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STATISTICALLY STORED DISLOCATIONS IN RATE-INDEPENDENT PLASTICITY

Abstract. Work hardening in crystalline materials is related to the accumulation of statistically stored dislocations in low-energy structures. We present here a model which includes dislocation dynamics in the rate-independent setting for plasticity. Three basic physical features are taken into account: (i) the role of dislocation densities in hardening; (ii) the relations between the slip velocities and the mobility of gliding dislocations; (iii)the energetics of self and mutual interactions between dislocations. The model unifies a number of different approaches to the problem presented in literature. Reaction-diffusion equation with mobility depending on the slip velocities are obtained for the evolution of the dislocations responsible of hardening.

1. Introduction

Slip lines and slip bands on the surface of a plastically deformed crystal are due to complicated phenomena which occur inside the crystal. When plastic deformation occurs, dislocations are generated : some of them move towards the crystal surface forming slip lines, others may be stored to harden the material and form more or less regular patterns ([1]-[16]). As reported in Fleck *et al.* [1], "dislocations become stored for two reasons : they accumulate by trapping each other in a random way or they are required for compatible deformation of various parts of the crystal. The dislocation which trap each other randomly are referred to as *statistically stored dislocations*...gradients of plastic shear result in the storage of *geometrically necessary dislocations*".

Taking into account both statistically stored dislocation (SSD) and geometrically necessary dislocations (GND), our purpose in this paper is to construct a model which is able, at least in the simple case of single slip, to describe dislocations patterns. The basic idea here is to introduce dislocation densities as independent variables in the framework of Gurtin's theory of gradient plasticity [17].

Total dislocation densities have been introduced frequently in the literature, both to describe hardening and the formation of patterns during plastic deformations ([18]-[26]).

In fact, materials scientists often describe hardening due to dislocation accumulation by means of the so-called Kocks' model (see [22]): the resistance to slip ζ is assumed to depend on the total dislocation density ϱ through a relation of the form

$$\zeta = \zeta(\varrho),$$

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and the accumulation of dislocations during plastic slip evolves according to an ordinary differential equation which can be rewritten in the form

$$\frac{d\varrho}{dt} = |\nu|(k_s\sqrt{\varrho} - k_r\varrho), \tag{1}$$

where ν is the resolved (plastic) shear strain rate and k_r, k_s are positive constants. In the right hand side of equation (1), the term $k_s\sqrt{\varrho}$ represents dislocation storage and the terms $k_r\varrho$ represents dynamic recovery. An important consequence of this approach is immediately recognizable by equation (1): the dislocation rate $\dot{\varrho}$ depends on the strain rate. Roughly, this means that dislocations are less mobile when the material hardens.

The above approach does not take into account dislocation density gradients and thus, while very efficient for small strain rates, it does not allow to study spatial variations of the density. One of the first approaches to *non-local* models, which should take into account both spatial and temporal variations of the dislocation density, is due to Holt [18], which obtains a Cahn-Hilliard equation for the total dislocation densities to describe patterning in a manner analogous to spinoidal decomposition in alloys. His model is based on a free energy density which takes into account dislocation interactions through higher gradients of the dislocation density, in conjunction with a gradient-flow derivation of a balance equation for such densities.

Other authors, for instance Aifantis (see for example [23]) and co-workers, model the complex phenomena due to dislocation interaction and annihilation by means of a reaction-diffusion system: in this approach two or more dislocation species are involved (e.g., mobile and immobile dislocations) and an evolution equation for each specie, say $\varrho(\mathbf{X}, t)$, is postulated

$$\frac{d\varrho}{dt} = D\Delta\varrho + g(\varrho) \tag{2}$$

where $g(\varrho)$ is a source term describing creation and annihilation of dislocations (e.g., $g(\varrho) = a\varrho - b\varrho^2$, with a and b phenomenological coefficients), D is a diffusive-like coefficient and Δ is the laplacian. Models like (2) may be used to describe various phenomena related to pattern formation, but they do not include (plastic) strain rate effects of the type described by (1).

