A comparison between strain gradient crystal plasticity and discrete dislocation dynamics *

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SUMMARY. We focus on the multislip behaviour of a long crystalline metal strip sheared between two bodies impenetrable to dislocations. On the basis of this benchmark, we identify the material parameters of a strain gradient crystal plasticity model by comparison with the pseudo-experimental results obtained from discrete Dislocation Dynamics (DD) simulations. The strain gradient plasticity model consists of a flow theory version of the deformation theory model developed in [1]; the model is of the higher-order type (see, e.g., Kuroda and Tvergaard [2] and references therein) and, in the limit of vanishing material length scales, particularises to the crystal plasticity model of Pierce et al. [3], within the small strain range. The strain gradient model is implemented into a user element subroutine (`uel`) for the finite element code ABAQUS [4]. The employed DD code is that developed as reported in [5] and references therein. We shall interpret the DD results at the light of the strain gradient model, with particular reference to the role of the material length scales involved. We shall show that the latent hardening effect is very large, and crucial, at the microscale. Also, we shall address some numerical issues emerged both in the implementation of the strain gradient model and in the comparison.

1 INTRODUCTION

We focus on the boundary value problem consisting of the simple shear of a crystalline strip constrained between two bodies in which dislocations cannot penetrate, unbounded along x_1 and x_3, of height H along the x_2-direction (see Figure 1).

The crystal is characterised by incompressible isotropic linear elasticity, with shear modulus μ, and by B couples of slip systems (the total number of systems is then $2B$), each couple β consisting of two possible glides symmetrically oriented with respect to any plane of constant x_2 by an angle θ_β. The strip is sheared by applying to the plane $x_2 = H$ a uniform displacement equal to ΓH in the x_1-direction (so that Γ is the applied shear).

The standard boundary conditions read

$$u_1(x_2 = 0) = 0; \quad u_1(x_2 = H) = \Gamma H \tag{1}$$

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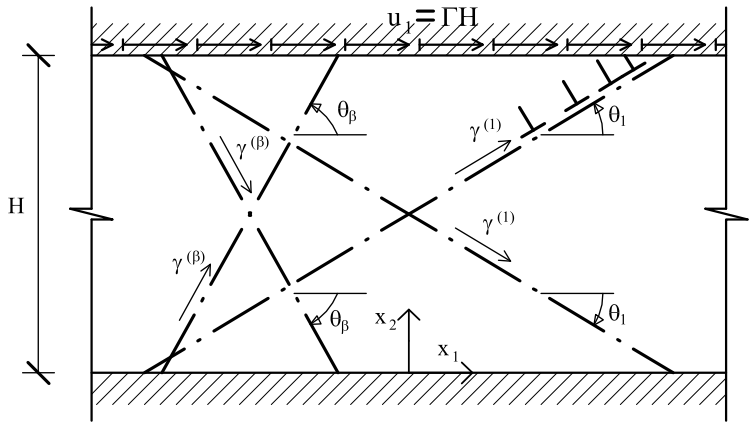

Figure 1: Simple shear of a constrained crystalline strip with multiple symmetric double slip systems.

$$u_2(x_2 = 0) = 0; \quad u_2(x_2 = H) = 0 \tag{2}$$

For this boundary value problem we aim at comparing the results of discrete Dislocation Dynamics (DD) simulations and strain gradient crystal plasticity.

We will first consider four strips of different height $H =$ (0.75 μm, 1.5 μm, 3. μm, 6. μm) endowed with one sole couple of systems inclined by $\theta_1 = \pi/8$. Then, we will analyse the effect of adding a second couple of systems inclined by an angle $\theta_2 = \pi/5$.

2 DISLOCATION DYNAMICS SIMULATIONS

DD simulations are run with the code developed as described, for instance, in Segurado et al. [5] (see also [6]). The model basically describes plasticity as the irreversible motion of dislocations into a linear elastic crystal. Dislocation glide, in our plane strain benchmark, is governed by:

$$v_\beta^i = \frac{b}{B_{\text{drag}}}\Big[\Big(\frac{\hat{\sigma}_{22} - \hat{\sigma}_{11}}{2} + \sum_{j\neq i}\frac{\sigma_{22}^j - \sigma_{11}^j}{2}\Big)\sin(2\theta_\beta) + \Big(\hat{\sigma}_{12} + \sum_{j\neq i}\sigma_{12}^j\Big)\cos(2\theta_\beta)\Big] \tag{3}$$

in which v_β^i is the velocity of the i dislocation on the β slip system, b is the Burgers vector length, B_{drag} is the drag coefficient, $\boldsymbol{\sigma}^i$ is the stress field exerted by the i dislocation in an unbounded medium, and $\hat{\boldsymbol{\sigma}}$ is the stress due to both the applied load and the image tractions applied at the boundary to make up for the use of the dislocation fields of the unbounded medium. At each time step along the loading history, $\hat{\boldsymbol{\sigma}}$ is obtained by means of a finite element analysis.

