Dislocation glide and deformation twinning as implemented in DisloTwin.f90

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PART I

Microstructure Parametrization

Dislocation structure

Internal variables:

- N^α edge dislocation densities $\varrho^\alpha_{\text{edge}}$
- N^α dipole densities $\varrho^\alpha_{\text{dipole}}$

Derived measures:

- τ^α_{c} threshold shear stress fordislocation glide
- λ^α mean distance between 2 obstacles seen by a dislocation

Morphology and topology of mechanical twins

Internal variables:

- N^β twin volume fractions f^β
- (N^β twin mean thicknesses s^β)

Derived measures:

- f total twin volume fraction
- $l^\beta = \frac{s^\beta (1-f)}{f^\beta}$ mean distance between neighboring twins β
- τ_c^β threshold shear stress for twinning
- λ^β mean distance between 2 obstacles seen by a growing twin

Threshold stress for glide activity

Threshold stress $\tau_{\mathrm{c}}^{\alpha}$:

$$\tau_{\mathrm{c}}^{\alpha} = k_{\mathrm{friction}}\, G_{\mathrm{iso}} \sqrt{c} + G_{\mathrm{iso}}\, b^{\alpha} \sqrt{\sum_{\tilde{\alpha}=1}^{N^{\alpha}} \xi^{\alpha\tilde{\alpha}} \left(\varrho_{\mathrm{edge}}^{\tilde{\alpha}} + \varrho_{\mathrm{dipole}}^{\tilde{\alpha}}\right)}$$

with:

- G_{iso} isotropic shear modulus
- c carbon concentration (at.%)
- k_{friction} adjusting parameter for solute atome friction stress
- b^{α} Burgers vector of slip system α
- $\xi^{\alpha\tilde{\alpha}}$ interaction strength (Kubin et al. 2008)

Threshold stress for twinning:

Threshold stress $\tau_{\mathrm{c}}^{\beta}$:

$$\tau_{\mathrm{c}}^{\beta} = \frac{\gamma_{\mathrm{sfe}}}{3\, b^{\beta}} + \frac{G_{\mathrm{iso}}\, b^{\beta}}{L_0}$$

with:

- γ_{sfe} temperature-dependant stacking fault energy
- b^{β} Burgers vector of twin system β
- L_0 twin source length

Dislocation mean free distance between two obstacles

Harmonic averaging:

$$\begin{aligned}\frac{1}{\lambda^\alpha} &= \frac{1}{d_\text{grain}} + \frac{\sqrt{\varrho^\alpha_\text{edge} + \varrho^\alpha_\text{dipole}}}{k_\lambda} + \frac{1}{d^{\alpha\beta}} \\ &= \frac{1}{d_\text{grain}} + \frac{\sqrt{\varrho^\alpha_\text{edge} + \varrho^\alpha_\text{dipole}}}{k_\lambda} + \sum_{\beta=1}^{N^\alpha} I^{\alpha\beta}\,\frac{1}{I^\beta}\end{aligned}$$

with:

- d_grain grain size
- $I^{\alpha\beta}$ slip–twin interactions (0 if α,β coplanars or cross-slip; 1 otherwise)

Twin mean free distance between two obstacles

Harmonic averaging:

$$\begin{aligned}\frac{1}{\lambda^{\beta}} &= \frac{1}{d_{\text{grain}}} + \frac{1}{d^{\beta}} \\ &= \frac{1}{d_{\mathrm{grain}}} + \sum_{\tilde{\beta}=1}^{N^{\beta}} I^{\beta\tilde{\beta}} \frac{1}{l^{\tilde{\beta}}}\end{aligned}$$

with:

- $I^{\beta\tilde{\beta}}$ twin–twin interactions (0 if β,$\tilde{\beta}$ coplanars; 1 otherwise)

PART II

Kinetics

Orowan's kinetics

Shear rate $\dot{\gamma}^\alpha$:

$$\dot{\gamma}^\alpha = \varrho^\alpha_\text{edge}\, b^\alpha\, v^\alpha_\text{glide}$$

Velocity v^α_glide:

$$v^\alpha_\text{glide} = v_0 \exp\left[-\frac{Q}{k_\text{B}\, T}\left(1 - \left(\frac{|\tau^\alpha|}{\tau^\alpha_\text{c}}\right)^p\right)^q\right] \operatorname{sign}(\tau^\alpha)$$

with:

