Full-field model for dynamic precipitation

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This is the documentation for the crystal plasticity constitutive law for DAMASK including dynamic precipitation available in:
`https://github.com/LightForm-group/Damask-KWN`.

The installation instructions for this version of DAMASK are provided elsewhere:
`https://lightform-group.github.io/wiki/software_and_simulation/kwn-damask`.

The purpose of the document is to describe the KWN-crystal plasticity coupled model used in the constitutive law `kwnpowerlaw`. The program inputs corresponding to the variables mentioned in this document are shown in Section 5.

1 Kampmann-Wagner Model

The KWN model used in this full field model is the one described in [1]. A ternary system is considered, with main element C and solute atoms A and B. The precipitate composition - considered as constant - is given by $A_xB_yC_z$.

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

$$N(t) = \int_0^\infty \phi(r,t)\,\mathrm{d}\,r, \tag{1}$$

the average radius, R, is given by

$$R(t) = \frac{1}{N(t)} \int_0^\infty r\phi(r,t)\,\mathrm{d}\,r, \tag{2}$$

and the volume fraction, f_v, is given by

$$f_v(t) = \int_0^\infty \frac{4}{3}\pi r^3 \phi(r,t)\,\mathrm{d}\,r. \tag{3}$$

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

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

where, $v(r, t)$ is the growth rate of the precipitates, and $S(r, t)$ is the source term representing the nucleation of precipitates.

1.1 Initial distribution

A pre-existing precipitate distribution is considered. The initial distribution $N(0)$ is assumed to follow a log-normal law, and is defined by its initial precipitate volume fraction $f_v(0)$, initial mean radius $R(0)$ and standard deviation σ^1 as [1]:

$$N(0) = f_v(0) \frac{\int_0^\infty f(r)dr}{\int_0^\infty f(r)\frac{4}{3}\pi r^3 dr} \tag{5}$$

where f is a function defined as:

$$f(r) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{R(0)^2}{2\sigma^2}\left(\ln(\frac{r}{R(0)}) + \frac{\sigma^2}{2R(0)^2}\right)^2\right] \tag{6}$$

1.2 Precipitate growth

The growth rate, $v(r, t)$ in Eq. (4) is assumed to be controlled by the slowest diffuser. Assuming the slowest diffuser is A, $v(r, t)$ is given by:

$$v(r, t) = \frac{D}{r} \cdot \frac{\overline{x}_A - x_A^r}{x_A^{pr} - x_A^r} \tag{7}$$

where D is the diffusion coefficient, calculated as detailed later, $\overline{x}_A$ is the average atomic fraction of A in the matrix, x_A^{pr} is the concentration in A in the precipitate ($x_A^{pr} = \frac{x}{x+y+z}$), and x_A^r is the concentration in A at the interface between the matrix and a precipitate of radius r, calculated as the solution of the following system of equations [1, 2]:

$$\begin{cases} x \cdot (x_B^0 - x_B^r) = y \cdot (x_A^0 - x_A^r) \\ \exp\left[(\frac{2\gamma v_m^{pr}}{rRT} + \frac{\Delta G_E \cdot v_m^{pr}}{RT}) \cdot (x + y + z)\right] \cdot (x_A^\infty)^x \cdot (x_B^\infty)^y = (x_A^r)^x \cdot (x_B^r)^y \end{cases} \tag{8}$$

where ΔG_E is the elastic strain energy, x_A^0 and x_B^0 are the bulk concentrations of the alloy in species A and B, respectively; x_A^∞ and x_B^∞ are the equilibrium concentrations in A and B, respectively; x_B^r - which is the second variable of the system in Eq. (8) - is the concentration at the interface between the matrix and a precipitate of radius r, and v_m^{pr} is the molar volume of the precipitate.

1.3 Source term

Using classical nucleation theory, the source term in Eq. (4) can be expressed as

$$S = \delta(r - r_c) I \tag{9}$$

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[1]the log-normal distribution is sometimes defined by a dimensionless dispersion parameter s defined as $s = \sigma/R(0)$

where $r_c(t)$ is the critical nucleus size, and $I(t)$ is the nucleation rate. The critical nucleus size $r_c(t)$ is calculated as the radius such that:

$$v(r_c, t) = 0 \tag{10}$$

The nucleation rate is given by

$$I(t) = N_s Z \beta \exp\left[-\frac{4\pi\gamma r_c^2}{3k_\mathrm{B}T}\right] \tag{11}$$

