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Crystal Plasticity Treated as a Quasi-Static Material Flow through Adjustable Crystal Lattice

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Considering high pressure torsion experiments as a motivation, plastic behavior of crystalline solids is treated as a highly viscous material flow through an adjustable crystal lattice. Instead of the traditional decomposition rule considering the deformation gradient as a product of the elastic and plastic parts, the proposed model is based on its rate form: the velocity gradient consists of the lattice velocity gradient and the sum of the velocity gradients corresponding to the slip rates of individual slip systems; the slip strains themselves are not defined in the model. The geometrical changes caused by material flow and the slip strains can be specified a posteriori. Crystal lattice distortions are measured with respect to a lattice reference configuration. In an adopted rigid plastic approximation the lattice distortions are reduced to rotations. Constitutive equations incorporate non-local hardening caused by close range interactions among dislocations.

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1. Introduction

After an initial adjustment to a tool, specimens twisted under high axial compression do not change their shape and withstand unlimited amount of plastic deformation. The initial non-steady material flow (up to strain ≈ 20 reported in [1–3]) is followed by a steady flow where no further work hardening and structural changes are observed. Looking at other severe plastic deformation experiments [4, 5] it seems that crystalline materials at yield behave as a special kind of incompressible, anisotropic, highly viscous fluids. The material flow through the crystal lattice has been regarded by Asaro [6] as crystal plasticity "basic tenet". The microscopic inspection reveals a structural adjustment of the crystal lattice to the material flow seen as a deformation substructure. High viscosity provides a possibility to describe the flow as a quasi-static process, where inertial forces can be neglected. The flow through the lattice is restricted to preferred crystallographic planes and directions causing anisotropy. In the deformation process the lattice is strained and rotated. Changes in the distances among lattice positions measured by the lattice strain are relatively small, therefore, in the outlined model the material is considered as rigid-plastic, the lattice can be adjusted to the flow by local reorientations.

2. Flow model

Kinematics of the model is characterized by the velocity field $\boldsymbol{v}(\boldsymbol{x},t)$, the slip rates $\nu^{(i)}(\boldsymbol{x},t)$, $i=1,2,\ldots,I$, and the lattice rotation $\boldsymbol{R}(\boldsymbol{x},t)$; $\boldsymbol{x}$ is a position in the current configuration and t means time. $\boldsymbol{v}$ and $\nu^{(i)}$ describe the material flow in the current configuration, and $\boldsymbol{R}$ controls the orientation of the lattice in the current configuration with respect to the lattice reference configuration. Instead of the traditional decomposition rule $\boldsymbol{F}=\boldsymbol{F}^{\mathrm{e}}\boldsymbol{F}^{\mathrm{p}}$ considering the deformation gradient $\boldsymbol{F}$ as a product of the elastic $\boldsymbol{F}^{\mathrm{e}}$ and plastic $\boldsymbol{F}^{\mathrm{p}}$ parts*, the proposed model is based on the rate form of this rule (a superposed dot means a material time derivative)

$$\boldsymbol{L}=\nabla\boldsymbol{v}=\dot{\boldsymbol{R}}\boldsymbol{R}^{\mathrm{T}}+\sum_{i=1}^{I}\nu^{(i)}\boldsymbol{s}^{(i)}\otimes\boldsymbol{m}^{(i)}, \tag{1}$$

where the velocity gradient $\boldsymbol{L}=\nabla\boldsymbol{v}$ has two parts: the lattice spin $\boldsymbol{\Omega}^{\mathrm{L}}=\dot{\boldsymbol{R}}\boldsymbol{R}^{\mathrm{T}}$ which measures the adjustment rate of the lattice, and the rate of material flow consisting of contributions of the individual slip rates $\nu^{(i)}$, $i=1,\ldots,I$. The vectors $\boldsymbol{s}^{(i)}(\boldsymbol{x},t)$ and $\boldsymbol{m}^{(i)}(\boldsymbol{x},t)$ in the current configuration are the slip directions and the unit normals to the slip planes, respectively. The vectors $\boldsymbol{s}^{(i)}$ and $\boldsymbol{m}^{(i)}$ rotate rigidly with the lattice, $\boldsymbol{s}^{(i)}=\boldsymbol{R}\boldsymbol{s}_0^{(i)}$, $\boldsymbol{m}^{(i)}=\boldsymbol{R}\boldsymbol{m}_0^{(i)}$, where $\boldsymbol{s}_0^{(i)},\boldsymbol{m}_0^{(i)}$ are the unit vectors fixed in the lattice reference configuration, they are determined by the crystallographic structure of the material.

