An Epitaxial SiON Layer on a SiC Surface Studied by the Density Functional Theory

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Formation of an insulating layer at surface is a crucial requirement for the application of a semi-conducting material to electronic devices. Very recently it was demonstrated experimentally that a silicon oxynitride (SiON) layer is epitaxially formed at a 6H-SiC(0001) surface. The surface leaves no dangling bonds as suggested by its structural analysis, and actually it is stable even under atmospheric pressure. Interestingly oxygen atoms in the second layer are reported to realize straight alignment of Si-O-Si atoms (see the left panel in Fig. 1) in contrast with most polymorphs and glasses of silica and tectosilicates where Si-O-Si angles distributes around 145°. Although the thickness of the SiON layer is only ~5 A , a typical STS I-V spectrum taken at the surface shows ~9 eV band gap, which is similar to that of bulk SiO_2.

In this study we theoretically investigate structural and electronic properties of the SiON-6H-SiC (0001) surface with first-principles calculation based on the density functional theory (DFT). We first test its structural stability and confirm that the 180° Si-O-Si angle is energetically stable against any small displacement of O atoms. Theoretically optimized atomic positions and those obtained by LEED analysis agree with each other with errors of 0.02-0.06 A. We also calculate its electronic local density of states (LDOS) at surface and bulk to find that wide band gap (~6eV in DFT calculation) is realized by a thin surface layer (Fig.1).

References

1) T. Shirasawa, K. Hayashi, S. Mizuno, S. Tanaka, K. Nakatsuji, F. Komori and H. Tochihara, Phys. Rev. Lett. **98**, 136105 (2007).

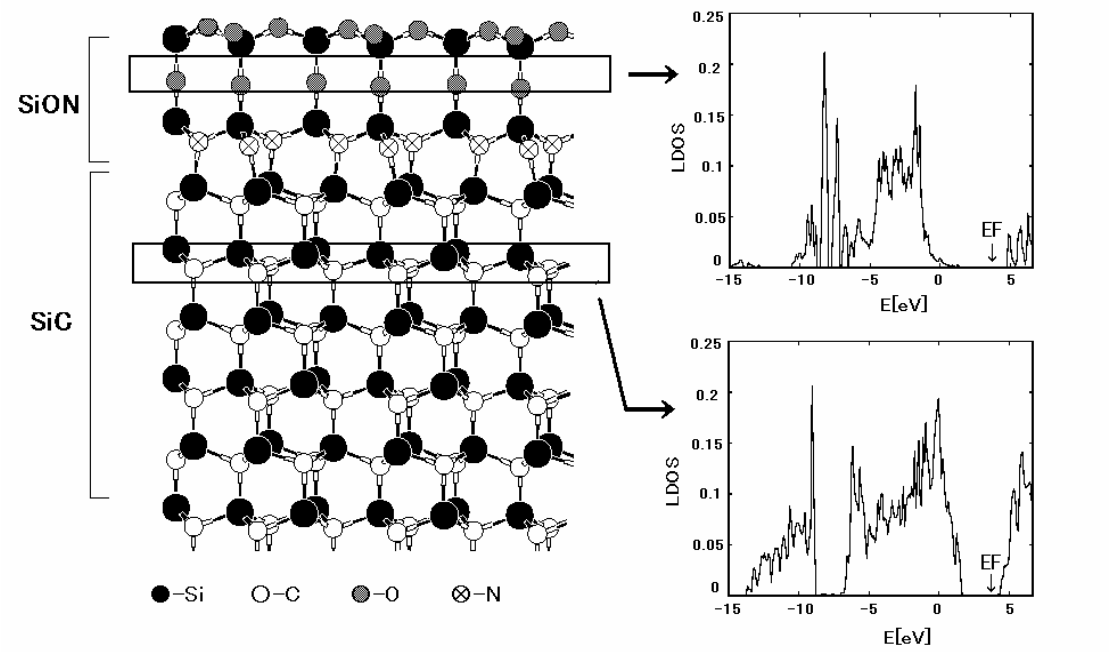

Fig.1. A side view of the structure of a SiON-6H-SiC (0001) surface and its electronic local density of states integrated within the slices near and deeply under the surface. Note that the present calculation based on DFT underestimates the band gap.