The main goal of our work is a unified model which includes all the basic features of the models described above, i.e., the dependence of (plastic) shear rate on dislocation density rate, the non-locality, and finally a term describing work and soft-hardening.

Using consistently the assumption of rate-independence (see Gurtin [17]), we obtain an equation for the total edge dislocation density of the form

$$\frac{d\varrho}{dt} = |\nu|\left(\epsilon\Delta\varrho - \frac{\partial\varphi}{\partial\varrho}\right) \tag{3}$$

where ϵ may be interpreted as a diffusive coefficient and $\varphi(\varrho)$ is a dislocation energy including work and soft-hardening behavior. Notice that equilibrium solutions satisfy

$$\epsilon\Delta\varrho - \frac{\partial\varphi}{\partial\varrho} = 0. \tag{4}$$

Those solutions may correspond to low energy dislocations structures (LEDS, see Kuhlmann-Wilsdorf [2]), or patterns forming during fatigue, where dislocations arrange themselves in such a way that their self and interaction energy are minimized, and their average density does not change with time, even if plastic flow does occur and $\nu \neq 0$.

If τ and $\zeta(\varrho)$ denote the resolved shear stress and the slip resistance respectively, then by regularization of the classical yield equation $\tau = (\mathtt{sgn}\,\nu)\zeta(\varrho)$, by letting $\tau = (\mathtt{sgn}\,\nu)|\nu|^{1/n}\zeta(\varrho)$ for a large positive integer n, we obtain

$$|\nu| = \left(\frac{|\tau|}{\zeta(\varrho)}\right)^n . \tag{5}$$

By substitution of ν, as given by (5), into (3), we obtain the non linear parabolic differential equation

$$\frac{d\varrho}{dt} = \left(\frac{|\tau|}{\zeta(\varrho)}\right)^n \left(\epsilon\Delta\varrho - \frac{\partial\varphi}{\partial\varrho}\right), \tag{6}$$

which can be solved if the resolved shear stress $\tau = \tau(\mathbf{X}, t)$ is known as a function of position and time.

2. Kinematics

Consider a body identified with its reference configuration $\mathcal{B}_R$, a regular region in $\mathbb{R}^3$, and let $\mathbf{X} \in \mathcal{B}_R$ denote an arbitrary material point of the body. A motion of the body is a time-dependent one-to-one smooth mapping $\mathbf{x} = \mathbf{y}(\mathbf{X}, t)$. At each fixed time t, the deformation gradient is a tensor field defined by

$$\mathbf{F} = \mathtt{Grad}\,\mathbf{y} \tag{7}$$

and consistent with $\mathtt{det}\,\mathbf{F}(\mathbf{X}, t) > 0$ for any $\mathbf{X}$ in $\mathcal{B}_R$. A superposed dot denotes material time derivative so that, for instance, $\dot{\mathbf{y}}$ is the velocity of the motion.

We assume that the classic elastic-plastic decomposition holds, i.e.,

$$\mathbf{F} = \mathbf{F}_e\mathbf{F}_p, \tag{8}$$

with $\mathbf{F}_e$ and $\mathbf{F}_p$ the elastic and plastic gradients, consistent with $J_e = \mathtt{det}\,\mathbf{F}_e > 0$ and $J_p = \mathtt{det}\,\mathbf{F}_p > 0$. The usual interpretation of these tensors is that $\mathbf{F}_e$ represents stretching and rotation of the atomic lattice embedded in the body, while $\mathbf{F}_p$ represents disarrangements due to slip of atomic planes.

