

## First Principle Calculations of Nucleation Free Energy Change for BCC Cu Precipitates in Fe–Cu System

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Abstract: A slight but crucial modification of the droplet model enables the first principles calculations of free energy change of precipitate nucleation. New treatment divides the free energy into cluster energy and entropy terms. The former, including the internal enthalpy change and the interface energy, is accurately calculated by ab initio methods. The latter simply estimated by the ideal solution model. Model calculations have been performed for bcc Cu clusters precipitated in bcc Fe matrix, and give reliable predictions of the free energies of small sizes around the critical radius.