Such electronic structure provides an explanation for the *n*-type conductivity in reduced $SrTiO_3$ and simultaneously for the visible light emission as well as the off-centered Ti antisite. Regarding electronic devices, how defects and impurities in gate dielectrics impact on metal-oxide-semiconductor (MOS) devices will be presented. High-k oxides are used as alternative gate dielectrics in MOS devices. Promising results have been achieved with Al_2O_3/III-V and HfO_2/Si MOS structures, which exhibit relatively low densities of interface states. However, the presence of carrier traps and fixed charges near the oxide/semiconductor interface still poses serious limitations in device performance, mainly due to native defects and impurities in the gate dielectric introduced during the deposition process. Using first-principles calculations, we investigate the effects of native defects and impurities in Al_2O_3 and HfO_2. By analyzing the position of the defect and impurity levels with respect to the semiconductor band edges, the role of the defects and impurities in the electrical properties of MOS devices is addressed. Our results show that the O vacancy and C impurity can act as carrier traps and/or lead to leakage current through the gate dielectric, while other native defects can be sources of fixed charge. N impurities are also a likely source of fixed charge, but may be effective in alleviating the problem of carrier traps and fixed charges associated with native defects.