We restrict attention to *plastic slip shear deformation*, i.e., deformations such that the decomposition (8) holds, with $\mathbf{F}_e$ arbitrary and with $\mathbf{F}_p$ of the form

$$\mathbf{F}_p = \mathbf{I} + \alpha\mathbf{s}\otimes\mathbf{m}, \qquad \mathbf{s}\cdot\mathbf{m} = 0, \tag{9}$$

with $\mathbf{I}$ the identity in $\mathbb{R}^3$, $\mathbf{s}$ and $\mathbf{m}$ constant unit vectors and $\alpha = \alpha(\mathbf{X}, t)$. In (9), $\dot{\alpha}$ may be interpreted as slip rate on the slip plane, defined by the glide direction $\mathbf{s}$ and the slip-plane normal $\mathbf{m}$. This plane is understood to be the only one active among all the available slip systems.

2.1. The geometrically necessary dislocation tensor

The presence of geometrically necessary dislocations in a crystal is usually described in terms of Burgers vector, a notion strictly related to the incompatibility of the elastic deformation.

DEFINITION 1. *Let S be a surface in the deformed configuration, whose boundary ∂S is a smooth closed curve. The Burgers vector of ∂S is defined as*

$$\mathbf{b}(\partial S) = \int_{\partial S} \mathbf{F}_e^{-1} d\mathbf{x}$$

where $d\mathbf{x}$ is the line element of the circuit ∂S. Stokes' theorem implies that

$$\mathbf{b}(\partial S) = \int_S \left(\mathtt{curl}\ \mathbf{F}_e^{-1}\right)^{\mathrm{T}} \mathbf{n} da,$$

where $\mathbf{n}$ is the unit normal to the surface S and $\mathtt{curl}$ and da are, respectively, the curl operator with respect to the point $\mathbf{x}$ and the area element in the deformed configuration.

Since $\mathtt{curl}\ \mathbf{F}_e^{-1} \neq 0$ is necessary to have non null Burgers vectors, the tensor $\mathtt{curl}\ \mathbf{F}_e^{-1}$ seems to be a candidate to measure geometrically necessary dislocations. As such, however, it suffers some drawbacks: for example, $\mathtt{curl}\ \mathbf{F}_e^{-1}$ is not invariant under superposed compatible elastic deformations; moreover, in view of applications to gradient theories of plasticity, it should be desirable to work in terms of a dislocation measure which can be expressed in terms of the plastic strain gradient also. In [27], Cermelli and Gurtin prove the existence of a dislocation tensor which satisfies both requirements above. We can rephrase their result as follows:

DEFINITION 2. *Let $\mathbf{y}$ be a deformation and $\mathbf{F} = \nabla\mathbf{y}$ its deformation gradient. If $\mathbf{F}_e$ and $\mathbf{F}_p$ are smooth fields satisfying (8), then the identity $\frac{1}{J_p}\mathbf{F}_p\mathtt{Curl}\ \mathbf{F}_p = J_e\mathbf{F}_e^{-1}\mathtt{curl}\ \mathbf{F}_e^{-1}$ holds: we define therefore the geometrically necessary dislocation tensor (GND tensor) as*

$$\mathbf{D}_G := \frac{1}{J_p}\mathbf{F}_p\mathtt{Curl}\ \mathbf{F}_p = J_e\mathbf{F}_e^{-1}\mathtt{curl}\ \mathbf{F}_e^{-1}. \tag{10}$$

By (10), we have an alternative plastic and elastic representation of $\mathbf{D}_G$. As pointed out in [27], in developing a constitutive theory "it would seem advantageous to use the representation of $\mathbf{D}_G$ in terms of $\mathbf{F}_p$, which characterizes defects, leaving $\mathbf{F}_e$ to describe stretching and rotation of the lattice". See [27] for an exhaustive discussion of the geometrical dislocation tensor defined by (10).

For single slip plastic deformations (9), the GND tensor has the form

$$\mathbf{D}_G = (\nabla\alpha \times \mathbf{m}) \otimes \mathbf{s} = s_g\mathbf{s} \otimes \mathbf{s} + e_g\mathbf{t} \otimes \mathbf{s} \tag{11}$$

where $\mathbf{t} = \mathbf{s} \times \mathbf{m}$ and

$$e_g = \nabla\alpha \cdot \mathbf{s}, \qquad s_g = -\nabla\alpha \cdot \mathbf{t}. \tag{12}$$

The quantities e_g and s_g can be interpreted as densities associated to geometrically necessary *edge* and *screw* dislocations, respectively, with Burgers vector parallel to $\mathbf{s}$.

