Precipitation in a multicomponent alloy: combining atomic and mesoscopic simulations

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Zr and Sc precipitate in aluminum alloys to form the compounds Al_3Zr, Al_3Sc, and $Al_3Zr_xSc_{1-x}$ which for low supersaturations of the solid solution have the $L1_2$ structure. The aim of the present study is to model at an atomic scale this kinetics of precipitation and to build a mesoscopic model so as to extend the field of supersaturations and annealing times that can be simulated. In this purpose, we use some ab-initio calculations and experimental data to fit an Ising model describing thermodynamics of the Al-Zr-Sc system. Kinetics of precipitation are studied using a kinetic Monte Carlo algorithm based on an atom-vacancy exchange mechanism.[1] These atomic simulations allow us to understand the experimentally observed structure of the precipitates in the ternary alloy as well as the different effect on the precipitation kinetics associated with a Sc or Zr addition. Cluster dynamics is then used to model at a mesoscopic scale all the different stages of homogeneous precipitation. This technique reproduces in a quantitative way kinetics of precipitation simulated with kinetic Monte Carlo as well as experimental data.[2]

[1] E. Clouet, M. Nastar, and C. Sigli. Nucleation of Al_3Zr and Al_3Sc in aluminum alloys: from kinetic Monte Carlo simulations to classical theory. *Phys. Rev. B*, 69:064109, 2004.

[2] E. Clouet, A. Barbu, L. Laé, and G. Martin. Precipitation kinetics of Al_3Zr and Al_3Sc in aluminum alloys modeled with cluster dynamics. *Acta Mater.*, in press, 2005.