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Energetic formulation of nonlocal crystal plasticity

We review an energetic solution to a problem of the rate-independent evolution of elasto-plastic materials subjected to external loads in the framework of large deformations and multiplicative plasticity. Our model includes gradients of the plastic strain and of hardening variables.

Keywords: Elasto-plasticity; Energetic solution; Plastic strain gradients

1. Introduction

The elastic–plastic behavior of crystalline materials poses a challenge for mathematical analysis on the microscopic, mesoscopic, and macroscopic scales. Here, we study a rate-independent model arising in crystal plasticity. A common and successful approach to the analysis of crystalline materials is via energy minimization. This is manifested for elastic crystals, even for those with the potential of undergoing phase transitions. The applicability of variational methods has been broadened to include *rate-independent* evolution. The rate-independent character of the evolution brings serious mathematical difficulties if one wants to show the existence of solutions since the problem generally leads to the so-called doubly nonlinear evolutionary inclusion. In their pioneering work, Mielke, Theil, and Levitas [1, 2] defined a generalized solution to these inclusions, nowadays called the energetic solution; cf. [3] for a closely related approach. Its main advantage is that it does not contain time-derivatives and therefore it allows for temporal non-smoothness. Moreover, it straightforwardly suggests numerical approximation schemes. This concept of solution is based on two requirements. First, as a consequence of the conservation law for linear momentum, all work put into the system by external forces or boundary conditions is spent on increasing the stored energy or it is dissipated. Secondly, the formulation must satisfy the second law of thermodynamics, which has in the present mechanical framework the form of a dissipation inequality. The last requirement enters the framework as the assumption of the existence of a non-negative convex potential of dissipative forces. As a consequence, the imposed deformation evolves in such a way that the sum of stored and dissipated energies is always minimized. This is reflected in the so-called stability inequality; see (1) below.

In this contribution, we apply this framework to strain gradient plasticity following earlier work of Dillon and Kratochvíl [4], Gurtin [5], Mainik and Mielke [6], and many others. In what follows, $\Omega \subset \mathbb{R}^3$ will be a smooth bounded domain representing the reference configuration of the material body. The overall deformation $y : \Omega \to \mathbb{R}^3$ maps the reference configuration to a deformed one. In the framework of multiplicative plasticity, we decompose $\nabla y = F_e F_p$ where F_e and F_p are the elastic and plastic parts of the deformation gradient, respectively. We suppose that the plastic deformation is incompressible, i.e., $\det F_p = 1$ at all times. The plastic strain tensor, jointly with hardening variables $p \in \mathbb{R}^m$ make a set of internal variables of our model. We denote $z := (F_p, p)$ and suppose that $z(t) \in \mathbb{Z}$, a set of plastic variables, for all time instants $t \in [0, T]$ of our process time interval. Similarly, $y(t) \in \mathbb{Y}$ where $\mathbb{Y}$ is typically a subset of a function space. We consider a separable material, where the energy density splits into elastic and plastic contributions, i.e.,

$$W(x, F_e, z, \nabla z) := W_e(x, F_e) + W_p(x, z, \nabla z) \tag{1}$$

subjected to external forces whose work on the body is described by

$$L(t, y) := \int_\Omega f(t, x) \cdot y(x)\,dx + \int_{\Gamma_1} g(t, x) \cdot y(x)\,dS \tag{2}$$

where f and g represent (time-dependent) body and surface force densities, respectively, and $\Gamma_1 \subset$ boundary (Ω). Moreover, we suppose that $y = y_0$ on $\Gamma_0 \subset$ boundary (Ω) for some fixed y_0. Altogether, the elasto–plastic energy functional $\mathcal{I}$ has the form

$$I(t, y, z) = \int_\Omega W(x, \nabla y(x)\, F_p^{-1}(x), z(x), \nabla z(x))\,dx - L(t, y(t)) \tag{3}$$

We are interested in the rate-independent evolution of the material. To this end, we assume the existence of a non-negative convex potential of dissipative forces $\delta = \delta(x, z, \dot{z})$, where $\dot{z}$ denotes the time derivative of z. In order to ensure rate-independence, δ must be positively one-homogeneous, i.e., $\delta(x, z, \alpha\dot{z}) = \alpha\delta(x, z, \dot{z})$ for all $\alpha \geq 0$. Following Mielke [7] we define a dissipation distance between two values of internal variables $z_0, z_1 \in \mathbb{Z}$ as $D(x, z_0, z_1) := \inf_z\{\int_0^1 \delta(x, z(s), \dot{z}(s))\,ds\colon\ z(0) = z_0, z(1) = z_1\}$, and set $\mathcal{D}(z_1, z_2) = \int_\Omega D(x, z_1(x), z_2(x))\,dx$.

2. Energetic solution

Suppose, that we look for the time evolution of $y(t) \in \mathbb{Y}$ and $z(t) \in \mathbb{Z}$ during the time interval $[0, T]$. The following two properties are key ingredients of the so-called energetic solution due to Mielke and Theil [2]

(i) Stability inequality: $\forall t \in [0, T]$, $\forall \tilde{z} \in \mathbb{Z}$, $\forall \tilde{y} \in \mathbb{Y}$:

$$\mathcal{I}(t, y(t), z(t)) \leq \mathcal{I}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}) \tag{1}$$

(ii) Energy balance: $\forall t \in [0, T]$:

$$\mathcal{I}(t, y(t), z(t)) + \mathrm{Var}(\mathcal{D}, z; [0, t]) = \mathcal{I}(0, y(0), z(0)) + \int_0^t \dot{L}(\xi, y(\xi))\, \mathrm{d}\xi$$

where $\mathrm{Var}(\mathcal{D}, z; [0, t]) := \sup\{\sum_{i=1}^N \mathcal{D}(z(t_i), z(t_{i-1}))$; $\{t_i\}$ partition of $[0, t]\}$. The stability inequality means that not only is the mere elastic energy minimized but the dissipation must be added. The energy balance says that work done by external loads is either dissipated or used to change the elastic energy. The mapping $t \mapsto (y(t), z(t)) \in \mathbb{Y} \times \mathbb{Z}$ is an energetic solution to the problem $(\mathcal{I}, \delta, L)$ if stability inequality and energy balance are satisfied for all $t \in [0, T]$. Its existence was established (under suitable assumptions) in [6, 8] by means of a sequence of incremental problems for a time discretization $0 = t_0 < \ldots < t_n = T$ with $\lim_{n\to\infty} \max_{1\leq i\leq n}(t_i - t_{i-1}) = 0$. Let a stable initial state $z^0 \in \mathbb{Z}$ be given. For $1 \leq k \leq n$, find $(y^k, z^k) \in \mathbb{Y} \times \mathbb{Z}$ such that this pair minimizes $\mathcal{I}(t_k, y, z) + \mathcal{D}(z^{k-1}, z)$, which is a discrete version of the stability inequality. Thus, this minimization amounts to solving a global optimization problem. A spatial discretization by finite elements, for instance, defines an algorithm for numerical solutions. We refer to [9] for closely related numerical issues.

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