2.2. The total dislocation tensor

Individual dislocations can be visualized by electron microscopy and their direction and Burgers vector can be determined experimentally. We thus assume that the microscopic arrangement of dislocations at each point is characterized by scalar densities of edge end screw dislocations, for any given Burgers vector. More precisely, assuming that only dislocations with Burgers vector $\mathbf{s}$

are present, and their line direction is contained in the slip plane $\mathbf{m}^{\perp}$, we introduce nonnegative functions

$$e_+ = e_+(\mathbf{X}, t), \quad e_- = e_-(\mathbf{X}, t), \quad s_+ = s_+(\mathbf{X}, t), \quad s_- = s_-(\mathbf{X}, t), \tag{13}$$

with the following interpretation : e_+ and e_- are the densities of dislocations with Burgers vector $\mathbf{s}$ and line direction $\mathbf{t}$ and $-\mathbf{t}$ respectively (edge dislocations); s_+ and s_- are the densities of dislocations with Burgers vector $\mathbf{s}$ and line direction $\mathbf{s}$ and $-\mathbf{s}$ respectively (screw dislocations).

Noting that all the information on a given system of dislocations may be summarized in one of the tensorial quantities (recall that $e\pm, s\pm \geq 0$)

$$e_+\mathbf{t} \otimes \mathbf{s}, \qquad -e_-\mathbf{t} \otimes \mathbf{s}, \qquad s_+\mathbf{s} \otimes \mathbf{s}, \qquad -s_-\mathbf{s} \otimes \mathbf{s},$$

we assume that the edge and screw densities above are related to the geometrically necessary dislocation tensor by a compatibility relation of the form

$$\mathbf{D}_G = (e_+ - e_-)\mathbf{t} \otimes \mathbf{s} + (s_+ - s_-)\mathbf{s} \otimes \mathbf{s} \tag{14}$$

from which it follows that

$$e_+ - e_- = e_g, \qquad s_+ - s_- = s_g.$$

DEFINITION 3. *Introducing the total edge and screw dislocation densities*

$$e := e_+ + e_-, \qquad s := s_+ + s_-,$$

we define the total dislocation tensor by

$$\mathbf{D}_S := e\,\mathbf{t} \otimes \mathbf{s} + s\,\mathbf{s} \otimes \mathbf{s}. \tag{15}$$

3. Dynamics

3.1. Standard forces and microforces

To describe the force systems associated to the motion of the body, plastic deformation and the evolution of the total dislocation densities, we introduce a tensor field $\mathbf{S}$, vector fields $\mathbf{b}^{ext}$, ξ, κ_e and κ_s, and scalar fields Π, Π^{ext}, M_e, M_e^{ext}, M_s and M_e^{ext}, all functions of $(\mathbf{X}, t)$.

These fields correspond to three physically distinct sets of forces acting on the body.

The first force system is standard, and is given by the usual Piola-Kirchhoff stress tensor $\mathbf{S}$ and the body force $\mathbf{b}^{ext}$.

The second force system has been introduced by Gurtin in his theory of gradient plasticity of single crystals (see [17]), to describe forces that perform work associated to plastic slip. This system consists in a vector microstress ξ, a scalar internal microforce Π, and a scalar external microforce Π^{ext}.

The last set of forces is introduced to account for the dynamics of the total screw and edge dislocation densities. It consists of a vector force κ_e, a scalar internal microforce M_e, and a scalar external microforce M_e^{ext} for edge dislocations, and corresponding quantities κ_s, M_s and M_s^{ext} for screw dislocations.

