MESOSCOPIC MODEL OF PHASE TRANSFORMATIONS AT FINITE STRAIN RATES WITH CONTINUUM PLASTICITY AND NONCLASSICAL HEAT TRANSFER

Roman Gröger*, **Turab Lookman****

***Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, 61662 Brno, Czech Republic; **Theoretical Division, Los Alamos National Laboratory, MS B262, Los Alamos, NM 87545, USA**

*groger@ipm.cz, **txl@lanl.gov

ABSTRACT We develop a mean-field model that can be used to study the evolution of microstructure in dynamically loaded crystalline materials. The Landau-Ginzburg functional and Rayleigh dissipation function are used to describe the thermoelastic and viscoelastic response of the body. A nonclassical heat conduction equation is derived to describe the propagation of the heat inside the body. The plasticity is introduced by the rate-dependent fully implicit backward Euler return mapping scheme with a phenomenological isotropic hardening. Within this model, the complex microstructural changes are consequences of the given Landau free energy functional, finite strain rates, heat conduction, and plasticity.

THEORETICAL BACKGROUND Any physically admissible theory must be consistent with the second law of thermodynamics. In continuum mechanics, this is represented by the Clausius-Duhem inequality [Gurtin and Williams, 1966]. The state of the system is described by a set of independent state variables, in our case $\{\boldsymbol{\epsilon}^e, \alpha^p, T\}$, where $\boldsymbol{\epsilon}^e$ is the elastic strain tensor, α^p the equivalent plastic strain, and T the temperature. By virtue of this choice of state variables, the Clausius-Duhem inequality can be written [Maugin, 1992] in the form of the specific Helmholtz free energy ψ, and the dissipation function, ϕ:

$$\begin{aligned} \rho\psi &= \boldsymbol{\sigma}^e : \boldsymbol{\epsilon}^e + A^p \alpha^p - \rho s T \\ \phi &= \phi_{intr} + \kappa \nabla^2 T \ , \end{aligned} \tag{1}$$

where $\phi_{intr} = \boldsymbol{\sigma}^v : \dot{\boldsymbol{\epsilon}}^e + \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p - A^p \dot{\alpha}^p$, $\rho = 1/V$ is the density, V the volume, κ the coefficient of thermal conduction, A^p the hardening force conjugate to the equivalent plastic strain α^p, and s the specific entropy. If we consider that the lattice has the cubic symmetry, the heat conduction is isotropic. The total stress is calculated as $\boldsymbol{\sigma} = \boldsymbol{\sigma}^e + \boldsymbol{\sigma}^v$, where $\boldsymbol{\sigma}^e$ is its reversible part that is conjugate to $V\boldsymbol{\epsilon}^e$, and $\boldsymbol{\sigma}^v$ the irreversible viscous part that is conjugate to the elastic strain rate $\dot{\boldsymbol{\epsilon}}^e$. The elastic and viscoelastic responses of the body to the external load applied at a given rate are described by the first terms on the right-hand sides of the two equations in (1), that is $\rho\psi^e = \boldsymbol{\sigma}^e : \boldsymbol{\epsilon}^e$ and $\phi^e = \boldsymbol{\sigma}^v : \dot{\boldsymbol{\epsilon}}^e$. Here, $\sigma^e_{ij} = c_{ijkl}\epsilon^e_{kl}$ and $\sigma^v_{ij} = \eta_{ijkl}\dot{\epsilon}^e_{kl}$, where c_{ijkl} is the elastic stiffness tensor and η_{ijkl} the viscosity tensor.

The rate of entropy production is proportional to the amount of internal energy converted into heat per unit time. In our case, this can be expressed as $T\dot{s} = \phi_{intr} + \kappa\nabla^2 T$. The specific entropy of a deformed lattice at the given temperature can be written as $s = s_0 + s_{def}$, where s_0 is the specific entropy of an undeformed lattice, and s_{def} the surplus entropy contributed by the deformation of the lattice at the constant temperature [Landau and Lifshitz, 1986]. This leads to a nonclassical isotropic heat conduction equation

$$c_V \dot{T} = \kappa \nabla^2 T + \phi_{intr} \ , \tag{2}$$

where we used the definition of the heat capacity $c_V/T = \partial s_0/\partial T$. In the special case of a quasistatic deformation, both the elastic and plastic strain rates vanish and thus $\phi_{intr} = 0$. In this case, one recovers the classical heat conduction equation $c_V \dot{T} = \kappa \nabla^2 T$.

