PRECIPITATION IN ALLOYS: A KINETIC MONTE CARLO AND CLASS MODEL STUDY

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Introduction

Breakthroughs and advances in materials science are closely connected to the basic research to interpret meso-, micro- and nano-scopic mechanisms. Many physical properties of the metals depend on the defects such as vacancies and their concentration in the crystals. Study of the precipitation kinetics from the saturated metastable solid solution can be divided into three regimes: (i) nucleation, (ii) diffusion controlled growth of clusters and (iii) cluster coarsening (Ostwald ripening) and coalescence where larger clusters grow on the expense of smaller. In reality those three idealized regimes often overlap consequentially making the interpretation of obtained results difficult.
Dynamic and kinetic development of molecular (atomic) systems using computational materials science is the main focus of this paper. Particular methods used here are a kinetic Monte Carlo (kMC) and a class model. The kMC is based on statistical mechanics [1-5], where development of the system is simulated in real time. The class model is based on classical nucleation and growth theory, [6], where precipitates are distributed in classes of size. These are then used to obtain time evolution of the particle size distribution. Results obtained with class model were compared to kMC simulations at atomic scale which gives precise evolution of precipitation, growth and coarsening in time. Both methods were performed on Fe, 1 at. % Cu alloy isothermally treated at 873 K.

Numerical model

Kinetic Monte Carlo model

Monte Carlo simulations in this work rely on the rigid lattice BCC residence time algorithm model. The vacancy diffusion simulations were performed on binary FeCu alloy with 1 at. % Cu on a fixed size of 80 periodic boundary conditions lattice constants. Evolution of the system is determined by eight first nearest jump probabilities around vacancy. Each probability is given by:

$$\Gamma_{XV} = \nu_X \exp\left(-\frac{E_{XV}}{kT}\right) \quad (1)$$

where ν_X represent attempt frequencies for particular atom and E_{XV} is the energy difference between stable position and the saddle point position of jumping atom. To calculate activation energies broken bond model was used [1, 2]. The activation energies depend on the saddle point energies and interatomic potentials of the first and second nearest neighbours of the jumping atom, calculated by:

$$\Delta E_{XV} = e_{SpX} - n_{XX}\varepsilon_{XX} - n_{XY}\varepsilon_{XY} - n_{XV}\varepsilon_{XV} \quad (2)$$

After calculation of eight possible jump probabilities around vacancy, the independent event is selected on the basis of the random number. The real time is calculated with correlation between vacancy concentration in the simulation box and reality, multiplied by averaged residence time and is given by

$$t = \left(\frac{c_{Vsim}}{c_{Vreal}}\right) \cdot \left(\frac{1}{\sum_{i=1}^{8} \Gamma_i}\right) \quad (3)$$

Simulation parameters are presented in Table 1.

Table 1: Simulation parameters

$\varepsilon^{(1)}_{FeFe} = -0.778$ eV	$\varepsilon^{(2)}_{FeFe} = -0.389$ eV
$\varepsilon^{(1)}_{CuCu} = -0.778$ eV	$\varepsilon^{(2)}_{CuCu} = -0.389$ eV
$\varepsilon^{(1)}_{FeCu} = -0.731$ eV	$\varepsilon^{(2)}_{FeCu} = -0.366$ eV
$\varepsilon^{(1)}_{FeV} = -0.335$ eV	$\varepsilon^{(1)}_{CuV} = -0.335$ eV
$e_{SpFe} = -9.557$ eV	$e_{SpCu} = -9.098$ eV
$\nu_{Fe} = 8.7\times10^{12}$ s^{-1}	$\nu_{Cu} = 8.7\times10^{12}$ s^{-1}

Class model

The class model for precipitation aims at describing the quantitative time evolution of the precipitation state, namely the particle size distribution, the volume fraction and the number density of precipitates. The precipitate size distribution is discretized into several size classes. The time evolution of the radius of each class is calculated as a function of temperature, solute content, solubility limit and diffusivity. Nucleation can eventually take place, thus adding new classes of precipitates. Time evolution of precipitates thus depends on diffusion controlled growth. In order to study the kinetics of the precipitation process a simulations for homogeneous precipitation were performed. For the sake of simplicity the model was restricted to spherical precipitates. Other parameters used were as follows; an interfacial energy of precipitates $\gamma = 0.25$ Jm^{-2}, diffusion constant $D_0 = 6\times10^{-8}$ m^{2}s^{-1}, activation energy for diffusion $Q = 166400$ Jmol^{-1}, and the simulation time used in model with 1 at. % of Cu was 10^6 s.