A balance law is associated to each force system. We consider first the standard system $(\mathbf{S}, \mathbf{b}^{ext})$, which is governed by the classical force balances, in local form given by

$$\mathtt{Div}\,\mathbf{S} + \mathbf{b}^{ext} = 0, \qquad \mathbf{S}\mathbf{F}^{\mathrm{T}} = \mathbf{F}\mathbf{S}^{\mathrm{T}}, \tag{16}$$

where we have omitted the inertial terms. To the second force system (ξ, Π, Π^{ext}), governing plastic slip, a corresponding microforce balance is associated (Gurtin, [17])

$$\text{Div}\,\xi + \Pi + \Pi^{ext} = 0. \tag{17}$$

Following Gurtin, [17] we shall see later that this relation replaces the usual yield condition for the single slip system under consideration.

In our theory two more balances must be introduced, in order to obtain a complete integrable set of equations once an adequate constitutive theory is developed. These new balances are associated to the force systems $(\kappa_e, \Pi_e, \Pi_e^{ext})$ and $(\kappa_s, \Pi_s, \Pi_s^{ext})$, and are given in local form by

$$\begin{aligned} \text{Div}\,\kappa_e + M_e + M_e^{ext} &= 0, \\ \text{Div}\,\kappa_s + M_s + M_s^{ext} &= 0. \end{aligned} \tag{18}$$

Each of the above force system is characterized by the way it expends power on the rate of change of the corresponding microstructural field : precisely, we assume that the working of the forces on an arbitrary portion $\mathcal{P}$ of the body is

$$\begin{aligned} W(\mathcal{P}) &= \int_{\partial\mathcal{P}} (\mathbf{Sn}\cdot\dot{\mathbf{y}} + \xi\cdot\mathbf{n}\dot{\alpha} + \kappa_e\cdot\mathbf{n}\dot{e} + \kappa_s\cdot\mathbf{n}\dot{s})da \\ &\quad + \int_{\mathcal{P}} (\mathbf{b}^{ext}\cdot\dot{\mathbf{y}} + \dot{\alpha}\Pi^{ext} + \dot{e}M_e^{ext} + \dot{s}M_s^{ext})dv. \end{aligned} \tag{19}$$

Notice that the microstress ξ and the corresponding external force, expend power on the slip velocity $\dot{\alpha}$, while the total dislocation forces κ_e and κ_s expand power on the rate of change of the corresponding dislocation densities.

We take the second law in the form of a dissipation inequality, stating that the time-derivative of the free energy relative to an arbitrary subregion $\mathcal{P}$ of the body may not exceed the working of the external forces acting on $\mathcal{P}$, i.e.,

$$\frac{d}{dt}\int_{\mathcal{P}} \psi\, dv \leq W(\mathcal{P}) \tag{20}$$

where ψ is the free energy, density per unit volume in the reference configuration. Using the balance equations, this inequality becomes, in local form,

$$\dot{\psi} \leq \mathbf{T}_e\cdot\dot{\mathbf{F}}_e + \xi\cdot\nabla\dot{\alpha} + \kappa_e\cdot\nabla\dot{e} + \kappa_s\cdot\nabla\dot{s} + \pi\dot{\alpha} - M_e\dot{e} - M_s\dot{s} \tag{21}$$

where

$$\mathbf{T}_e = \mathbf{SF}_p^T \qquad \pi = \tau - \Pi, \qquad \tau = \mathbf{S}\cdot(\mathbf{F}_e\mathbf{s}\otimes\mathbf{m}). \tag{22}$$

Notice that τ is the *resolved shear stress* on the slip system under consideration.

