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On microstructures occuring in a model of finite–strain elastoplasticity involving a single slip–system.

Starting from a novel variational principle the flow theory of elastoplasticity can be formulated as a minimization problem with respect to the total deformation and the update of the plastic deformation gradient. For a specific model involving a single slip-system the latter quantity can be eliminated. The resulting minimization problem with respect to the total deformation only turns out to be not quasiconvex, thus giving rise to the occurrence of layered microstructures. Finite element calculations indeed show these layers. The results are, however, mesh-dependent. To overcome this effect a partial rank one convexification of the potential given is performed.

1. Finite elastoplasticity

We assume the now well established multiplicative split of the deformation gradient $\mathbf{F} = \mathrm{D}\phi$ into a plastic and an elastic part: $\mathbf{F} = \mathbf{F_e}\mathbf{F_p}$. Then the internal energy W of an elastoplastic material is supposed to depend only on $\mathbf{F_e}$ and a set of hardening parameters p. This means we have

$$W(\mathbf{F},\mathbf{F_p},p) = \overline{W}(\mathbf{F}\mathbf{F_p}^{-1},p) = \overline{W}(\mathbf{F_e},p). \tag{1}$$

Next we are going to introduce thermodynamically conjugate forces to the independent variables $\mathbf{F},\mathbf{F_p}^{-1},p$ via

$$\mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}, \quad \mathbf{Q} = -\frac{\partial W}{\partial \mathbf{F_p}^{-1}}, \quad q = -\frac{\partial W}{\partial p}. \tag{2}$$

Here $\mathbf{T}$ is the first Piola–Kirchhoff stress–tensor. Furthermore we assume that the yield–function φ depends only on those forces and on $\mathbf{P} = \mathbf{F_p}^{-1}$. At the same time φ should, like the internal energy, only depend on $\mathbf{F_e}$ and p. This leaves us with

$$\varphi(\mathbf{T},\mathbf{Q},q) = \overline{\varphi}(\overline{\mathbf{Q}},q), \qquad \text{where} \qquad \overline{\mathbf{Q}} = (\mathbf{F_p}^{-1})^T\mathbf{Q} = -\mathbf{F_e}^T \mathrm{D}_{\mathbf{F_e}}\overline{\mathrm{W}}(\mathbf{F_e},\mathrm{p}) = \mathbf{P}^T\mathbf{Q}. \tag{3}$$

The material model is completed by evolution laws for the internal parameters, the so–called flow–rules

$$\mathbf{P}^{-1}\dot{\mathbf{P}} = \dot{\lambda}\frac{\partial\overline{\varphi}}{\partial\overline{\mathbf{Q}}}, \qquad \dot{p} = \dot{\lambda}\frac{\partial\overline{\varphi}}{\partial q}, \tag{4}$$

$\dot{\lambda} \geq 0$, which can be put in the form $(\mathbf{P}^{-1}\dot{\mathbf{P}},\dot{p}) \in \partial J(\overline{\mathbf{Q}},q)$, where $J(\overline{\mathbf{Q}},q) = \begin{cases} 0 & \text{for } \overline{\varphi}(\overline{\mathbf{Q}},q) \leq 0, \\ \infty & \text{else.} \end{cases}$.

2. Variational formulation

Let us now proceed to a time–discretized formulation by replacing the time–derivatives in (4) by time–increments of the form $\Delta(\mathbf{P},\mathbf{P}_0) = (\theta\mathbf{P}_0 + (1-\theta)\mathbf{P})^{-1}(\mathbf{P}-\mathbf{P}_0)$ or $\Delta(\mathbf{P},\mathbf{P}_0) = (\theta\mathbf{P}_0^{-1} + (1-\theta)\mathbf{P}^{-1})(\mathbf{P}-\mathbf{P}_0)$ for $0 \leq \theta \leq 1$. Then equations (2) and (4) (in a discretized version) as well as the equilibrium conditions $\mathrm{div}\mathbf{T} + \mathbf{f} = 0$, $\mathbf{f}$ being a body–force, and the respective boundary conditions (we have for simplicity assumed only displacement boundary conditions) can be obtained by variation of the functional (here τ denotes the length of the time–step considered)

$$I(\phi,\mathbf{P},p,\overline{\mathbf{Q}},q) = \int_\Omega \left[\overline{W}(\mathrm{D}\phi\,\mathbf{P},p) - \mathbf{f}\cdot\phi + \overline{\mathbf{Q}}{:}\Delta(\mathbf{P}_0,\mathbf{P}) + q\cdot(p-p_0) - \tau J(\overline{\mathbf{Q}},q)\right]\mathrm{dx}. \tag{5}$$

