pcpsim
MODEL FOR HOMOGENEOUS PRECIPITATION KINETICS in GNU OCTAVE

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1 Introduction

The model for homogeneous isothermal precipitation is partly based on the model by Langer and Schwartz, modified by Kampmann and Wagner (MLS model). In this model, we treated the nucleation and growth of the precipitation.

2 Thermodynamics of the model

As a first step we need to define the driving force for precipitation at any given time of the aging process.

$$\Delta g = -\frac{kT}{V_{at}} \cdot S \tag{1}$$

with

$$S = X_p \ln(\frac{X_C}{X_{eq}}) - (1 - X_p) \ln(\frac{1 - X_C}{X_{eq}}) \tag{2}$$

where V_{at} is the atomic volume (considered as constant for all species), S is a thermodynamical function giving the driving force for nucleation (based on the hypothesis of a diluted and regular solid solution), X_{eq} is the equilibrium solute mole fraction in the matrix, X_p the nitrogen mole fraction in the precipitate, and X_C the current solute mole fraction of the matrix.

The nucleation rate as the derivative of the precipitation density N is:

$$\frac{dN}{dt} = N_0 Z \beta^* \exp(-\frac{\Delta G^*}{kT}) \exp(-\frac{\tau}{t}) \tag{3}$$

where N_0 is the number of nucleation sites per unit volume ($\approx l/vat = 2/a^3$ for a bcc structure with lattice parametera), Z is the Zeldovich factor ($\approx 1/20$), τ is the incubation time. The other parameters of equation are expressed as follows:

$$\beta^* = \frac{4\pi R^{*2} D X_{C0}}{a^4} \tag{4a}$$

$$R^* = \frac{R_0}{S} \tag{4b}$$

$$R_0 = \frac{2\gamma V_{at}}{kT} \tag{4c}$$

$$\Delta G^* = \frac{16}{3}\pi \frac{\gamma}{\delta g} \tag{4d}$$

$$\tau = \frac{1}{2\beta^* Z} \tag{4e}$$

$$\tag{4f}$$

where R^* is the nucleation critical radius, R0 is a thermodynamical parameter which has the dimension of a length, γ is the matrix/precipitate interfacial energy, D is the diffusion coefficient of solute atoms in the matrix, X_{C0} is the initial solute mole fraction.

The precipitate size increase during a time increment dt is then calculated as:

$$\frac{dR}{dt} = \frac{D}{R} \cdot \frac{X_C - X_{eq} exp(R_0/(X_p R))}{X_p - X_{eq} exp(R_0/(X_p R))} + \frac{1}{N}\frac{dN}{dt} \cdot (\alpha R^* - R) \tag{5}$$

The first term corresponds to the growth of existing precipitates (including the Gibbs-Thomson effect) and the second term to the appearance of the new nuclei of size R^*. The numerical factor $\alpha = 1.05$ results from the fact that new precipitates only grow if their size is slightly larger than the nucleation size. Finally, the coupling between the precipitation density and their mean radius is made through the solute balance:

$$X_c = \frac{X_{C0} - (4/3)\pi(X_p N R^3)}{1 - (4/3)\pi(N R^3)} \tag{6}$$

Now are defined the new dimensionless variables which are more easy to use for programming.

References