3.2. Constitutive equations

Letting $\sigma = (\mathbf{F}_e, e_+, e_-, s_+, s_-, \nabla e_+, \nabla e_-, \nabla s_+, \nabla s_-)$ and $v = (\dot{\alpha}, \dot{e}, \dot{s})$ we consider constitutive equations of the form

$$\psi = \hat{\psi}(\sigma), \qquad \mathbf{T}_e = \hat{\mathbf{T}}_e(\sigma), \qquad \xi = \hat{\xi}(\sigma), \qquad \kappa_e = \hat{\kappa}_e(\sigma), \qquad \kappa_s = \hat{\kappa}_s(\sigma) \tag{23}$$

and

$$\pi = \hat{\pi}(\sigma, \upsilon), \qquad M_e = \hat{M}_e(\sigma, \upsilon), \qquad M_s = \hat{M}_s(\sigma, \upsilon). \tag{24}$$

Requiring the consistency of the constitutive equations with the dissipation inequality for any process, we obtain by the classical Coleman-Noll procedure the result that the constitutive functions above cannot depend on $\nabla e_+,\ \nabla e_-,\ \nabla s_+$ and ∇s_-, but only on ∇e and ∇s, i.e., we can rewrite the constitutive relations (23) in terms of the list

$$\sigma' = (\mathbf{F}_e, e_+, e_-, s_+, s_-, \nabla e, \nabla s)$$

or, equivalently,

$$\sigma'' = (\mathbf{F}_e, e_g, s_g, e, s, \nabla e, \nabla s).$$

Furthermore, the constitutive relations in (23) must satisy the requirements

$$\begin{aligned} \mathbf{T}_e &= \frac{\partial \hat{\psi}}{\partial \mathbf{F}_e}, & \xi &= \frac{\partial \hat{\psi}}{\partial e_g}\mathbf{s} + \frac{\partial \hat{\psi}}{\partial s_g}\mathbf{m} \times \mathbf{s}, \\ \kappa_e &= \frac{\partial \hat{\psi}}{\partial \nabla e}, & \kappa_s &= \frac{\partial \hat{\psi}}{\partial \nabla s}, \end{aligned} \tag{25}$$

while the internal microforces M_e and M_s decompose as

$$M_e = -M_e^{dis} - \frac{\partial \hat{\psi}}{\partial e}, \qquad M_s = -M_s^{dis} - \frac{\partial \hat{\psi}}{\partial s} \tag{26}$$

where $M_e^{dis},\ M_s^{dis}$ and π must satisfy the residual dissipation inequality

$$\delta = \pi\dot{\alpha} + M_e^{dis}\dot{e} + M_s^{dis}\dot{s} \geq 0 \tag{27}$$

for all processes (σ, υ).

3.3. Rate independence

Notice that, under a time scale transformation defined by $t \to t/\theta$, $\theta > 0$, the fields $\dot{\alpha},\ \dot{e}$ and $\dot{s}$ transform according to $\dot{\alpha} \to \theta\dot{\alpha},\ \dot{e} \to \theta\dot{e}$ and $\dot{s} \to \theta\dot{s}$. Following Gurtin, we assume that the constitutive equations for $M_e^{dis},\ M_s^{dis}$ and π are rate-independent, in the sense that they satisfy

$$M_e^{dis}(\sigma, \upsilon) = M_e^{dis}(\sigma, \theta\upsilon), \quad M_s^{dis}(\sigma, \upsilon) = M_s^{dis}(\sigma, \theta\upsilon), \quad \pi(\sigma, \upsilon) = \pi(\sigma, \theta\upsilon),$$

for any (σ, υ) and for all $\theta > 0$.

4. A nonlinear model

For the applications presented in this paper, we choose a particular form of the free energy function ψ, namely

$$\psi = \psi_e(\mathbf{F}_e) + \varphi(e_g, s_g, e, s) + \frac{1}{2}\epsilon_1|\nabla e|^2 + \frac{1}{2}\epsilon_2|\nabla s|^2 \tag{28}$$

where ψ_e and φ are non-negative functions and ϵ_1 and ϵ_2 are positive constants.

