

## First principles calculations on vibration free energies of SiC polytypes

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SiC has been recently focused on the next generation materials for the power electronic devices due to its excellent physical and chemical properties. SiC shows many polytypes such as, 3C, 4H and 6H. The phase stabilities of these polytypes are still under discussions. The novel crystal growth method of SiC polytypes, so-called Metastable Solvent Epitaxy(MSE), has recently been developed by the authors, in which a similar mechanism to that of the high-pressure synthesis of diamond is used. The driving force of the epitaxial growth of stable 4H-SiC is the metastability of the polytype of SiC.

The stability of the polytypes have been explored by the first principles calculations with the phonon free energy, but the difference is very small. In this research, the authors investigate the accuracy of the calculations. The VASP (Vienna Ab-initio Simulation Package) code has been used.

After adjusting some parameters of the VASP code, the major controlling parameter on the total energy has been appeared to be the cut-off energy. Fig.1 shows the cut-off energy dependence of the total energy of 3C-SiC; the energies approach to a value of 1000eV or above of the cut-off energy. Fig.2 shows the temperature dependency of the phase stabilities of 3C-SiC measured from 4H-SiC. Two lines calculated by the cut-off energies of 600eV and 400eV are shown by the solid and dashed lines, respectively. The dashed line with the cut-off energy of 400eV shows that 4H-SiC is more stable than 3C-SiC on the entire temperature range. The solid line with the cut-off energy of 600eV shows

- (i) 3C-SiC is stable at the lower temperatures,
- (ii) 4H-SiC is stable at the higher temperatures, and
- (iii) the transition temperature is located around at 1000K.

These results are consistent with the experimental ones.

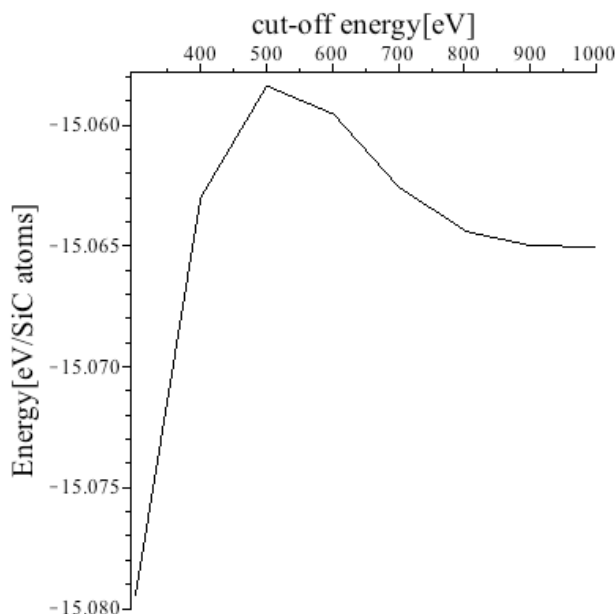


Fig.1 Cut-off energy dependence of the total energy of 3C-SiC.

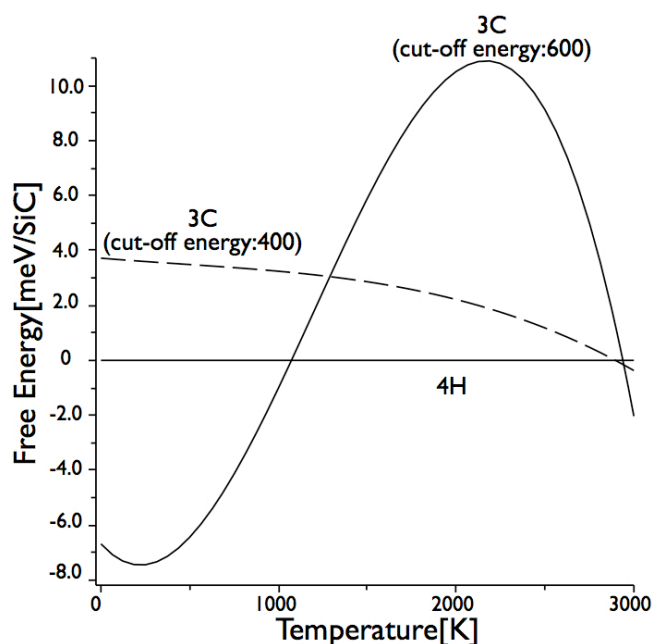


Fig.2 Temperature dependency of the phase stabilities of 3C-SiC measured from 4H-SiC. The solid and dashed lines were calculated with the cut-off energies of 600eV and 400eV, respectively.