"Atomistic simulation of internal interfaces in copper matrix alloys"

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Copper matrix alloys are widely used in applications which require both high strength and high electrical conductivity. Further improvement of these materials demands a detailed understandig of the effect of alloying elements on the mechnical strength and the electrical conductivity. Usually these materials contain several types of precipitates and dissolved foreign atoms. High strengths are obtained with precipitates hindering dislocation motion effectively. This can be achieved by suitable chemical compositions and interface structures of the precipitates. The electrical conductivity is mainly decreased by a high number of dissolved foreign atoms. Candidates for materials which contain suitable precipitates and few dissolved foreign atoms are Cu-Ag and Cu-Ni-Si-X where X represents an additional alloying element.

In this work the precipitation processes in Cu-Ag and Cu-Ni-Si-X are simulated using the kinetic Monte Carlo (KMC) method. Parameters needed for the KMC model are determined by ab initio calculations. In case of Cu-Ni-Si-X the KMC simulations show that Cr and Fe reduce the number of dissolved foreign atomsmost effectively. In agreement with experimental results the KMC simulations with Mg confirm that Mg diffuses to the interfaces between Ni-Si precipitates and copper matrix. Ab initio calculations of these interfaces reveal favourable Mg sites and a strongly enhanced misfit strain due to Mg. In case of Cu-Ag classical molecular dynamics (MD) is used to investigate stresses and strains at Cu-Ag interfaces and to study the interaction of a dislocation with silver precipitates. The MD simulations show that the shape of the precipitate and the coherency of the interface has a strong influence on the strengthening.