Free Energy from Density Functional Calculations

S. R. Nishitani

Two kind of free energy changes obtained from the electron density calculations will be given in the presentation; the first is the free energy change due to the precipitates nucleation of Fe-Cu system, and the second is the vibrational free energy of SiC polytypes.

Free energy change of the nucleation process is generally constructed with the volume and the interface energy changes. For the precipitation from the super saturated solid solution, which is the typical example of the solid-solid transitions, the free energy change is alternatively obtained from the purely enthalpic and the purely entropic changes; the former is calculated by the first principles calculations and the latter is obtained from the statistical thermodynamics. The first principles calculations show the reliable estimation of the critical free energy change for bcc Cu precipitates in Fe-Cu system.

The second example, the vibrational free energy difference of SiC polytypes, is the driving force of the newly investigated process of SiC single crystals. The growth mechanism of the new process is understood by the stable and metastable double phase diagram; the equilibrium 4H SiC is deposited from the super saturated Si(C) solvent which is obtained from the metastable 3C SiC. The first principles calculations of phonon DOS predict the stable region of 4H SiC at the low temperatures.