Surface Energy and Configurations of *SiC* by First Principles Calculation

Yosuke Yamamoto, S. R. Nishitani, R. Takeda, K. Terai, T. Kaneko and Noboru Ohtani

SiC is a strong candidate for the next generation materials of power electric devices, due to its superior physical and chemical properties. *SiC* wafer is very expensive due to the chemical vapor deposition.

The authors have reported quite new method, called 'Metastable Solvent Epitaxy (MES)', so as to avoid these problems. 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. However MSE possesses unknown points in the crystal growth mechanisms; kinetic or energetic mechanism determing surface morphology.

We have tried to calculate the surface energies of (11-20), (1-100) and (0001) for 4H and 6H-*SiC* by a first principles calculation code. Furthermore for revealing the surface diffusion path, we calculated the energy differences of the carbons attached at some typical sites on *Si*-face and *Si* terminated C-face.