First principles calculations of relaxed and reconstructed surfaces of SiC

Hideki Otubo, Y.Yamamoto, H.Takekuni, and S.R.Nishitani,

Department of Informatics, Kwansei Gakuin University, Gakuen 2-1, Sanda, 669-1337 Japan

Commercial SiC single crystals for the device substrate are being produced by Lely-method, where the micropipes on the {0001} surface are easily included. These defects induce severe damages of the current leak occasionally. On the other hand, newly developed metastable epitaxy method (MSE) makes defect-free single crystals. The growth environments are much different between them, C-rich for Lely-method and Si-rich for MSE.

The authors have been proposed a model describing the environmental dependence of the micropipe formation. The key difference should be on the surface energy, where Si-rich environment makes {0001} surface stabilized against other orthogonal surfaces, and C-rich environment makes opposite tendency. When {0001} surface is most stable, attached atoms diffuse to cover the micropipe for enlarging the {0001} surface. We have calculated some surface energies using the first principles method under the unrelaxed conditions. In this research, we include the effects of relaxation and reconstruction of the near surface region.

We used the slab models of specific surfaces for the polytypes of 3C, 4H and 6H SiC. The surface relaxations are included for the surfaces orthogonal to {0001} face. For the {0001} face, a surface reconstruction of 3x3 type has been reported as shown in Fig.1[1]. First principles calculations were performed with VASP code, and Projector Augmented Wave(PAW) potentials was used.

Figure 2 shows the calculated results of surface energies. The {0001} face shows environmental dependence due to the changes of Si and C chemical potentials. {11-20} and {1-100} faces, orthogonal to {0001} face, however, are non-polarized, and show no environmental dependence. The surface energy of {0001} face in Si-rich environment shows most stable and that in C-rich shows most unstable, which is the same tendency for the unrelaxed calculations done before. The results are consistent with the experimental results and the model of the micropipe formation.

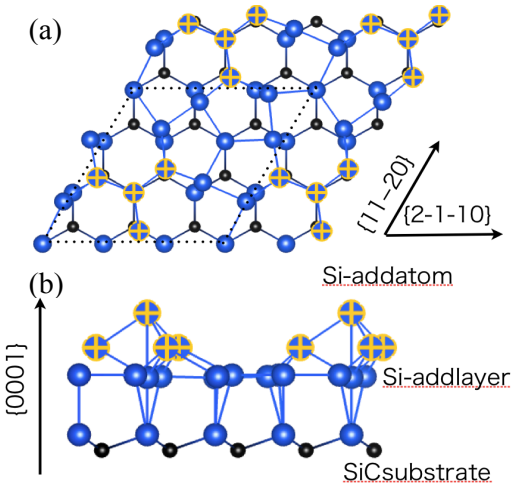

Fig.1 (a) top view and (b) side view of the surface reconstruction for {0001} face of SiC[1].

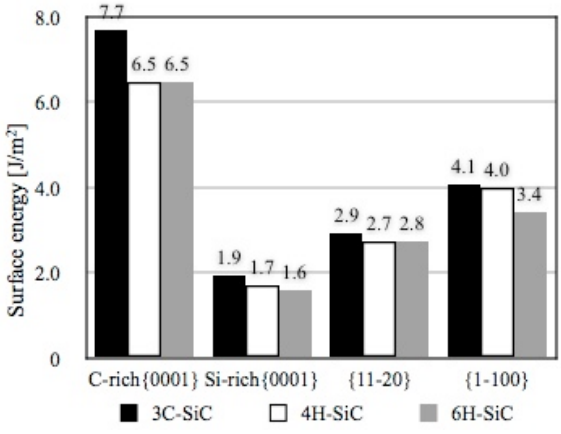

Fig.2 Surface energy of SiC considering the relaxation and reconstruction effects.

References

[1] Y. Li, L. Ye, X.Wang, *Surface Science,* **600**, 298–304 (2006).