

First-principles study of the effect of lattice vibrations on Cu nucleation free energy in Fe–Cu alloys

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Abstract: The effects of lattice vibration on Cu nucleation in Fe-Cu alloys have been investigated by a first-principles technique. We find that the vibrational effect is comparable ($\sim 36\%$) to be configurational entropy. Lattice vibration increases the activation barrier of Cu precipitates by 5.3 eV, where the resulting activation barrier is estimated to be 0.62 eV at critical number n^* of 12 atoms, which is in satisfactory agreement with the previous experimental prediction. Within the description of classical treatment, this increase is interpreted in terms of the associated decrease of driving force due to lattice vibration.