3.3.15 First Principles Calculations on Phase Stability of SiC Polytypes

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The authors have recently proposed new single crystal growth method, named metastable solvent epitaxy, which is developed for *SiC*, the next generation power device materials. The driving force of this crystal growth mechanism is the thermal stability differences of *SiC* polytypes of 3C, 4H and 6H. In this research, we will show the vibrational free energies of *SiC* polytypes from the first principles calculations.

In the new method, epitaxial layer of 4H *SiC* is grown using the feed of polycrystalline 3C *SiC*. The solvent of liquid *Si* used for carbon transfer is very thin, such as a few tens or a few hundreds micrometers, and kept at a constant temperature. The solute concentration difference of the liquid *Si* solvent between the interfaces facing feed and seed *SiC* is the driving force and is rooted in the difference of stable and metastable phases. The energy differences among the polycrystals of *SiC*, however, are subtle, and hardly determined from the experiments. Thus the first principles calculations are powerful estimation tools.

The first principles calculations are performed by VASP, and the phonon calculations are performed by preprocessor software of MedeA. The vibrational free energy are obtained under thermal expansion allowed. At the ground state calculations, the stabilities are 3C>4H>6H. However, including the zero point vibration, they become 3C>6H>4H. At the higher temperatures, the stability of 6H overtakes that of 4H. These results are consistent with the experimental ones.

1. S.R.Nishitani and T.Kaneko, J. Crystal Growth, 210 (2008), 1815-1818.