We are able to eliminate $\overline{\mathbf{Q}}$ and q from this functional by introducing the Legendre–transform $J^*(\mathbf{S},s)$ $= \sup\left\{\overline{\mathbf{Q}}{:}\mathrm{S} + q\cdot s - J(\overline{\mathbf{Q}},q)\right\} = \sup\left\{\overline{\mathbf{Q}}{:}\mathrm{S} + q\cdot s \,\middle|\, \overline{\varphi}(\overline{\mathbf{Q}},q) \leq 0\right\}$ which leads to the functional

$$\mathcal{I}_{\mathbf{f},\mathbf{P}_0,p_0}(\phi,\mathbf{P},p) = \int_\Omega \left\{\overline{W}(\mathrm{D}\phi\mathbf{P},p) - \mathbf{f}\cdot\phi + J^*(\Delta(\mathbf{P}_0,\mathbf{P}),p-p_0)\right\}\mathrm{dx}. \tag{6}$$

$\mathcal{I}_{\mathbf{f},\mathbf{P}_0,p_0}$ has now the advantage of being stationary at a minimum with respect to ϕ, $\mathbf{P}_0$ and p_0, see [1] for details.

3. A model with a single slip system

Let us apply the formalism derived above to a specific model with internal energy and yield function given by

$$\overline{W}(\mathbf{F}_e, p) = U(\det \mathbf{F}_e) + \mathrm{tr}\mathbf{F}_e^T\mathbf{F}_e + \frac{a}{2}p^2 \qquad \text{and} \qquad \overline{\varphi}(\overline{\mathbf{Q}}, q) = |\mathbf{m}\cdot\overline{\mathbf{Q}}\,\mathbf{n}| - r - q, \tag{7}$$

where $U(j) = \frac{\Lambda}{4}j^2 - \frac{\Lambda+2}{2}\log j$. Here $\Lambda \geq 0$ is a Lamé–parameter, $a > 0$ is a parameter describing isotropic hardening and p is a single scalar variable. The internal energy corresponds to compressible neo–Hookean material. The vectors $\{\mathbf{m},\mathbf{n}\}$, $\mathbf{m}\cdot\mathbf{n} = 0$, constitute a so called slip–system. Equations (7) form a typical description of an elastoplastic metal–crystal. The flow rule (4) becomes in this case $(\mathbf{P}^{-1}\dot{\mathbf{P}}, \dot{p}) = \dot{\lambda}\,(\mathrm{sign}(\mathbf{m}\cdot\overline{\mathbf{Q}}\mathbf{n})\,\mathbf{m}\otimes\mathbf{n}, -1)$ from which we can conclude that the plastic strain $\mathbf{P}$ assumes the form $\mathbf{P} = \mathbf{1} + \gamma\,\mathbf{m}\otimes\mathbf{n}$, where γ is a scalar parameter. The Legendre–transform can now be calculated explicitly and the functional (6) becomes

$$\mathcal{I}_{\mathbf{f},\gamma_0,p_0}(\boldsymbol{\phi},\gamma) = \int_\Omega \left\{U(\det\mathbf{F}) + \mathrm{tr}\mathbf{F}^T\mathbf{F} + 2\gamma C_{mn} + \gamma^2 C_{mm} + \frac{a}{2}(\gamma-\gamma_0)^2 + (r - ap_0)|\gamma-\gamma_0| - \mathbf{f}\cdot\boldsymbol{\phi}\right\}dx, \tag{8}$$

