Electronic Supplementary Material (ESI) for Nanoscale

Supporting Information

Phase transformations in nanograin materials under high pressure and plastic shear: nanoscale mechanisms

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1. The total system of equations for interaction between phase transformation and dislocation evolution[1]

We designate contractions of tensors $\boldsymbol{A}$ and $\boldsymbol{B}$ over one and two indices as $\boldsymbol{A}\cdot\boldsymbol{B}$ and $\boldsymbol{A}:\boldsymbol{B}$; the transpose of $\boldsymbol{A}$ is $\boldsymbol{A}^T$, $\boldsymbol{I}$ is the unit tensor, and $\otimes$ is a dyadic product.

Below we described coupled system of PFA equations for martensitic PT and dislocation evolution developed in[1]. This theory combines the most advanced PFA for dislocations[2] and PT[3] with additional coupling terms[1]. Both PFAs[2,3] are the only available large strain formulations; current letter is based on fully geometrically nonlinear formulation as well. Current work keeps also other advantages of[2,3]: advanced thermodynamic potential that describes some conceptual features of the effect of the stress tensor, reproducing, in particular, stress-independent transformation strain tensor and Burgers vector and desired local stress-strain curves. Also, the desired, mesh-independent, dislocation height is introduced for any slip orientation, leading to well-posed formulation. Coupling between PT and dislocations includes nonlinear kinematics and corresponding mechanical driving forces, inheritance of dislocation during PT, and dependence of all material parameters for dislocations on the order parameter η that describes PT, which results also in the extra driving force for PT due to change in dislocation energy during the PT.

Let the motion of elastoplastic material with PT be described by equation $\boldsymbol{r} = \boldsymbol{r}(\boldsymbol{r}_0, t)$, where $\boldsymbol{r}$ and $\boldsymbol{r}_0$ are the positions of a material point at time t (deformed configuration V) and t_0 (undeformed configuration V_0, which is in A state). All equations are considered in V_0. Multiplicative decomposition of the deformation gradient into elastic, transformational, and plastic parts is used: $\boldsymbol{F} = \partial\boldsymbol{r}/\partial\boldsymbol{r}_0 = \boldsymbol{F}_e\cdot\boldsymbol{F}_t\cdot\boldsymbol{F}_p$. Transformation $\boldsymbol{F}_t$ and plastic $\boldsymbol{F}_p$ deformation gradients are described by equations[2,3]:

$$\mathbf{F}_t = \mathbf{I} + \boldsymbol{\varepsilon}_t(a\eta^2(1-\eta)^2 + (4\eta^3 - 3\eta^4)), \tag{1}$$

$$\dot{\boldsymbol{F}}_p \cdot \boldsymbol{F}_p^{-1} = \sum_{\alpha=1}^{p}\sum_{\omega=1}^{m_\alpha} \frac{1}{H^\alpha}\boldsymbol{b}^{\alpha\omega} \otimes \boldsymbol{n}^\alpha \dot{\phi}(\bar{\xi}_{\alpha\omega}), \tag{2}$$

The order parameter η for PT varies from 0 (in A) to 1 (in M); the order parameter for dislocations in the α^{th} plane with the unit normal $\boldsymbol{n}^{\alpha}$ along the ω^{th} slip direction with the Burgers vector $\boldsymbol{b}^{\alpha\omega}$, $\xi_{\alpha\omega}$, varies from 0 to n when n dislocations appear; $Int(\xi_{\alpha\omega}) = n$ and $\bar{\xi}_{\alpha\omega} := \xi_{\alpha\omega} - Int\,(\xi_{\alpha\omega}) \in [0,1]$ are the integer and fractional parts of $\xi_{\alpha\omega}$. In Eqs.(1) and (2), $\boldsymbol{\varepsilon}_t = \boldsymbol{F}_t(1) - \boldsymbol{I}$ is the transformation strain, a is the parameter, $\phi(\bar{\xi}) = \bar{\xi}^2(3-2\bar{\xi})$, and H^{α} is the dislocation height. For compactness, we consider single M variant only; generalization for multiple M variants can be done as in[3]. The Helmholtz free energy per unit undeformed volume is accepted as the sum of elastic, thermal, crystalline, and gradient energies related to PT and dislocations:

