

Comparison of Electronic and Optical Properties of the α and κ Phases of Alumina Using Density Functional Theory

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κ -Al₂O₃ is a metastable phase of alumina. We have investigated the electronic structure and optical properties of κ -Al₂O₃ by a first-principles calculation in the framework of density functional theory (DFT) and the full potential linearized augmented plane wave (FP-LAPW) with three different potentials: the generalized gradient approximation (GGA), the local density approximation (LDA), and the Engle-Vosco approximation (EVA). The results were compared with the stable phase α -Al₂O₃. Our calculated value for the direct band gap of α -Al₂O₃ is 7.2 eV, which is very close to its experimental measurement. A direct band gap of 5.95 is obtained for κ -Al₂O₃ which is about 1.25 eV smaller than that of α -Al₂O₃. The calculated optical reflectivity, optical conductivity, and electron energy loss spectrum for α - and κ -Al₂O₃ are similar on the whole, and for α -Al₂O₃ are in excellent agreement with the experimental measurements.

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I. INTRODUCTION

Alumina (Al₂O₃) is one of the most important ceramic materials, having exceptional properties. It has many industrial and technological applications because of its hardness, abrasion resistance, mechanical strength, corrosion resistance, good electrical insulation, useful optical properties, fine particle size, large surface area, and catalytic surface activity. Besides the stable phase α -Al₂O₃, alumina exhibits a number of different metastable or transition phases, such as γ , κ , λ , η , θ , and χ alumina. The metastable alumina can be divided into two major groups, depending on the stacking of their O anions: face-centered cubic (fcc) packing (γ , θ , η , and λ) and hexagonal close packing (hcp) (κ and χ) [1]. The electronic structure of alumina (Al₂O₃) is increasingly of interest for its variety of applications in optical, electronic, and structural devices. For instance, α -Al₂O₃ is used in electronics and κ -Al₂O₃ in wear-resistant coatings on cemented-carbide cutting tools. The κ -phase can be produced by heat treatments of hydrated aluminas, but is technologically most often produced by chemical vapor deposition (CVD). The advantages of the κ -phase over α -Al₂O₃ are its smaller grain size, lower pore density, and epitaxial growth when produced using CVD. Although metastable, κ -Al₂O₃ appears to be very stable, maintaining