First Principles Calculations of SiC vibrational free energy

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SiC is well known compounds with many polymorphs. In this research the vibrational free energies of SiC are estimated by the first principles calculations. The first principle calculation is performed by VASP, and the preprocessor of MedeA is used for the phonon dispersion and density of states calculations.

Three typical types of the polymorphs of SiC are calculated, 3C, 4H and 6H. The phonon density of states are shown in Fig.1, and show very similar shapes due to their similarity of the local atomic configuration. When we use the quasi-harmonic approximation under their stable volumes fixed, the vibrational free energies are calculated.

6H SiC is the most stable phase at the intermediate temperatures. The stability of 3C and 4H SiC are very close and depends on the cell size and k-points. More careful calculations are being performed.

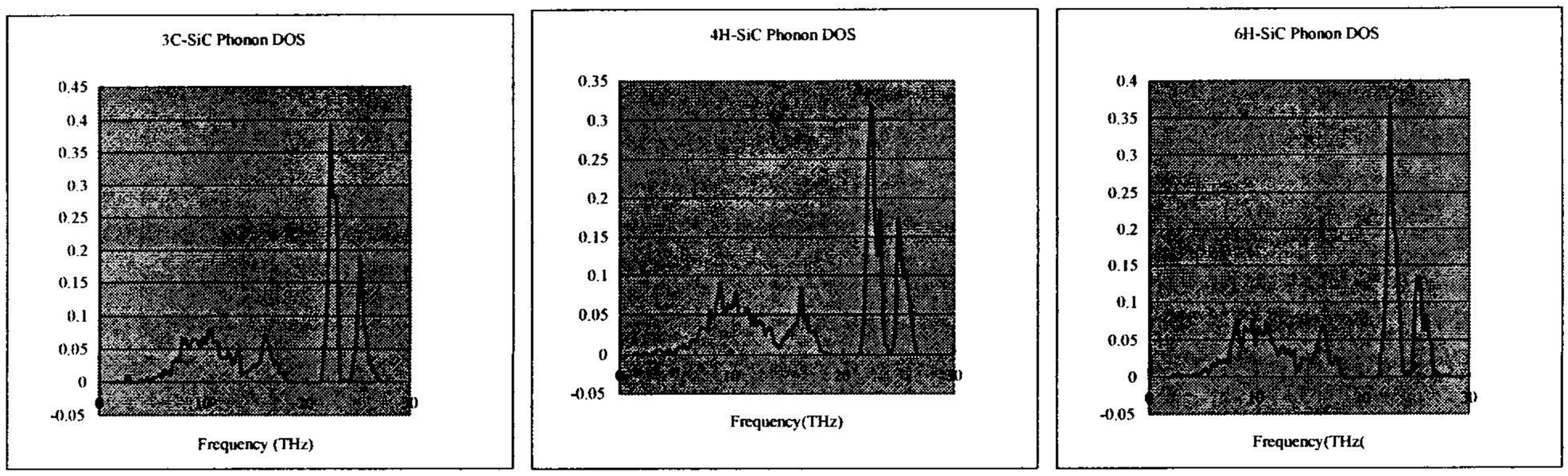

Fig.1 phonon density of states of 3C, 4H and 6H SiC.