Moreover, we shall assume that the dissipative fields M_e^{dis}, M_s^{dis} and π are given by

$$
\begin{aligned}
M_e^{dis}(\sigma, v) &= a(e,s)\frac{\dot e}{|\dot\alpha|},\\
M_s^{dis}(\sigma, v) &= b(e,s)\frac{\dot s}{|\dot\alpha|},\\
\pi(\sigma, v) &= \zeta(e,s)\,\mathtt{sgn}\,\dot\alpha,
\end{aligned}
\tag{29}
$$

where $a(e,s)$, $b(e,s)$ and $\zeta(e,s)$ are positive functions. This choice guarantees rate-independence, and yields a dissipation density Δ quadratic in the rates of change of the total dislocation densities. Moreover, as we shall see, when $\dot\alpha = 0$, equations $(29)_1$ and $(29)_2$ are well-defined.

Following Gurtin [17], the function ζ may be interpreted as the *slip resistance*. In [17], ζ is introduced as internal variable, whose evolution is given by an ordinary differential equation, called the *hardening equation*, of the form

$$\dot\zeta = f(\lambda, \dot\alpha),$$

where λ is a list possibly containing the fields $\mathbf{F}_e$, $\mathbf{F}_p$, $\nabla\mathbf{F}_p$ and ζ. As shown in [17], when restricted by rate independence, the hardening equation becomes

$$\dot\zeta = K(\lambda)|\dot\alpha|. \tag{30}$$

Our approach to hardening is substantially different from that based on internal variables: we assume in fact that ζ is given by a constitutive relation compatible with the dissipation inequality and the hypothesis of rate independence. Therefore it is not necessary to introduce the hardening equation *a priori*, since, as shown below, it is a consequence of the constitutive choices $(29)_1$ and $(29)_2$ for M_e^{dis} and M_s^{dis}.

To write explicitly the evolution equations for our model, we assume that no external forces are present, and choose a cartesian coordinate system (X, Y, Z) in the reference configuration such that

$$(1,0,0) = \mathbf{s}\times\mathbf{m} \qquad (0,1,0) = \mathbf{s} \qquad (0,0,1) = \mathbf{m}.$$

The balance equations are then

1) the balances of linear and angular momentum

$$\mathtt{Div}\left(\frac{\partial\psi_e}{\partial\mathbf{F}_e}\mathbf{F}_p^{-T}\right) = 0, \qquad \text{and} \qquad \frac{\partial\psi_e}{\partial\mathbf{F}_e}\mathbf{F}_e^T = \mathbf{F}_e\left(\frac{\partial\psi_e}{\partial\mathbf{F}_e}\right)^T. \tag{31}$$

2) the yield equation

$$\tau = (\mathtt{sgn}\,\dot\alpha)\zeta - \frac{\partial^2\varphi}{\partial e_g^2}\frac{\partial^2\alpha}{\partial Y^2} + 2\frac{\partial^2\varphi}{\partial e_g\partial s_g}\frac{\partial^2\alpha}{\partial X\partial Y} - \frac{\partial^2\varphi}{\partial s_g^2}\frac{\partial^2\alpha}{\partial X^2}, \tag{32}$$

Notice that the yield condition is modified by the presence of geometrically necessary dislocations (we have used (12) to express the geometrically necessary dislocation densities in terms of the derivatives of the plastic slip α), which can be thought as inducing isotropic hardening-softening.

3) a reaction-diffusion system for the total dislocation densities

$$\dot e = \frac{|\dot\alpha|}{a}\left(\epsilon_1\Delta e - \frac{\partial\varphi}{\partial e}\right), \qquad \dot s = \frac{|\dot\alpha|}{b}\left(\epsilon_2\Delta s - \frac{\partial\varphi}{\partial s}\right). \tag{33}$$

Notice that the dislocation mobility is proportional to the modulus of the slip velocity $\dot{\alpha}$. Henceforth, two characteristic features of dislocation dynamics are immediately recognizable from (33):

(i) one can have equilibrium configurations for edge dislocations, i.e.,

$$\epsilon_1 \Delta e - \frac{\partial \varphi}{\partial e} = 0$$

such that $\dot{e} = 0$ and dislocations are "locked" in low energy structures, but plastic flow does occur, and the slip velocity does not vanish: $\dot{\alpha} \neq 0$. A similar discussion applies to screw densities.

