Vacancy effect on the precipitate nucleation in Fe-Cu alloy

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The activation energy barrier height of bcc-Cu precipitates in Fe-Cu alloy has been predicted using the first principles calculations. The predicted values of the critical number of 12 atoms and the critical free energy barrier of 0.6eV show good agreements with the experimentally estimated ones for the annealing temperature of 773K and the initial concentration of 1.4at%Cu. This approach also predicted that the vacancy prefers inside not at the interface of clusters.