First principles calculations on surface energy of SiC

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SiC is a strong candidate for the next generation material of power electronic devices. For getting cheap SiC wafers, an alternative process to the current expensive one of the chemical vapor deposition is highly required. The current authors have recently proposed a quite new method of the SiC crystal growth, which utilizes the solution method. To understand the growth of crystal in this process, it is necessary to clarify the orientation dependency of SiC surface energy.

The first principles calculations using VASP, Vienna Simulation Package, are performed on the surfaces of {0001}, {11-20} and {1-100} in 4H and 6H-SiC. In 3C-SiC, we performed on the surfaces of {111}, {1-10} and {11-2} which show equivalent local configurations with those of 4H and 6H-SiC. For describing the chemical potential dependency of the silicon rich environment, the method proposed by Qian *et al.* is applied. The results shown in Fig.1 are summarized as follows; the surface energies are very close among the equivalent local configuration of different polytypes. The surface energies of {0001} are lower than those of the other surfaces, that is consistent with the experimental observation of the initial shapes of 4H-SiC single crystals.

References:
1 S.R.Nishitani, T.Kaneko, J.Cryst. Growth, 310 (2008), 1815.
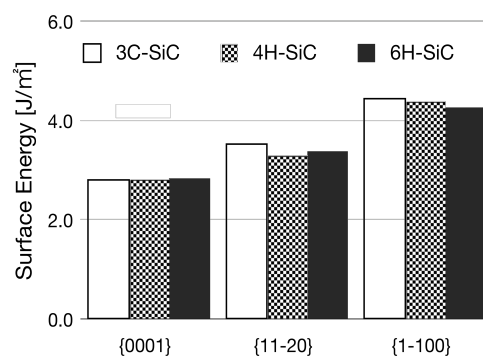2 G.-X. Qian, R. M. Martin, D. J. Chadi, Phys. Rev. B, 38 (1988), 7649.

Fig.1 Surface energies of SiC polytypes.