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Electronic structure and scattering property of 4H-SiC(0001)/SiO_2 interface TOMOYA ONO, CHRISTOPHER KIRKHAM, Center for Computational Sciences, University of Tsukuba, Japan, SHIGERU IWASE, Department of Precision Science and Technology, Osaka University, Japan — SiC is attracted much attention as a promising material for the high-power electronics devices. We carried out a first-principles calculations to reveal the relationship between the electronic structure and the interface defects appearing in the thermal oxidation. We found interlayer the states along the SiC conduction band edge (CBE), whose location changes depending on which of two possible lattice sites, h or k, is at the interface. Excess O atoms at the interface lead to defect structures which alter the electronic structure. Changes to the valence band edge are the same whether h or k sites are at the interface. On the other hand, defects remove the interlayer state of the CBE between the first and second SiC bilayers if an h site is at the interface, but have no effect when there is a k site. The scattering property of the defects was also examined by electron-transport calculations. Carriers at the CBE of the h-type interface are easily scattered by the defects because of the absence of the interlayer states while those at the k-type interface is not. Since recent SiC-MOSFETs mainly use the conduction band as a channel, the behavior of these interlayer states at the CBE might play an important role in the performance of these devices.

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