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Investigation of 3C-SiC/SiO_2 interfacial point defects from ab initio g-tensor calculations and electron paramagnetic resonance measurements T. A. NUGRAHA, Max-Planck-Inst. fuer Eisenforschung, M. ROHRMUELLER, U. GERSTMANN, University of Paderborn, S. GREULICH-WEBER, Solar Weaver GmbH, A. STELLHORN, University of Paderborn, J. L. CANTIN, J. VON BARDELEBEN, Pierre and Marie Curie University, W. G. SCHMIDT, University of Paderborn, S. WIPPERMANN, Max-Planck-Inst. fuer Eisenforschung — SiC is widely used in high-power, high-frequency electronic devices. Recently, it has also been employed as a building block in nanocomposites used as light absorbers in solar energy conversion devices. Analogous to Si, SiC features SiO_2 as native oxide that can be used for passivation and insulating layers. However, a significant number of defect states are reported to form at SiC/SiO_2 interfaces, limiting mobility and increasing recombination of free charge carriers. We investigated the growth of oxide on different 3C-SiC surfaces from *first principles*. Carbon antisite Csi defects are found to be strongly stabilized in particular at the interface, because carbon changes its hybridization from sp^3 in the SiC-bulk to sp^2 at the interface, creating a dangling bond inside a porous region of the SiO^2 passivating layer. Combining *ab initio* g-tensor calculations and electron paramagnetic resonance (EPR) measurements, we show that Csi defects explain the measured EPR signatures, while the hyperfine structure allows to obtain local structural information of the oxide layer. Financial support from BMBF NanoMatFutur grant 13N12972 and DFG priority program SPP-1601 is gratefully acknowledged.

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