where N_s is the number density of nucleation sites, calculated as

$$N_s = \frac{\overline{x}_\mathrm{A} + \overline{x}_\mathrm{B}}{V} \tag{12}$$

where V is the atomic volume of the matrix. In Eq. (11), the Zeldovich factor, Z, is given by

$$Z = \frac{V}{2\pi r_c^2}\sqrt{\frac{\gamma}{k_\mathrm{B}T}}, \tag{13}$$

β is given by

$$\beta = 4\pi D(\overline{x}_\mathrm{A} + \overline{x}_\mathrm{B})\frac{r_c^2}{a^4}, \tag{14}$$

where a is the lattice parameter of the product phase.

1.4 Solute conservation

The precipitate solute concentration in element i (where i=A or B), x_i^pr , is assumed to be constant, and the matrix solute concentration satisfies:

$$x_i^0 = f_v(t)x_i^\mathrm{pr} + (1 - f_v(t))\,\overline{x}_\mathrm{i}(t), \tag{15}$$

2 Crystal plasticity model

A crystal plasticity constitutive model is used and the plastic strain rate is given by [3]:

$$\mathbf{L}_\mathrm{p} = \sum_{\alpha=1}^{12} \dot{\gamma}^\alpha n^\alpha \otimes s^\alpha \tag{16}$$

where the indices α refer to the 12 FCC slip systems, defined by the slip plane normal n^α and the slip direction s^α, and $\dot{\gamma}^\alpha$ is the slip rate. The slip rates are given by an empirical power law [4]:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{\tau_*^\alpha}\right)^n \tag{17}$$

where $\dot{\gamma}_0$ and n are constants, τ^α is the resolved shear stress on the slip system, and the slip resistance, τ_*^α, is given by [5]:

$$\tau_*^\alpha = \tau_s + \sqrt{(\tau_p)^2 + (\tau_d^\alpha)^2} \tag{18}$$

where τ_s, τ_p and τ_d^α are the contributions of the atoms in solid solution, of the reinforcing precipitates, and of the dislocations, respectively. τ_s is given by:

$$\tau_s = k_s \cdot (\overline{x}_A + \overline{x}_B)^{2/3} \tag{19}$$

where k_s is an empirical constant [5]. The precipitation hardening contribution τ_p, is given by [5]:

$$\tau_p = \mu\sqrt{\frac{3f_v}{2\pi}} \cdot \frac{k_p}{R \cdot \sqrt{r_t}} \left(\int_0^{r_t} r \cdot \phi(r,t)\,\mathrm{d}r + \int_{r_t}^\infty r_t \cdot \phi(r,t)\,\mathrm{d}r \right)^{3/2} \tag{20}$$

where μ is the shear modulus, k_p is an empirical constant, and r_t is the transition radius between shearing and Orowan looping [6]. In Eq. (18), τ_d^α is the resistance to slip due to forest dislocations, and the hardening rate is given by [4]:

$$\dot{\tau}_d^\alpha = h_0 \sum_{\beta=1}^N q_{\alpha\beta} \, \dot{\gamma}^\beta \left[1 - \frac{\tau_d^\beta}{\tau_\infty} \right]^m , \tag{21}$$

where h_0, τ_∞ and m are hardening parameters, and $q_{\alpha\beta}$ is the latent hardening between the slip systems α and β. The initial value of τ_d^α (considered as identical for all slip systems and labelled $\tau_d(0)$) is a model input.

3 Excess vacancy model

Plastic deformation produces vacancies which enhance diffusivity and accelerate precipitation kinetics. A phenomenological model [1, 7, 8] is used to calculate the excess vacancy concentration as a function of temperature and deformation conditions. The rate of generation and annihilation of vacancies is given by

$$\dot{c}_V = \chi \frac{V}{E_V} \sum_{\alpha=1}^N \dot{\gamma}^\alpha \tau^\alpha + 0.5 \cdot \frac{c_j V}{4b^3} \sum_{\alpha=1}^N \dot{\gamma}^\alpha - \frac{D_V}{L^2} c_V, \tag{22}$$

where χ is the fraction of plastic work converted into vacancies; E_V, is the vacancy formation energy; $D_V = D_{V0} \exp\left[-\frac{M_V}{k_B T} \right]$ is the vacancy diffusion coefficient in terms of the vacancy migration energy, M_V; b the burgers vector of screw dislocations; and c_j is the dislocation jog concentration, calculated as $c_j = \exp\left[\frac{-E_j}{k_B T} \right]$, where E_j is the jog formation energy. L is the average spacing between vacancy sinks, and is given by the minimum of dislocation spacing and grain size d_g

