Free Energy Calculation of Precipitate Nucleation

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Our recently proposed calculating method reliably predicts the nucleation free energy barrier of the homogeneous and coherent precipitations. Helmholtz free energy change is clearly defined and calculated by the purely enthalpic and entropic contributions between the initial state of the isolated solute atoms scattering around the matrix and the final state of the cluster of size n traveling around the matrix. The enthalpic term is calculated by the reliable first principles method and the entropic term is estimated by the ideal solution model. The vibrational free energy is also included by the quasi-harmonic approximation. The model calculation was performed on bcc Cu precipitations in the Fe-Cu system. The predicted values of the critical number of 12 atoms and the critical free energy barrier of 0.6eV show good agreement with the experimentally estimated ones for the annealing temperature of 773K and the initial concentration of 1.4at%Cu.