

Full-field Kampmann-Wagner Models

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1 Kampmann-Wagner Model

A number density distribution of precipitates, $\phi(r, t)$, is defined. The total number density of precipitates, N , is given by

$$N(t) = \int_0^\infty \phi(r, t) \, dr, \quad (1)$$

the average radius, R , is given by

$$R(t) = \frac{1}{N(t)} \int_0^\infty r \phi(r, t) \, dr, \quad (2)$$

and the volume fraction, f , is given by

$$f(t) = \int_0^\infty \frac{4}{3} \pi r^3 \phi(r, t) \, dr. \quad (3)$$

The conservation of precipitates is then represented by the following conservation law

$$\frac{\partial \phi}{\partial t} + \frac{\partial [v\phi]}{\partial r} = S \quad (4)$$

where, $v(r, t)$ is the growth rate of the precipitates, and $S(r, t)$ is the source term representing the nucleation of precipitates. Using classical nucleation theory, the source term can be expressed as

$$S = \delta(r - r_c) I \quad (5)$$

where $r_c(t)$ is the critical nucleus size, and $I(t)$ is the nucleation rate. The critical nucleus size is given by

$$r_c(t) = -\frac{2\gamma}{\Delta G_E + \Delta G_V}, \quad (6)$$

and the nucleation rate is given by

$$I(t) = N_s Z \beta \exp \left[-\frac{4\pi\gamma r_c^2}{3k_B T} \right] \exp \left[-\frac{\tau}{t} \right]. \quad (7)$$

The elastic misfit energy, ΔG_E , is assumed to be constant. The chemical energy change, ΔG_V , is given by

$$\Delta G_V = \frac{RT}{V} c_P \ln \frac{c_M}{c_{eq}} \quad (8)$$

where, the precipitate solute concentration, c_P , is assumed to be constant, $c_M(t)$ is the matrix solute concentration satisfying

$$c_M(t=0) = f c_P + (1-f) c_M(t), \quad (9)$$

and c_{eq} is the equilibrium matrix composition. In Eq. (7), the Zeldovich factor, Z , is given by

$$Z = \frac{V}{2\pi r_c^2} \sqrt{\frac{\gamma}{k_B T}}, \quad (10)$$

β is given by

$$\beta = 4\pi D_M c_M \frac{r_c^2}{a^4}, \quad (11)$$

in terms of the solute diffusion coefficient, D_M , and the incubation time, τ , is given by

$$\tau = \frac{1}{2Z^2\beta}. \quad (12)$$

Finally, the growth rate, $v(r, t)$ in Eq. (4) is given by

$$v(r, t) = \frac{D}{r} \frac{c_M - c_I}{c_P - c_I}, \quad c_I = c_{eq} \exp \frac{2\pi\gamma}{RT r}. \quad (13)$$

2 Crystal Plasticity

A crystal plasticity constitutive model is a representation of the plastic strain rate (velocity gradient)

$$\mathbf{L}_p = \sum_{\alpha=1}^N \dot{\gamma}^\alpha n^\alpha \otimes s^\alpha \quad (14)$$

in terms of the slip rates, $\dot{\gamma}^\alpha$, on slip system α defined by slip plane normal, n^α , and slip direction s^α . The slip rates are given by a power law,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left(\frac{\tau^\alpha}{\tau_r^\alpha + \tau_p^\alpha} \right)^{1/m} \quad (15)$$

where τ^α is the resolved shear stress on the slip system, and the strain-hardening contribution to slip resistance, τ_r^α , is given by

$$\dot{\tau}_r^\alpha = h_0 \sum_{\beta=1}^N h_{\alpha\beta} \dot{\gamma}^\beta \left[1 - \frac{\tau_r^\beta}{\tau_\infty^\beta} \right], \quad (16)$$

and the precipitate-hardening contribution to slip resistance, τ_p^α , is given by

$$\tau_p^\alpha = \frac{1}{bL^\alpha} \int_0^\infty \phi(r, t) F(r, t) dr, \quad (17)$$

which accounts for precipitate shearing, with $F(r, t) = kGbr$ for $r < b/k$, and Orowan looping, with $F(r, t) = Gb^2$ for $r > b/k$. L^α is the average particle spacing on the dislocation line, and is obtained from Friedel's statistics as

$$L^\alpha = \left[\frac{4\pi R^2 G b^2}{3fb\tau_p^\alpha} \right]^{\frac{1}{3}}, \quad (18)$$

where R and f are given by Eq. (2) and Eq. (3) respectively.

Furthermore, vacancy generation due to plastic deformation is considered. The rate of generation and annihilation of vacancies is given by

$$\dot{c}_V = \chi \frac{\Omega}{E_V} \sum_{\alpha=1}^N \dot{\gamma}^\alpha \tau^\alpha - \frac{D_V}{L^2} c_V, \quad (19)$$

where, χ is the fraction of plastic work converted into vacancies, Ω is the atomic volume, E_V is the vacancy formation energy, and $D_V = D_{V0} \exp\left[-\frac{M_V}{k_B T}\right]$, is the vacancy diffusion coefficient in terms of the vacancy migration energy, M_V . L is the average spacing between vacancy sinks, and is given by the minimum of dislocation spacing and interstitial (c_{int} assumed to be constant) spacing

$$L = \min \left[\frac{Gb}{\tau_r^\alpha - \tau_{r0}^\alpha}, \frac{1}{\sqrt[3]{c_{int}}} \right]. \quad (20)$$

Currently, the solute diffusion coefficient in Eq. (11) and Eq. (13) is related to the vacancy concentration through

$$D_M = c_V D_{M0} \exp \left[-\frac{M}{k_B T} \right] \quad (21)$$

In the future, the influence of dislocation density on the nucleation site density, N_s in Eq. (7), through the elastic misfit energy, ΔG_E , and the solute diffusion coefficient, D , through pipe diffusion, might be worth looking into.

3 Mass Transport

The solute and vacancy balance in Eq. (10) and Eq. (19) respectively local. In addition long-range transport can be incorporated by including diffusional fluxes

$$\dot{c}_V = \nabla D_V \nabla c_V + \chi \frac{\Omega}{E_V} \sum_{\alpha=1}^N \dot{\gamma}^\alpha \tau^\alpha - \frac{D_V}{L^2} c_V \quad (22)$$

$$\dot{c}_M = \nabla D_M \nabla c_M + \frac{\dot{f}}{1-f} (c_M - c_P) \quad (23)$$