

SiC polar surface growth by first principles calculations

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SiC is receiving particular attention as the next generation materials for new power electronic devices. At the moment, the main SiC crystal growth is performed by the vapor-method called 'improved Lely-method'¹⁾. In this method, it utilizes the phenomenon that vapor constituted by Si and C, sublimed from 'feed', deposit out of inert gas to the 'seed' whose temperature is lower than that of 'feed'. Authors have recently developed a new method which is 'Metastable Solvent Epitaxy'(MSE)²⁾. In this method, C dissolved from 'feed'(3C-SiC) transports to 'seed'(4H-SiC) through thin Si solvent.

We could observe large micropipes³⁾ at (0001)-face in the case of the vapor-method. On the other hand, (0001)-face shows flat and wide surfaces in the case of MSE. We thought that the difference of polar surface growth of SiC depends on the environment around 'seed'. Thus, we paid attention surface energies as factors for growing crystal shape. Thus, we calculated those by the first principles calculations code.

In this calculation, we selected 3C, 4H and 6H-SiC in SiC polytypes, {0001}, {11-20} and {1-100}-faces hexagonal crystals. {0001}-face is the polar surface and another faces are surfaces orthogonal the polar surface. In the case of cubic crystal, we selected {111}, {1-10} and {11-2} because equivalent to those of hexagonal crystals. The first principles calculations are performed by VASP code. bulk and slab-models of SiC are constructed by 'MedeA'. We calculated surface energies using chemical potentials⁴⁾.

Fig.1 shows our results. As the results, the polar surface is most stable surface in (a)Si-rich, and is most unstable surface in (b)C-rich. Thus, polar surface grown in Si-rich should show largest than another surfaces. If micropipes appears on the (0001)-face in C-rich, micropipes does not close, and that spreads.

Reference:

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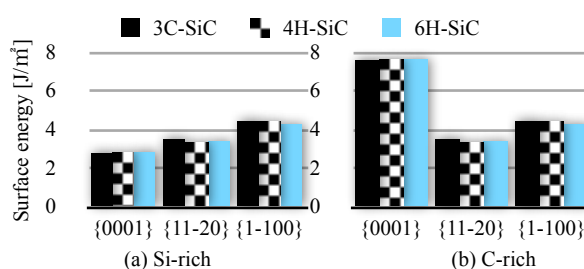


Fig. 1. Surface energies in each environment