Surface energy of SiC by first principles calculation

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SiC has more excellent physical properties than Si. For example, its band gap is about three times larger than that of Si and thermal conductivity is about four times larger. Thus, SiC is a strong candidate for the next generation materials of power electronic devices. For the cost cut of SiC wafer making, the alternative process to the current expensive process of the chemical vapor deposition is highly required. The production from liquid phases has been thought to be very difficult due to low growth rate resulting from the low carbon solubility in liquid Si.

'Metastable Solvent Epitaxy(MSE)' [1] is a quite new method of the SiC crystal growth from the solution developed by the authors. In this new method, 4H-SiC is used as the 'seed' and 3C-SiC is used as the 'feed', and thin film of melt Si is placed between them. To control the growth of crystal in this process, it is necessary to clarify the orientation dependency of SiC surface. We have thus performed the first principles calculation of the typical surface energies of SiC polytypes.

Specific targets of the first principles calculations performed by VASP, Vienna Simulation Package, are SiC polytypes of 3C, 4H and 6H-SiC and the surfaces of {0001}, {11-20} and {1-100} in 4H and 6H-SiC. In 3C-SiC which shows cubic structure, we performed on the surfaces of {111}, {1-10} and {11-2} which shows equivalent local configurations with those of 4H and 6H. The preliminary results shows as follows; the surface energies are very close among the equivalent local configuration of different polytypes, and the surface energy of {0001} 4H-SiC, which is expected to be low from the experimental observation of the initial shapes of 4H-SiC single crystals, is not so low.

References:

[1]S.R.Nishitani and T.Kaneko, J.Cryst. Growth, Vol 310/7-9 (2008), pp 1815-1818..