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Effects of solute concentration on the stacking fault energy in copper alloys at finite temperatures

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Abstract

Stacking-fault energy (SFE) is a critical parameter that influences plastic deformation of Cu alloys. Here, the SFEs of Cu solid solutions at various temperatures and solute concentrations were studied by using first-principles calculations. The interaction energies of 18 substitutional atoms and 5 interstitial atoms with stacking fault (SF) in Cu were obtained for the first time. The results show that the interactions can extend to the second layer with respect to the SF. Substitutional atoms Sn, Al, Zn, P, Si, Ge as well as interstitial atoms Be, C, N, O, H have large attraction energies with the SF; whereas, substitutional atoms Ti, Mn, Cr are repelled by the SF, and the rest of the atoms have small interaction energies. Then, the effects of uniform and Fermi-Dirac distribution of solute atoms on the SFE of Cu