Precipitation strengthening in Cu-Ni-Si alloys modelled with ab initio based interatomic potential

Cu-Ni-Si alloys with δ-Ni_2Si and β-Ni_3Si precipitates are widely used for electric and electronic applications such as connectors or lead frames because they combine high strength and high electrical conductivity.
Effective interaction potentials suitable for Cu/δ-Ni_2Si and Cu/β-Ni_3Si are developed. We optimise potential parameters of an embedded atom method (EAM) potential to reproduce forces, energies and stresses obtained by ab initio calculations. Details of the potential generation are given and its validation is demonstrated. The potentials are used in molecular dynamics simulations of shear tests to study the interactions of edge dislocations with coherent δ-Ni_2Si and β-Ni_3Si precipitates embedded in a copper matrix. In spite of significantly different crystallographic structures of copper and δ-Ni_2Si which usually result in Orowan circumvention, we also observed cutting processes in our simulations. Cutting is found for a specific orientation of the δ-Ni_2Si precipitate and in some cases where Orowan loops originating from previous circumvention processes are present in the glide plane. It is found that β-Ni_3Si precipitates have a similar effect on precipitation strengthening as δ-Ni_2Si. Dislocations usually cut β-Ni_3Si but increased coherency strain can lead to circumvention processes.