475i First-Principles Studies of the Electronic Properties of Hfo_2 on Sic

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Silicon carbide (SiC) has attracted much attention as a promising wide-bandgap semiconductor material due to its excellent physical and electrical properties. Although thermal SiO_2 is the most widely studied gate dielectric on SiC, it displays large density of defect states at the interface, low channel mobility and a fundamentally low dielectric strength that limit its application. Ultrathin HfO_2 films were demonstrated to be a viable high-k gate dielectric alternative to SiO_2 for use in SiC power metal-oxide-semiconductor field effect transistors. In this work, we present the bulk, surface and interface properties of hexagonal SiC using the density functional theory within local density approximation. The investigated electronic properties include the density of states, band structures, and the effect of surface geometries. We find the conduction-band minimum of SiC is affected significantly by the polytype difference, while the valence band maximum is not sensitive, resulting in the difference in the band gaps of hexagonal polytypes of SiC. Surface calculations show the (0001) surface reconstruction of SiC depending on the atomic termination. The silicon-terminated surface does not display reconstruction leading to the metallic character of the surface, whereas the carbon-terminated structure undergoes the 2x1 surface reconstruction resulted from the C-C dimer formation, thereby removing the metallic state completely. These reconstructions give useful information to assess the interface properties because interface bonding geometries and cation-anion coordinations are influenced by the reconstructed surface structures. We also performed photoconductivity measurements to investigate bulk properties, such as band gap and defect states, of SiC. The band alignment at the HfO_2/SiC interface was investigated by x-ray photoelectron spectroscopy and photoconductivity measurements. These results are compared to density functional theory (DFT) calculations of a monoclinic HfO_2/4H-SiC interface, where SiC (0001) was terminated at the interface with either Si or C atoms for comparison. The Si-terminated (C-terminated) structure resulted in valence and conduction band offsets of 2.09 eV (1.47 eV) and 0.35 eV (0.97 eV), respectively. Finally, we discuss the effect of nitrogen incorporation on the electronic structure of hafnium oxynitrides by density functional theory. Recent studies show that the incorporation of nitrogen in HfO_2 films helps prevent recrystallization of dielectric thin films at high temperatures, which allows the diffusion of dopants through the grain boundaries. The simulation results demonstrated that, as the N concentration increases, the N 2p state extends toward the conduction band and the ionic character of Hf-N bonding is less pronounced, resulting in the reduction of the band gap.