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Ab initio based atomistic modeling pre-precipitation in Al-Cu alloys

by

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Discovered a long time ago, age-hardenable aluminium alloys are still very important for light-weight constructions. The strengthening of these alloys is mainly due to the formation of coherent, metastable, and nano-sized precipitates. Thermodynamics and atomic structures of pre-precipitates in dilute Al–based alloys are studied using Metropolis Monte Carlo simulations as well as the master equation approach with many-body effective cluster interactions that have been systematically derived from ab initio supercell calculations. We show that many-body interactions, including the contributions due to lattice relaxations around the solute atoms, are mainly responsible for the formation of metastable planar atomic arrangements known as Guinier-Preston zones (GPZ). Interaction terms up to four-body clusters are shown to be necessary to correctly reproduce the structures of GPZs in Al–Cu solid solutions. The atomistic simulations yield very reasonable ordering temperatures and kinetics of pre-precipitation.

Date: **17 October 2018**

Time: **14:00**

Venue: **Building C1 Vědeckotechnický park, room TC 211, Teslova 5B, Pilsen**

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