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Stochastic statistical theory of nucleation and evolution of nano-sized precipitates in alloys with application to the precipitation of copper in iron

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Kinetics of nucleation and evolution of nano-sized precipitates in alloys is studied basing on the earlier-developed stochastic statistical approach (SSA), with the use of the Fe-Cu alloy models as an example. Comparison of results of the SSA-based simulation employing the simplified direct atomic exchange model to the available results of the atomistic Monte Carlo simulation in which a more realistic, vacancy-mediated exchange model is used, shows a good agreement in all microstructural features, including the sizes, morphology and the number of precipitates, when temporal variation of an effective direct atomic exchange rate due to the vacancy trapping effect is taken into account, while using our approach considerably reduces the computation time. Kinetics of very first stages of nucleation is studied in detail, and evolution of microstructure at these stages is found to have little in common with the classical nucleation theory notions. We also investigate dependences of various characteristics of precipitation, including sizes and density of precipitates and the incubation time, on temperature, concentration and on solute-solute interaction type. We found these dependences to be typically very sharp and to qualitatively agree with the classical nucleation theory ideas.

Mardi 6 janvier 2009 à 14h30

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