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First-principles study of SiON/SiC(0001) surface insulating layer
YASUNOBU ANDO, University of Tokyo, KAZUTO AKAGI, WPI-AIMR, Tohoku university, SHINJI TSUNEYUKI, University of Tokyo, TETSUROH SHIRASAWA, ISSP, University of Tokyo, HIROSHI TOCHIHARA, Kyushu university — Silicon oxynitride (SiON) formed on a 6H-SiC (0001) surface could be an ideal insulating layer in the application of SiC for future semiconductor devices: it is not amorphous but crystalline with only three-atomic-layer (5A) thickness, while STS-IV measurements show that the surface has a band gap as large as crystalline SiO2 (Shirasawa et al., Phys. Rev. Lett. 98, 136105(2007)). In this study, we precisely calculated band gap profile of the system in the surface normal direction with a first-principles method based on density functional theory to find reasonable agreement with that obtained by the element-specific XAS and XES measurements. In view of its application to a metal-oxide-semiconductor (MOS) structure, we also investigated the effect of aluminum atoms deposited on the insulating layer at low coverage. Starting from several candidate structures, we optimized the structure and investigated the band gap profile. We found that adsorbate-originated states appeared within the large band gap at the surface, though the states are confined within a very thin layer apparently preserving the surface insulating layer.

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