$$\psi = \psi^e + f + \psi_\eta^\nabla + \psi_\xi + \psi_\xi^\nabla; \quad \psi_\eta^\nabla = 0.5\beta_\eta |\boldsymbol{\nabla}\eta|^2; \tag{3}$$

$$\psi_\xi = \sum_{\alpha=1}^{p}\sum_{\omega=1}^{m_\alpha} A_\alpha(\eta)\bar{\xi}^2_{\alpha\omega}(1-\bar{\xi}_{\alpha\omega})^2;$$

$$\psi_\xi^\nabla = \frac{\beta_\xi(\eta)}{2}\sum_{\alpha=1}^{p}\sum_{\omega=1}^{m_\alpha}\left\{\boldsymbol{\nabla}\bar{\xi}^2_{\alpha\omega} + [M(1-\bar{\xi}_{\alpha\omega})^2 - 1](\boldsymbol{\nabla}\bar{\xi}_{\alpha\omega}\cdot\boldsymbol{n}_\alpha)^2\right\};$$

$$f = A_c\eta^2 + (\Delta G - 2A_c)\eta^3 + (A_c - 3\Delta G)\eta^4. \tag{4}$$

Here $A_c = A_0(\theta - \theta_c)$ and $\Delta G = \Delta_z(\theta - \theta_e)$; θ, θ_e, and θ_c are the temperature, the phase equilibrium temperature for A-M, and the critical temperature for the loss of A stability; β_ξ and β_η are the gradient energy coefficients, and A_0 and M are parameters. The coefficient A_α, which determines the yield strength for dislocations, is a periodic step-wise function of the coordinate along the normal to the slip plane $\boldsymbol{n}_\alpha$[2]. The thermodynamic procedure similar to that in[2–4] results in the elasticity rule for the nonsymmetric Piola-Kirchhoff stress tensor (force per unit area in V_0) $\boldsymbol{P}\cdot\boldsymbol{F}_p^T\cdot\boldsymbol{F}_t^T = \frac{\partial\psi}{\partial\boldsymbol{F}_e}$ and expressions for the dissipation rate to due PTs $D_\eta = X_\eta\dot{\eta} \geq 0$ and dislocations $D_\xi = X_{\alpha\omega}\dot{\xi}_{\alpha\omega} \geq 0$. Then the simplest linear relationships between thermodynamic forces and rates leads to the Ginzburg-Landau equations

$$\frac{1}{L_\eta}\frac{\partial\eta}{\partial t} = X_\eta = \boldsymbol{P}^T\cdot\boldsymbol{F}_e : \frac{\partial\boldsymbol{F}_t}{\partial\eta}\cdot\boldsymbol{F}_p + \boldsymbol{\nabla}\cdot\left(\frac{\partial\psi}{\partial\boldsymbol{\nabla}\eta_i}\right) - \frac{\partial\psi}{\partial\eta}, \tag{5}$$

$$\frac{1}{L_\xi(\eta)}\frac{\partial\xi_{\alpha\omega}}{\partial t} = X_{\alpha\omega} = \boldsymbol{P}^T\cdot\boldsymbol{F}_e : \boldsymbol{F}_t\cdot\frac{\partial\boldsymbol{F}_p}{\partial\xi_{\alpha\omega}} + \boldsymbol{\nabla}\cdot\left(\frac{\partial\psi}{\partial\boldsymbol{\nabla}\xi_{\alpha\omega}}\right) - \frac{\partial\psi}{\partial\xi_{\alpha\omega}}, \tag{6}$$

where L_ξ and L_η are the kinetic coefficients. All parameters in equations for dislocations depend on η according to the rule $B = B_A + (B_M - B_A)\phi(\eta)$, where B_A and B_M are the value of a parameter in A and M. This in turn leads to contributions of the dislocation-related terms in Ginzburg-Landau Eq.(5) for PT. In addition, both processes are coupled through the mechanical driving force (stress power) in Eqs.(5),(6) and evolving stress field.

