Precipitation Kinetics from EAM Potentials:
Influence of the Vacancy Jumps Activation Barriers

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We have studied diffusion and precipitation kinetics in dilute $Fe_{1-x}Cu_x$ alloys, using both static relaxation of a many body EAM potential and kinetic Monte Carlo simulations. We first show that for dilute Fe-Cu alloys, the configurational energies predicted by the EAM potential relaxation can be described by a simple pair interaction model on a rigid lattice. Then, the saddle point energy for vacancy migration is shown very sensitive to both the nature of the jumping atom and that of the first nearest neighbors of the atom at the saddle point position. Finally, the interaction energies and the saddle point energies obtained from the EAM potential are integrated in a Monte Carlo scheme. The dependence

of the saddle point energies on the local atomic configurations modifies the relative mobility of small Cu clusters and Cu monomers. At high temperature, it leads to a slowing down of the precipitation by a constant ratio of on the time scale, but at low temperature, the kinetic path is completely modified.