where $C_{mm} = \mathbf{m}\cdot\mathbf{F}^T\mathbf{F}\mathbf{m}$ and $C_{mn} = \mathbf{m}\cdot\mathbf{F}^T\mathbf{F}\mathbf{n}$ are the components of the right Cauchy–Green–tensor in the directions given by $\mathbf{m}$ and $\mathbf{n}$. We further take the variation of $\mathcal{I}_{\mathbf{f},\gamma_0,p_0}$ with respect to γ, solve for γ and thus are able to eliminate γ (see again [1]) ending up with a functional with $\boldsymbol{\phi}$ as the only independent variable

$$\hat{\mathcal{I}}_{\mathbf{f},\gamma_0,p_0}(\boldsymbol{\phi}) = \int_\Omega \left\{U(\det\mathbf{F}) + \mathrm{tr}\mathbf{F}^T\mathbf{F} + 2\gamma_0 C_{mn} + \gamma_0^2 C_{mm} - \frac{(2|C_{mn} + \gamma_0 C_{mm}| - r + ap_0)_+^2}{2(2C_{mm} + a)} - \mathbf{f}\cdot\boldsymbol{\phi}\right\}dx. \tag{9}$$

4. Convexity properties and microstructures

Let us denote the $\mathbf{F}$–dependent part of the integrand in (9) by $\hat{W}_{\gamma_0,p_0}(\mathbf{F})$. This constitutes a formal elastic internal energy. Let us consider $\hat{W}_{\gamma_0,p_0}(\mathbf{F})$ for the parameter values $\gamma_0 = 0$, $p_0 = 0$ and the rank one–family of deformation gradients $\mathbf{F} = \mathbf{1} + \frac{\lambda}{2}(\mathbf{m}+\mathbf{n})\otimes(\mathbf{n}-\mathbf{m})$. This yields $\tilde{W}(\lambda) = \lambda^2 - \frac{1}{2}\frac{(|\lambda|-r)_+^2}{1+a+(1-\lambda)^2}$. For a small enough it is easy to see that $\tilde{W}(\lambda)$ is not convex, hence $\hat{W}_{\gamma_0,p_0}(\mathbf{F})$ is not rank one convex and by virtue not quasiconvex indicating the possibility of the occurrence of microstructures, see [2], [3].

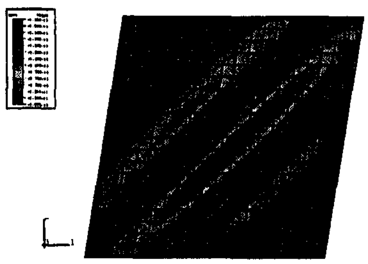

Figure 1

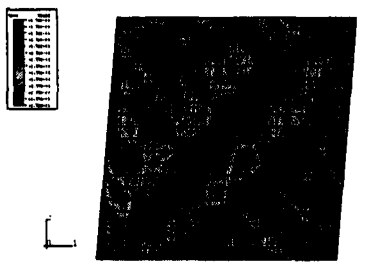

Figure 2

A finite element calculation of a simple shear deformation of a square–shaped body (under plane strain assumptions) clearly shows those microstructures. Figure 1 shows a plot of the internal parameter γ. The slip system $\{\mathbf{m},\ \mathbf{n}\}$ is rotated by an angle of 45 degrees with respect to the coordinate axes. These results, however, are mesh–dependent. In order to avoid this phenomenon we calculated a relaxed energy by the partial rank one–convexivication given by

$$R_1\hat{W}(\mathbf{F}) = \sup\left\{\,(1-\lambda)\hat{W}(\mathbf{F} - \lambda\,\mathbf{a}\otimes\mathbf{b}) + \lambda\,\hat{W}(\mathbf{F} + (1-\lambda)\,\mathbf{a}\otimes\mathbf{b})\;\middle|\; 0 \leq \lambda \leq 1,\quad |\mathbf{a}| = 1\,\right\}, \tag{10}$$

compare the exposition in [3]. We used the NAG–library subroutine E04JAF which employs a gradient line–search algorithm in order to solve the constraint optimization problem given in (10). A typical result of this procedure is depicted in figure 2; once again γ is plotted. One should note that the variations in figure 2 are less than 5 % of those in figure 1. The results are essentially mesh–independent now.

5. References

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