(ii) if the material behaves elastically, so that $\dot{\alpha} = 0$, then dislocations cannot move.

Besides, by derivations with respect the time of the constitutive relation $\zeta(e, s)$ for the slip resistance, and using equations $(33)_1$ and $(33)_2$, we obtain a hardening equation

$$\dot{\zeta} = \left[\frac{1}{a} \frac{\partial \zeta}{\partial e} \left(\epsilon_1 \Delta e - \frac{\partial \varphi}{\partial e} \right) + \frac{1}{b} \frac{\partial \zeta}{\partial s} \left(\epsilon_2 \Delta s - \frac{\partial \varphi}{\partial s} \right) \right] |\dot{\alpha}| \tag{34}$$

which is a generalization of the classical equation (30).

5. One dimensional model

In this section we describe some simplifying assumptions which allow to reduce the reaction-diffusion system for the total dislocation densities, to a single one-dimensional equation for the total edge density.

ASSUMPTIONS

(i) We assume that the geometrically necessary dislocation densities vanish, i.e.,

$$e_g = s_g = 0,$$

which implies that $e_+ = e_-$, $s_+ = s_-$ and thus, by (12), α only depends on (Z, t) .

(ii) Screw dislocations densities are assumed to vanish identically, and the total edge dislocation density e is constant on each slip plane, so that e depends only on (Z, t). Thus e is the only non-vanishing dislocation density.

(iii) The resolved shear stress τ is assumed to be constant with respect to $(\mathbf{X}, t)$.

(iv) The constitutive relation for the slip resistance has the form

$$\zeta(e) = \zeta_0 + c\sqrt{e}$$

where ζ_0 and c are positive constants. This relation is well known in the materials science literature (cf. Livingston [4], Van Drunen and Saimoto [5], Staker and Holt [6]).

(v) We approximate $\mathtt{sgn}\,\dot{\alpha}$ for $\dot{\alpha} \neq 0$ by

$$|\dot{\alpha}|^{\frac{1}{n}} \mathtt{sgn}\,\dot{\alpha}$$

with n large (viscoplastic regularization).

(vi) Assuming that the body $\mathcal{B}$ is an infinite layer between the planes $Z = 0$ and $Z = L$, we take natural boundary conditions for the microstress associated to the total edge dislocation density,

$$\left.\frac{\partial e}{\partial Z}\right|_{Z=0} = \left.\frac{\partial e}{\partial Z}\right|_{Z=L} = 0.$$

5.1. A particular energy dislocation function

We further choose $\varphi(e)$ in the form

$$\varphi(e) = \frac{1}{4}[e(e - e_m)]^2, \tag{35}$$

with $e_m > 0$ a constant. The function $\varphi(e)$ is non-convex and non-negative with a local minimum at $e = 0$ and $e = e_m$ and a local maximum at $e = e_m/2$.

5.2. The model

Assuming that the standard balance of momentum (31) is identically satisfied, the previous assumptions reduce the general model to the following two equations

$$\tau = (\mathtt{sgn}\,\dot{\alpha})|\dot{\alpha}|^{1/n}(\zeta_0 + c\sqrt{e}), \tag{36}$$

and

$$\dot{e} = \frac{1}{a}|\dot{\alpha}|\left(\epsilon_1 \frac{\partial^2 e}{\partial Z^2} - e(e - e_m/2)(e - e_m)\right). \tag{37}$$

Using (36), equation (37) becomes

$$\dot{e} = \frac{1}{a}\left(\frac{|\tau|}{\zeta_0 + c\sqrt{e}}\right)^n \left(\epsilon_1 \frac{\partial^2 e}{\partial Z^2} - e(e - e_m/2)(e - e_m)\right), \tag{38}$$

supplemented by the natural boundary conditions discussed above. Equation (38), which is the basic result of this work, is a non-linear partial differential equation which may be solved numerically: a complete discussion of the behavior of the solutions to (38) will be published elsewhere.

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