Results and Discussion

In figure 1, results obtained from class model for homogeneous precipitation are shown. Figure depicts nucleation rate, volume fraction, critical and average radius versus time.

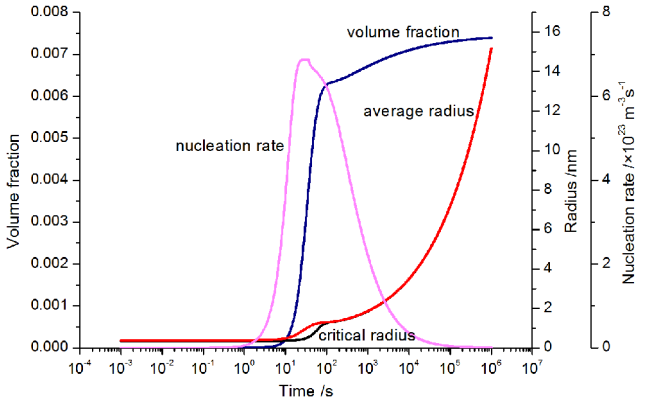

Fig. 1. Class model predicted precipitation kinetics at 873 K.

It is evident from the volume fraction diagram that long holding times, precipitation process has not reached equilibrium conditions. The average radius starts to increase significantly immediately after the nucleation rate reaches its maximum value. At this point the intensive growth of precipitates starts. After plateau the nucleation rate starts to drop. Short time is needed for the size of the critical radius to reaches the average radius. At this point the nucleation is already finished and process of growth commences. Larger precipitates are growing on the expense of smaller precipitates.

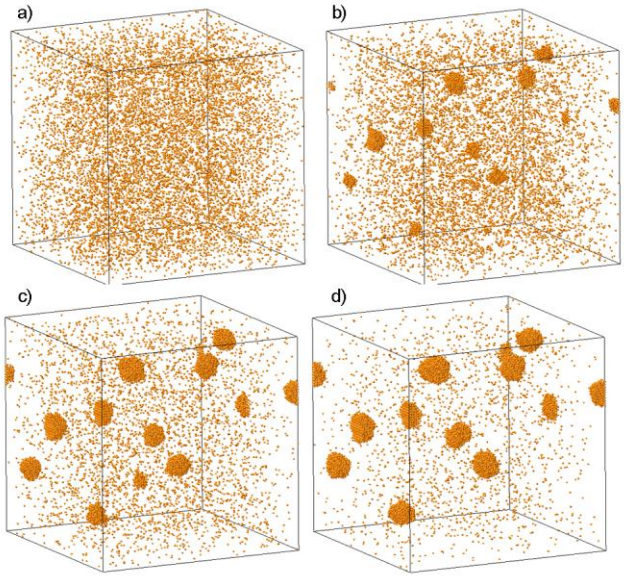

Fig. 2. kMC simulation at 873 K of precipitation and growth at; a) 0 s, b) 44 s, c) 87 s and d) 257 s.

Class model results were then compared to results obtained with kMC simulations on a BCC simulation box of size $L = 80^3$ lattice constants with size length in reality of 22.96 nm populated with a total 1024000 atoms. In figure 2 only Cu atoms for the kMC simulation performed at 873 K are shown. Cu atoms are dissolved in the matrix at the beginning (figure 2a). As simulation progresses and the time advances, precipitates start to nucleate (figure 2b). They are small in size, however further on they start to grow (figure 2c and 2d) as was predicted with class model. At the end of kMC simulation (figure 2d) nine precipitates with Cu concentration 0.81 at. % and mean diameter of 2 nm were found.

Conclusions

Class model for precipitation used here is powerful tool capable of describing precipitation process. Kinetic Monte Carlo simulations of precipitation at atomistic level can contribute to a better understanding of nucleation, growth and coarsen regimes. Result presented here were obtained on simple binary alloy isothermally treated at 873 K. Compared to kMC which starts with randomly distributed atoms on lattice the class model can be used to quickly calculate kinetic properties of desired alloys. Necessities for correct results are high quality input parameters in both models.

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