$$L = \min\left[\frac{0.27\mu b}{\max(\tau_d^\alpha) \cdot \kappa^2}, d_g \right]. \tag{23}$$

where κ is a constant between 1 and 10 related to the dislocation arrangement ([1, 7]). The solute diffusion coefficient D in Eq. (14) and Eq. (7) is related to the vacancy concentration through

$$D = D_{th}(1 + \frac{c_v - c_{eq}}{c_{eq}}) \tag{24}$$

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where c_{eq} is the equilibrium vacancy concentration, calculated as $c_{\text{eq}} = 23 \exp[-\frac{E_f}{k_{\text{B}}T}]$ [1], and D_{th} is the solute diffusion coefficient in the absence of any deformation, calculated as $D_{\text{th}} = D_0 \exp(-E_s/k_{\text{B}}T)$, where E_s is the solute migration energy. It is assumed that $c_v(0) = c_{\text{eq}}$.

4 To improve the model

In the future, the influence of dislocation density on the nucleation site density, N_s in Eq. (11), through the elastic misfit energy, ΔG_E, and the solute diffusion coefficient, D, through pipe diffusion, might be worth looking into.

4.1 Mass Transport

The solute and vacancy balance in Eq. (15) and Eq. (22) respectively local. In addition long-range transport can be incorporated by including diffusional fluxes

$$\dot{c}_{\text{V}} = \nabla D_{\text{V}} \nabla c_{\text{V}} + \chi \frac{\Omega}{E_{\text{V}}} \sum_{\alpha=1}^{N} \dot{\gamma}^{\alpha} \tau^{\alpha} - \frac{D_{\text{V}}}{L^2} c_{\text{V}} \tag{25}$$

$$\dot{c}_{\text{M}} = \nabla D_{\text{M}} \nabla c_{\text{M}} + \frac{\dot{f}}{1-f} \left(c_{\text{M}} - c_{\text{P}} \right) \tag{26}$$

4.2 Decreasing calculation time

Currently, the equilibrium composition at the interface between matrix and precipitate is calculated at each time step for all bins of the distribution. As the equilibrium concentration at the interface does not depend on time, the code could be modified to calculate the equilibrium composition only at the beginning.

4.3 Improve readability

Readability might be improved by converting all units in the `phase_mechanical_plastic_kwnpowerlaw.f9` source file to international unit system (for now, several variables are normed).

5 Model inputs

Symbol	Variable	Unit
m	a_sl	-
V	atomic_volume	m^3
b	burgers_vector	m
$[x_{\mathrm{A}}^0, x_{\mathrm{B}}^0]$	c0_matrix	at
$[x_{\mathrm{A}}^\infty, x_{\mathrm{B}}^\infty]$	ceq_matrix	at
$[x_{\mathrm{A}}^{pr}, x_{\mathrm{B}}^{pr}]$	ceq_precipitate	at
κ	dislocation_arrangement	-
$\dot{\gamma}_0$	dot_gamma_0_sl	m^{-1}
γ	gamma_coherent	Jm^{-2}
h_0	h_0_sl_sl	Pa
$q_{\alpha\beta}$	h_sl_sl	-
$R(0)$	initial_mean_radius	m
$f_v(0)$	initial_volume_fraction	-
E_j	jog_formation_energy	eV
a	lattice_parameter	m
ΔG_E	misfit_energy	Jm^{-3}
v_{m}^{pr}	molar_volume	m^{3}mol^{-1}
n	n_sl	-
k_p	precipitate_strength_constant	-
μ	shear_modulus	Pa
D_0	solute_diffusion0	m^{2}s^{-1}
E_s	solute_migration_energy	eV
k_s	solute_strength	-
σ	standard_deviation	m
[x,y,z]	stoechiometry	-
r_t	transition_radius	m
$\tau_d(0)$	xi_0_sl	Pa
τ_∞	xi_inf_sl	Pa
$D_{\mathrm{V}0}$	vacancy_diffusion0	m^{2}s^{-1}
E_{V}	vacancy_energy	eV
χ	vacancy_generation	-
M_{V}	vacancy_migration_energy	eV
d_g	vacancy_sink_spacing	m

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