The distortion of the body discretized into a finite number of cells is calculated in two steps. First, the distortion of each cell is predicted using linear elasticity. The calculated internal stresses are employed in a suitable yield criterion to check whether the predicted state of the body is elastic. If it is not, the predicted stress state is mapped back onto the yield surface using the rate-dependent fully implicit backward Euler return mapping scheme, while acquiring plastic strains [Simo and Hughes, 1998, Belytschko et al., 2000]. One defines a modified dissipation function,

$$\Omega = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p - A^p \dot{\alpha}^p - \dot{\lambda} f \ , \tag{3}$$

where $\dot{\lambda}$ is a plastic Lagrange multiplier, and f the yield function. For close-packed crystals, one can take the yield function as $f = \bar{\sigma} - (\sigma_Y + A^p)$, where $\bar{\sigma} = \sqrt{(3/2) s_{ij} s_{ij}}$ is the von Mises stress, $s_{ij} = \sigma_{ij} - \delta_{ij}\sigma_{kk}/3$ the components of the deviatoric stress tensor, and σ_Y the initial yield stress. We maximize the dissipation Ω with respect to both thermodynamic forces $\boldsymbol{\sigma}$ and A^p. This yields a set of equations for the increments of the state variables:

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\lambda} \boldsymbol{r}(\boldsymbol{s}, \alpha^p) \qquad \dot{\alpha}^p = -\dot{\lambda} h(\boldsymbol{s}, \alpha^p) \ , \tag{4}$$

where $\boldsymbol{r} = \partial f/\partial \boldsymbol{s}$ and $h = \partial f/\partial A^p$. In elastic-viscoplastic materials the finite viscosity of the material permits the stress state to lie outside of the volume in the principal stress space that is bounded by the yield surface. In this case, the plastic multiplier $\dot{\lambda}$ is obtained from the constitutive equation $\dot{\lambda} = \Phi(\boldsymbol{s}, \alpha^p)/\eta$, where Φ is an overstress function, and η the viscosity. The simplest form of the overstress function is represented by the ramp function $\Phi(\boldsymbol{s}, \alpha^p) = (f + |f|)/2$, where f is the yield function and η the viscosity. Details on how this plastic integration can be implemented can be found, for example, in the book of Belytschko et al. [2000] and in the paper of Dorgan and Voyiadjis [2007].

SIMULATIONS In the following, we will consider that both the impact flyer and the sample are made of the same material and that this can undergo a displacive phase transformation from its high-symmetry cubic phase to a tetragonal phase. The three basic modes of deformation are described by the elastic-plastic strain parameters: (i) hydrostatic strain $e_1 = (\epsilon_{11} + \epsilon_{22})/\sqrt{2}$, (ii) change of shape $e_2 = (\epsilon_{11} - \epsilon_{22})/\sqrt{2}$, and (iii) shear $e_3 = \epsilon_{12}$. The thermoelastic part of the Helmholtz free energy as well as the viscoelastic part of the dissipation function are both harmonic. To allow for the phase transformation to occur, we add higher order terms containing the order parameter e_2. Hence, the thermoelastic part of the Helmholtz free energy is represented by the Landau-Ginzburg functional, $\rho\psi^e = \sum_i A_i(T)(e_i^e)^2 + B(e_2^e)^4 + C(e_2^e)^6 + K_2(\nabla e_2^e)^2$, where $A_i(T)$ are linear combinations of the temperature-dependent elastic moduli, and B, C and K_2 are parameters describing the phase change and the cost of an inhomogeneous deformation of the body [Shenoy et al., 1999]. We adopt the Rayleigh dissipation functional, $\phi^e = \sum_i A'_i(\dot{e}^e_i)^2$, where A'_i are linear combinations of the components of the viscosity tensor [Landau and Lifshitz, 1986].

At time $t = 0$, the impact flyer hits the sample with velocity 1 m/s, thereby inducing a predominantly uniaxial compression in the direction of the impact velocity. The positions and temperature of the nodes of the mesh are evolved according to the equation of motion $\rho\ddot{\boldsymbol{u}} = \nabla \cdot \boldsymbol{\sigma}$, together with the heat conduction equation (2) and the plastic corrector step described above. The density of the deformed body is calculated as $\rho = \rho_0 J$, where ρ_0 is the density of the undeformed lattice and J the determinant of the deformation gradient tensor. Periodic boundary conditions are applied on the upper and lower faces while the left and right faces of the block are traction-free. In Fig. 1, we show the results of our simulations.

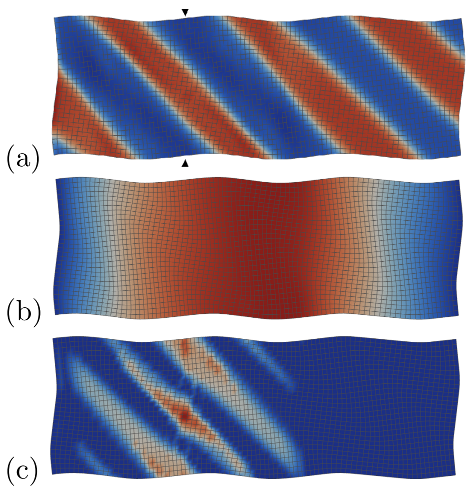

Figure 1: The simulated block 0.24 μs after the impact. (a) shows the field e_2 (red=positive, blue=negative), (b) the temperature field (deep blue=temperature of the heat bath to red=peak temperature), (c) equivalent plastic stress A^p (deep blue=none to red=maximum). The boundary between the flyer (left) and the sample (right) is shown in (a) by the triangles. The yield criterion is reached (and thus the plasticity sets in) first inside the two tetragonal variants along the plane of impact. The equivalent plastic stress (A^p) and thus also the actual yield stress $\sigma_Y + A^p$ decay away from this plane, as shown in (c).

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