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Atomic and electronic structure of polar oxide-wide band gap semiconductor interfaces: MgO(111)/SiC(0001) VLADO LAZAROV, PHIL HASNIP, University of York, KATE ZIEMER, Northeastern University, KOHJI NAKAMURA, Mie University, MICHAEL WEINERT, University of Wisconsin-Milwaukee, UNIVERSITY OF YORK TEAM, NORTHEASTERN UNIVERSITY COLLABORATION, MIE UNIVERSITY COLLABORATION, UNIVERSITY OF WISCONSIN COLLABORATION — Atomically sharp polar oxide/semiconductor heterostructures are characterized by the abrupt change of the electrostatic potential across these junctions. This inherent property provides opportunities to tailor the functional properties of these heterojunctions by engineering their atomic interface structure. In this work we present a combined experimental and theoretical study on model MgO(111)/SiC(0001) polar interface. Thin MgO(111) films with rock salt structure were grown by molecular beam epitaxy on two surface reconstructions of SiC(0001). Atomic imaging of the film/substrate interface(s) reveals that chemically abrupt interfaces determined by either O or Mg can be formed, depending on the substrate surface preparation. The density functional theory calculations show that screening of the interfacial dipole moment is the driving force for atomic stacking at the interface, which in turn determines the electronic properties of the MgO(111)/SiC(0001) interfaces. The electronic structure calculations show that O and Mg terminated interface have valence band offsets of 1.0 eV and 3.5 eV, respectively. These results demonstrate the large electronic tunability of this heterostructure, and indicate potentials for number of other polar oxide/semiconductor interfaces.

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