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First-principles study on atomic and electronic structures of 4H-SiC(0001)/SiO_2 interface TOMOYA ONO, CHRISTOPHER KIRKHAM, CCS, University of Tsukuba — SiC is attracted much attention as a promising material for the high-power electronics devices. However, the carrier mobility of the SiC/SiO_2 interface is poor compared with bulk SiC. This reduction in carrier mobility is attributed to the high density of defects formed at the interface during thermal oxidation. The atomic structure of SiC and SiO_2 directly at the interface affects its electronic properties. Although extensive experimental efforts have been undertaken to reveal the interface atomic structure, there still remains much to be learned. In this study, we combine experimental results, obtained from transmission electron microscope, with first-principles calculations, to identify the SiO_2 polymorph directly at the (0001) face of the 4H-SiC/SiO_2 interface. We screen candidate polymorphs based on several different parameters; the lattice mismatch between SiC and SiO_2, lateral spacing of the atomic layers within and between the SiC and SiO_2 regions, and examining the local density of states for lack of gap states. The latter also allows for a qualitative analysis of band offsets. We find that when all three parameters are taken together β-tridymite matches closest to the experimental results.

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