The first principles calculations on the surface diffusion of SiC

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SiC is a strong candidate for the next generation materials of power electronic devices, due to its superior physical and electronic properties. Conventionally SiC has been produced by chemical vapor deposition, which causes the cost of SiC wafer very high.

The authors have very recently reported quite new method, called 'Metastable Solvent Epitaxy(MSE)' [1)]. SiC single crystals are deposited from the thin layer of Si melt containing supersaturated carbon under the constant temperatures. The uniqueness of the new method is the driving force of its crystal growth, which is the chemical potential difference between 3C and 4H-SiC polytypes. MSE possesses unclear points in the crystal growth mechanism; typically the outer shape of the initial single crystals shows six-fold mushroom like.

The origin of this query shape should be either due to the static effect of orientation dependency of surface energy, or the kinetic effect of surface growth. To evaluate the kinetic effect, we should know the surface diffusion behavior, which is controlled by the activation energies of diffusing process of the carbon ad-atom on typical surfaces. Thus we have performed the first principles calculations of the surfaces using the slab model with a carbon atom attached at some typical sites on Si-face and Si terminated C-face. The activation energy of carbon diffusion on the {0001} surface is very low, which suggests that the flat surfaces appear on SiC single crystals.

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