- v_0 velocity pre-factor
- Q activation energy for dislocation glide
- $k_\text{B}\, T$ Boltzmann energy

Twin nucleation law

Shear rate $\dot{\gamma}^\beta$:

$$\dot{\gamma}^\beta = \gamma_\mathrm{c}^\beta \, \dot{f}^\beta = \gamma_\mathrm{c}^\beta \, (1 - f) \, V^\beta \, \dot{N}^\beta$$

Nucleation rate $\dot{N}^\beta$:

$$\dot{N}^\beta = \dot{N}_0 \, \exp\left[- \left(\frac{\tau_\mathrm{c}^\beta}{\tau^\beta} \right)^r \right]$$

with:

- γ_c^β characteristical twin shear
- V^β volume of grown-up twins
- $\dot{N}_0$ constant twin nucleation rate per time and volume

Spontaneous twin growth

Volume of grown-up twins V^β:

$$V^\beta = \frac{\pi}{6}\, s^\beta\, {\lambda^\beta}^2$$

PART III

Evolution laws for microstructure

Dislocation multiplication

Multiplication:

$$\dot{\varrho}^{\alpha}_{\text{multiplication}} = \frac{|\dot{\gamma}^{\alpha}|}{b^{\alpha}\,\lambda^{\alpha}}$$

Dipole formation

Dipole formation:

$$\dot{\varrho}^{\alpha}_{\text{formation}} = 2\,\frac{2\,\max(\hat{d}^{\alpha},\check{d}^{\alpha})}{b^{\alpha}}\,\frac{\varrho^{\alpha}_{\text{edge}}}{2}\,|\dot{\gamma}^{\alpha}|$$

Upper stability limit for dipoles $\hat{d}^{\alpha}$:

$$\hat{d}^{\alpha} = \frac{1}{8\,\pi}\,\frac{G_{\text{iso}}\,b^{\alpha}}{1-\nu}\,\frac{1}{|\tau^{\alpha}|}$$

Spontaneous annihilation of 2 single dislocations

Single–single annihilation:

$$\dot{\varrho}^{\alpha}_{\text{single–single}} = 2\,\frac{2\,\check{d}^{\alpha}}{b^{\alpha}}\,\frac{\varrho^{\alpha}_{\text{edge}}}{2}\,|\dot{\gamma}^{\alpha}|$$

Lower stability limit of dipoles $\check{d}^{\alpha}$:

$$\check{d}^{\alpha} \propto b^{\alpha}$$

Spontaneous annihilation of one single dislocation with a dipole constituent

Single–dipole constituent annihilation:

$$\dot{\varrho}^{\alpha}_{\text{single–dipole}} = 2\,\frac{2\,\check{d}^{\alpha}}{b^{\alpha}}\,\frac{\varrho^{\alpha}_{\text{dipole}}}{2}\,|\dot{\gamma}^{\alpha}|$$

Dipole climb

Dipole climb:

$$\dot{\varrho}^{\alpha}_{\text{climb}} = \varrho^{\alpha}_{\text{dipole}} \frac{2\, v_{\text{climb}}}{(\hat{d}^{\alpha} - \check{d}^{\alpha})/2}$$

Climb velocity $v^{\alpha}_{\text{climb}}$:

$$v^{\alpha}_{\text{climb}} = \frac{D\, \Omega^{\alpha}}{b^{\alpha}\, k_{\text{B}}\, T} \frac{G_{\text{iso}}\, b^{\alpha}}{2\, \pi\, (1 - \nu)} \frac{1}{(\hat{d}^{\alpha} + \check{d}^{\alpha})/2}$$

Evolution of dislocation densities

Edge dislocation density rate:

$$\dot{\varrho}^{\alpha}_{\text{edge}} = \dot{\varrho}^{\alpha}_{\text{multiplication}} - \dot{\varrho}^{\alpha}_{\text{formation}} - \dot{\varrho}^{\alpha}_{\text{single–single}}$$

Dislocation dipole density rate:

$$\dot{\varrho}^{\alpha}_{\text{dipole}} = \dot{\varrho}^{\alpha}_{\text{formation}} - \dot{\varrho}^{\alpha}_{\text{single–dipole}} - \dot{\varrho}^{\alpha}_{\text{climb}}$$