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SiC polar surface energy by the 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 SiC crystal growth is mainly performed by the vapor deposition called 'improved Lely-method'[1]. In this method, it utilizes the phenomenon that vapor constituted by Si and C, sublimated from 'feed', deposits out of inert gas on 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, carbon dissolved from 'feed'(3C-SiC) transports to 'seed'(4H-SiC) through thin Si solvent. Large micropipes are often observed at (0001)-face in the case of the vapor-method[3]. On the other hand, (0001)-face shows flat and wide surfaces in the case of MSE. We thought that the difference of the polar surface growth of SiC depends on the environment around 'seed'. Thus, we performed the first princeples calculations of the surface energies as the controling factor for growing crystal shape. In this calculation, we selected 3C, 4H and 6H-SiC in SiC polytypes, {0001}, {11-20} and {1-100}-faces hexagonal crystals. The {0001}-face is the polar surface and another faces are surfaces orthogonal to that. In the case of cubic crystal, we selected {111}, {1-10} and {11-2} because of the equivalence 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 with the consideration of the chemical potential dependency[4]. As shown in the results of Figs.1, the polar surface is the most stable surface in (a) Si-rich, but is the most unstable surface in (b)C-rich. Thus, the results indicated that the polar surface grown in Si-rich environment should show larger area than those of another surfaces.

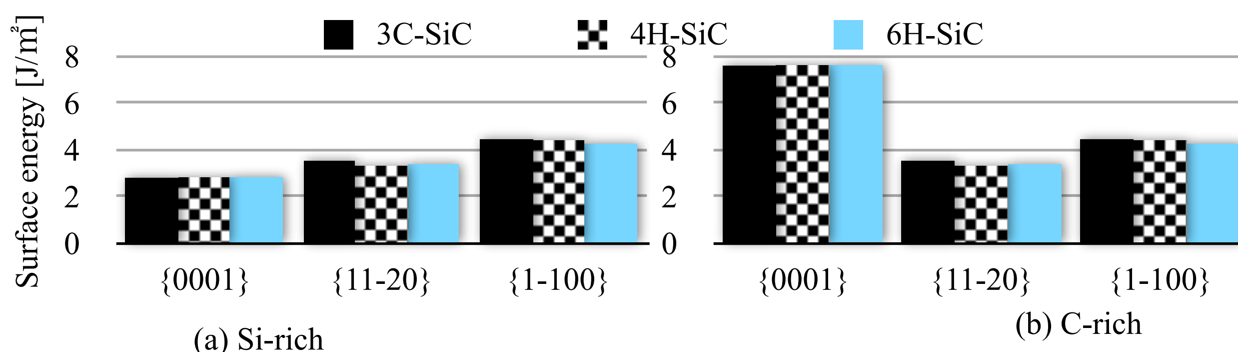

Fig.1. Surface energies in each environment.

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