The symmetric part of (1) yields the quasistatic flow equations represented by the stretching $\boldsymbol{D}$,

$$\boldsymbol{D}=\left(\nabla\boldsymbol{v}+\nabla\boldsymbol{v}^{\mathrm{T}}\right)/2 =\sum_{i=1}^{I}\nu^{(i)}(\boldsymbol{s}^{(i)}\otimes\boldsymbol{m}^{(i)}+\boldsymbol{m}^{(i)}\otimes\boldsymbol{s}^{(i)})/2. \tag{2}$$

The antisymmetric part of (1) provides the evolution

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* The gradient $\boldsymbol{F}$ and slips $\gamma^{(i)}$ are not defined in the model. If needed, they may be recovered a posteriori. For a chosen reference configuration $\boldsymbol{F}$ can be revealed by time integration of the velocity gradient field, $\dot{\boldsymbol{F}}\boldsymbol{F}^{-1}=\boldsymbol{L}$. Similarly, the slip strains carried by individual slip systems could be obtained from the corresponding slip rates $\nu^{(i)}$ by a posteriori time integration.

equations for $\boldsymbol{R}$ representing adjustment of the lattice

$$\dot{\boldsymbol{R}} = \Big[(\nabla \boldsymbol{v} - \nabla \boldsymbol{v}^{\mathrm{T}})/2 - \sum_{i=1}^{I} \nu^{(i)} (\boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)} - \boldsymbol{m}^{(i)} \otimes \boldsymbol{s}^{(i)})/2\Big] \boldsymbol{R}. \tag{3}$$

Generally, $\boldsymbol{R}$ does not correspond to a gradient of a vector field, i.e. $\boldsymbol{R}$ may be incompatible. As seen by an observer in the current configuration a measure of incompatibility is the density tensor $\boldsymbol{\Lambda}$ of excess dislocations (called usually geometrical necessary dislocations (GNDs)), (cf. [7] eq. (6.6))

$$\boldsymbol{\Lambda} = \Big[\mathrm{curl}\, \boldsymbol{R}^{\mathrm{T}}\Big] \boldsymbol{R}^{\mathrm{T}}. \tag{4}$$

In the present model the GND density tensor $\boldsymbol{\Lambda}$ represents the result of the fragmentation process modeling misoriented deformation substructures seen in electron micrographs.

Dynamics of the deformation process is governed by the Cauchy stress $\boldsymbol{T}(\boldsymbol{x},t)$ and critical resolved shear stresses $\tau_y^{(i)}(\boldsymbol{x},t)$. The stress has to satisfy quasistatic stress equilibrium

$$\mathrm{div} \boldsymbol{T} = 0. \tag{5}$$

The Cauchy stress $\boldsymbol{T}$ controls the slip rates $\nu^{(i)}$ through the resolved shear stresses $\tau^{(i)}$

$$\tau^{(i)} = \boldsymbol{s}^{(i)} \cdot \boldsymbol{T} \boldsymbol{m}^{(i)}. \tag{6}$$

Constitutive equations. In the rigid-viscous-plastic version of the flow model the resolved shear stresses $\tau^{(i)}$ are assumed to be coupled with the slip rates $\nu^{(i)}$ through a power law constitutive equation

$$\nu^{(i)} = \left| \frac{\tau^{(i)}}{\tau_y^{(i)}} \right|^{1/r} \mathrm{sgn}\, \tau^{(i)}, \tag{7}$$

where $r > 0$ is a scalar material parameter, which controls the rate sensitivity; for $r \to 0$ the constitutive relation (7) represents a rate independent limit, i.e. the material is idealized as rigid-plastic.

The critical resolved shear stresses $\tau_y^{(i)} > 0$ representing dissipative internal forces that oppose slip are assumed to be governed by the evolution equations

$$\dot{\tau}_y^{(i)} = \sum_{j=1}^{I} H_{ij} |\nu^{(j)}| + \sum_{j=1}^{I} K_{ij} (\boldsymbol{s}^{(i)} \cdot \nabla)(\boldsymbol{s}^{(j)} \cdot \nabla) \nu^{(j)}, \tag{8}$$

where H_{ij} is a local hardening matrix. In (8) the terms $(\boldsymbol{s}^{(i)} \cdot \nabla)(\boldsymbol{s}^{(j)} \cdot \nabla)\nu^{(j)}$ introduce non-local effects; K_{ij} is a non-local hardening matrix. The gradient terms model short range interactions among dislocations. The attempts to specify the local and non-local hardening effects, based on a statistical treatment of ensembles of discrete dislocations [8–10], resulted in a whole spectrum of gradients and revealed the complexity of the problem. In [10] it is argued that the GND density tensor $\boldsymbol{\Lambda}$ is insufficient to describe the hardening process. The non-local interactions can be expressed as integral terms dependent on close range correlations among dislocations. However, specification of the correlation functions and an approximation of the integral terms by gradients remain an open problem. Therefore, the gradient term in (8) derived for parallel dislocation segments should be understood as a rough approximation.

