Nucleation, growth, coarsening equations

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1 Intro

The formulas in this note have been collected from a number of papers & books:

- Wagner et al. [1], a comprehensive review of theory and experiments
- Russell [2], good explanation of nucleation
- Calderon et al. [4], growth and coarsening in concentrated alloys with second phase precipitate concentration $\neq 1$
- Deschamps and Brechet [3], example application of theory to Al-Mg-Si
- Perez and Deschamps [5], example application to Fe-C

2 Definitions

α Solid solution phase

β Precipitate phase

C_0 Average atomic solute concentration

$C_e^{\alpha,\beta}$ Equilibrium concentration in α or β

C_∞^{α} Concentration in the α matrix (far from the precipitate)

$\hat{C}^{\alpha,\beta}$ Concentration in α or β at the precipitate/matrix interface (modified by surface tension)

N Number of precipitates per unit volume

R Precipitate radius

γ Surface energy (J/m^2)

V_0 Atomic volume

a Lattice constant

D Solute diffusion coefficient

Z Zeldovitch factor, typically $Z \approx 1/20$

3 Model Parameters

The value of γ is mostly used as a model parameter to fit experimental data. From γ the following central quantities can be obtained:

$$R_0 = \frac{2\gamma V_0}{k_B T} \tag{1}$$

$$\Delta G_0 = \frac{4}{3}\pi R_0^2 \gamma \tag{2}$$

In one case [3] both the values of γ and ΔG_0 were used as fitting parameters. However the authors did not specify exactly how they did it. We assume that R_0 is calculated from γ and ΔG_0 is used in the calculation of free energy, ΔG^*.

4 Nucleation

The "driving force for nucleation" is proportional to

$$S = C_e^\beta \log \frac{C_\infty^\alpha}{C_e^\alpha} + (1 - C_e^\beta) \log \frac{1 - C_\infty^\alpha}{1 - C_e^\alpha} \tag{3}$$

The critical nucleation radius is

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

and the associated free energy barrier

$$\Delta G^* = \Delta G_0 / S^2 \tag{5}$$

The nucleation rate is

$$\frac{dN}{dt} = \frac{1}{V_0} Z \beta^* \exp\left(-\frac{\Delta G^*}{k_B T}\right) \exp\left(-\frac{1}{2Z\beta^* t}\right) \tag{6}$$

where

$$\beta^* = \frac{4\pi R^{*2} D C_0}{a^4} \tag{7}$$

5 Growth

By solving the steady-state diffusion equation $\nabla^2 C(r) = 0$ in the region around the precipitate the following equation is obtained

$$\frac{dR}{dt} = \frac{D}{R} \frac{C_\infty^\alpha - \hat{C}^\alpha}{\hat{C}^\beta - \hat{C}^\alpha} \tag{8}$$

In the *ideal solution* approximation the concentration at the interface is given by

$$\hat{C}^{\alpha,\beta} = C_e^{\alpha,\beta} \cdot \exp\left\{ \frac{R_0}{R} \frac{1 - C_e^{\alpha,\beta}}{C_e^\beta - C_e^\alpha} \right\} \tag{9}$$

When nucleation & growth occur simultaneously the following term has to be added to dR/dt to account for the arrival of new particles of radius R^*

$$\frac{dR}{dt} = -\frac{1}{N} \frac{dN}{dt} \left(\delta \cdot R^* - R\right) \tag{10}$$

The factor $\delta \sim 1.05$ accounts for the fact that the radius of new nuclei is slightly higher than R^*. In numerical solutions the initial value of R should be $R(t = 0) = \delta \cdot R^*$.

6 Coarsening

In the coarsening region the average radius grows as

$$R^3(t) = K \cdot t \tag{11}$$

where K is given in the *ideal solution* approximation by

$$K \approx K_{\mathrm{IS}} = \frac{4DR_0}{9} \frac{C_e^\alpha (1 - C_e^\alpha)}{(C_e^\beta - C_e^\alpha)^2} \tag{12}$$

Thus the time differential of R is given by

$$\frac{dR}{dt} = \frac{4}{27} \frac{DR_0}{R^2} \frac{C_e^\alpha (1 - C_e^\alpha)}{(C_e^\beta - C_e^\alpha)^2} \tag{13}$$

References

[1] Richard Wagner, Reinhard Kampmann, and Peter W. Voorhees. Homogeneous second-phase precipitation. In G Kostorz, editor, *Phase Transformations in Materials*, pages 309–407. Wiley-VCH, Weinheim, FRG, 1 2005. doi: 10.1002/352760264x.ch5. URL `https://doi.org/10.1002/352760264X.ch5`.

[2] Kenneth C. Russell. Nucleation in solids: The induction and steady state effects. *Advances in Colloid and Interface Science*, 13(3-4):205–318, 9 1980. doi: 10.1016/0001-8686(80)80003-0. URL `https://doi.org/10.1016%2F0001-8686%2880%2980003-0`.

[3] A. Deschamps and Y. Brechet. Influence of predeformation and ageing of an al–zn–mg alloy—II. modeling of precipitation kinetics and yield stress. *Acta Materialia*, 47(1):293–305, 12 1998. doi: 10.1016/s1359-6454(98)00296-1. URL `https://doi.org/10.1016%2Fs1359-6454%2898%2900296-1`.

[4] H.A. Calderon, P.W. Voorhees, J.L. Murray, and G. Kostorz. Ostwald ripening in concentrated alloys. *Acta Metallurgica et Materialia*, 42(3):991–1000, 3 1994. doi: 10.1016/0956-7151(94)90293-3. URL `https://doi.org/10.1016%2F0956-7151%2894%2990293-3`.

[5] Michel Perez and Alexis Deschamps. Microscopic modelling of simultaneous two-phase precipitation: application to carbide precipitation in low-carbon steels. *Materials Science and Engineering: A*, 360(1–2):214–219, 1 2003. doi: 10.1016/S0921-5093(03)00431-3. URL `http://www.sciencedirect.com/science/article/pii/S0921509303004313`.