It is assumed for simplicity that dislocations are inherited when diffuse A-M interface passes through them, their Burgers vector and normal to slip plane transform to $\boldsymbol{b}_M^{\alpha\omega} = \boldsymbol{F}_t \cdot \boldsymbol{b}_A^{\alpha\omega}$ and $\boldsymbol{n}_M^{\alpha\omega} = \boldsymbol{n}_A^{\alpha\omega} \cdot \boldsymbol{F}_t^{-1}/|\boldsymbol{n}_M^{\alpha\omega} \cdot \boldsymbol{F}_t^{-1}|$. That means that in the undeformed state V_0 slip systems of A and M coincides. Equilibrium equation $\boldsymbol{\nabla} \cdot \boldsymbol{P} = 0$ completes our system. Cubic-tetragonal PT was considered. Isotropic quadratic elastic potential ψ^e in terms of Lagrangian elastic strain $\boldsymbol{E}_e = (\boldsymbol{F}_e^T \cdot \boldsymbol{F}_e - \boldsymbol{I})/2$ with shear modulus $\mu = 71.5 GPa$ and bulk modulus $K = 112.6 GPa$ (the same for both phases) was used for simplicity below. The following parameters for PT and all slip systems have been used in all problems: $L_\xi = 2600 (Pa \cdot s)^{-1}$, $M = 0.05$, $H = 0.7nm$, $|\boldsymbol{b}| = 0.35nm$, $\gamma = 0.5$, $\beta_\xi = 7.5 \cdot 10^{-11} N$, $A_\alpha = 0.75 GPa$ for A, $A_\alpha = 2.25 GPa$ for M, $\beta_\eta = 2.59 \cdot 10^{-10} N$, $L_\eta = 2600 (Pa \cdot s)^{-1}$, $A_0 = 20.6 MPa/K$, $\Delta_z = 5.05 MPa/K$, $\theta = 298K$, $\theta_e = 100K$, $\theta_c = -90K$, $\bar{\theta}_c = 504K$, $\epsilon_t^x = \epsilon_t^y = -0.05$, $\epsilon_t^{xy} = 0.1$ (i.e., $\varepsilon_{0t} = -0.1$ and $\gamma_t = 0.2$). For such material parameters, the phase equilibrium pressure $p_e = 10$, the critical pressure for instability of the low pressure phase (LPF) is $p_{cl} = 20$, and the critical pressure for instability of the high pressure phase (HPF) is $p_{ch} = -10$. Negative p_{ch} was chosen because otherwise reverse PT would occur at pressure release to zero through homogeneous nucleation, even if interfaces were arrested.

2. Pressure-induced PT at a single dislocation

First, we created one dislocation in the left grain by applying shear displacement, and we arrested it at the grain boundary by stopping to solve the Ginzburg-Landau equation for dislocations. Then the applied shear stress was reduced to zero, and we obtained a sample with a single dislocation per two nanograins, which mimics initially annealed material. After this, all mechanical boundary conditions were substituted with homogeneous stresses (pressure) normal to the deformed surface. It was found that the lowest pressure at which the nucleus appears is $p_h = 15.75$ (which is in the middle between p_e and p_{cl}), after which it grows and fills essential part of the grain (Fig. S1). This is reasonable, because 15.75 is significantly higher than p_e, which determines the local interface propagation pressure. Thus, even one dislocation significantly reduces the pressure required to nucleate HPP, but it is still much higher than p_e; $k = -p_h \varepsilon_{t0} = 1.575$. PT is not completed because pressure in the transformed region and at the interface reduces below p_e due to the transformation volume decrease.

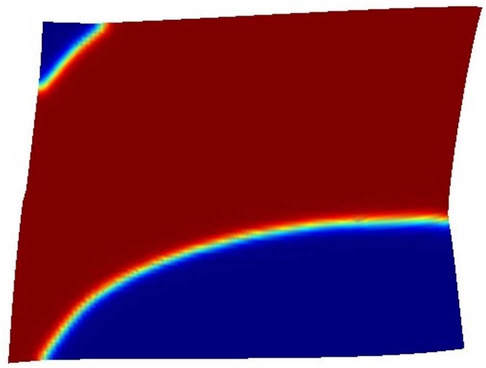

Figure 1: Stationary distribution of high pressure phase in the presence of a single dislocation and under the hydrostatic pressure $\bar{p} = 15.75$.

References

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