3. Results and discussion

In summary: *a flow-adjustment boundary value problem* involves the following system of equations: the quasi static flow Eqs. (2), the constitutive Eq. (7) incorporating (6) and the equilibrium Eq. (5) accompanied by the evolution equations for $\boldsymbol{R}$ and $\tau_y^{(i)}$ given by (3) and (8). The problem has to be supplemented by initial and boundary conditions. The initial value of $\boldsymbol{R}(\boldsymbol{x},0)$ is either compatible, i.e. it corresponds to a gradient of a vector field, or $\boldsymbol{R}(\boldsymbol{x},0)$ is incompatible and the corresponding $\boldsymbol{\Lambda}(\boldsymbol{x},0)$ given by Eq. (4) represents the initial distribution of GNDs. Typical boundary conditions of high pressure torsion (HPT) experiments can be taken as an example. HPT process seen in the direction perpendicular to the torsion axis is approximately viewed as a plane-strain simple shear [11]. HPT sample can be idealized as an infinite slab of the height h. During deformation the bottom of the slab is fixed and the upper surface is driven by velocity $\rho\dot{\theta}$; ρ is the distance from the torsion axis, and $\dot{\theta}$ the rate of torsion angle per unit height of the specimen.

In a prospective incremental solution procedure for fields $\boldsymbol{R}_k$ and $(\tau_y^{(i)})_k$ known in the k-time step, the velocity field $\boldsymbol{v}_k$ can be evaluated in principle from Eqs. (2), (5)–(7). Then Eqs. (3) and (8) yield rates $\dot{\boldsymbol{R}}_k$ and $(\dot{\tau}_y^{(i)})_k$. The values $\boldsymbol{R}_{k+1}$ and $(\tau_y^{(i)})_{k+1}$ needed in the next time step δt_{k+1} are expressed as $\boldsymbol{R}_{k+1} = \boldsymbol{R}_k + \dot{\boldsymbol{R}} \delta t_{k+1}$ and $(\tau_y^{(i)})_k + (\dot{\tau}_y^{(i)})_{k+1} \delta t_{k+1}$. Let us note that assuming the constitutive equation of type (7) all slip systems become activated.

The outlined approach is designed to model a deformation substructure represented by the adjusted lattice. The substructure formation can be modeled as an instability of the homogeneous flow, e.g. [9]. However, similarly as the standard crystal plasticity, the flow model without the gradient terms in (8) predicts singular physically non-realistic substructure features: singular substructure orientation and zero size of their patterns. To reach a better agreement with the observations the model should be enriched by dislocation mechanisms which control the plastic flow. At present there is no unique recipe how to formulate an adequate model. In principle, in crystalline materials a spectrum of the mechanisms may be activated, however, for a particular instability mode and loading conditions usually one of the mechanisms becomes dominant, e.g. the width of persistent slip bands is controlled by an inner structure of the bands [12], the close range dislocation interactions control the orientation and size of misoriented patterns [9]. As an example, the outlined model is enriched by the statistically motivated higher gradients of slip rates introduced in the hardening Eq. (8). In Ref. [9] it has been shown that such gradient terms lead to a finite dislocation pattern size and a more realistic substructure misorientation. The line tension of dislocations introducing higher gradients through the dislocation line curvature seems to be another mechanism [13].

Nevertheless, in the outlined flow model an important ingredient is still missing. Besides the incorporated polar dislocation substructure, i.e. GNDs, there exist dipolar dislocation clusters not accompanied by the crystal lattice misorientations. They consist mainly of dislocation dipoles and loops (tangles, veins, walls), e.g. [12], which serve as a storage of dislocations and places of their annihilation and generation.

4. Conclusion

Using an allegory, a ductile material in a plastic regime tries to build a highway system of misoriented regions and lamellae of localized shear to minimize the energy cost of the plastic traffic. In the system the dipolar clusters serve as service stations which provide fresh carriers of plastic deformation and store or destroy out-of-service carriers (the dipolar clusters provide often a subsidiary service only, as polar boundaries can annihilate and generate glide dislocations as well). The art of metallurgy is to hinder the plastic traffic as much as possible and to allow it only at higher applied stresses and temperatures, but not to stop the traffic entirely. Hindering the traffic raises material strength, but stopping it could result in a dangerous brittleness.

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