A random distribution of sources is set in the strip such that in any source a dislocation dipole nucleates when the resolved shear stress reaches the nucleation stress for a certain minimum lapse of time, called the nucleation time. Dislocations of opposite sign gliding on the same slip system are annihilated when they are closer than the so-called annihilation length. Dislocation pinning by obstacles is accounted for by a random distribution of obstacles where dislocations get blocked if their driving shear stress is lower than the obstacle strength.

The parameters involved in the simulation are set as follows: $b = 0.25$ nm, $B_{\rm drag}$ = 1.E-4 Ns/m^2, source density = 42 μm^{-2}, obstacle density = 126 μm^{-2}, nucleation stress = 25 MPa (with a standard deviation of 5 MPa), nucleation time = 0.01 μs, obstacle strength = 300 MPa, annihilation length $= 6b$, slip system spacing $= 100b$.

2.1 *The results of DD simulations*

The results of the analyses in which one sole couple of slip systems is considered show that, within the range of about $\Gamma \in [0, 0.01]$, decreasing the height H leads to an increase in strain hardening, while no strengthening (i.e., an increase in what is recognised as the initial yield stress) is observed.

The addition of a second couple of systems provides an extremely high latent hardening, as the stress-strain curve results higher than that with one sole couple for about the whole range of Γ considered. This means that the compliance introduced by the possibility of slip given by the second couple of systems is much less important than the obstruction to glide provided on the first (less inclined) couple of systems by dislocations nucleating on the second couple.

3 THE STRAIN GRADIENT CRYSTAL PLASTICITY MODEL

In order to describe the behaviour observed in the DD simulations, we exploit and extend the strain gradient crystal plasticity model developed in [1] (see also [7], [8], [9]). In fact, that model includes a higher-order coupling among different systems through the defect energy, defined as a quadratic function of Nye's dislocation density tensor (Nye [10], Gurtin [7]). However, preliminary simulations have shown that such a coupling is not enough in order to describe the DD results. Hence, we extend that strain gradient crystal plasticity by also including the standard latent hardening proposed by Pierce et al. [3].

In the boundary value problem described in section 1, within the context of crystal plasticity and contrariwise to the DD analyses, all the fields are independent on both x_1 and x_3 and for each couple β of slip systems the two slips are equal and we call both of them $\gamma^{(\beta)}$. The sole non-vanishing components of the plastic strain and Nye's tensor are, respectively:

$$\varepsilon^p_{12} = \sum_{\beta=1}^{B} \gamma^{(\beta)} \cos(2\theta_\beta) \qquad \alpha_{23} = 2\sum_{\beta=1}^{B} (\gamma^{(\beta)})' \sin^2\theta_\beta \tag{4}$$

where the symbol $'$ denotes a partial derivative computed with respect to x_2 and α_{23} expresses the Burgers vector component in the x_2-direction due to edge dislocations lying along x_3.

The standard balance equation states that both σ_{12} and σ_{22} must be spatially uniform. Then, the boundary conditions (2) imply that u_2 (and σ_{22}) must be zero everywhere, so that the problem is essentially uni-dimensional and henceforth, when possible, we will simplify the notation by dropping some indexes, as follows:

$$x \equiv x_2 \qquad \varepsilon^p \equiv \varepsilon^p_{12} \qquad \alpha \equiv \alpha_{23} \qquad \sigma \equiv \sigma_{12} \qquad u \equiv u_1 \tag{5}$$

and so on, as specified in the text when needed.

The displacement u can be expressed as

$$u' - 2\sum_{\beta=1}^{B} \gamma^{(\beta)} \cos(2\theta_\beta) = \frac{\sigma}{\mu} \tag{6}$$

The higher-order balance equations written in terms of kinematic variables read

$$\underbrace{H^{(\beta)}\left(\frac{\dot\gamma^{(\beta)}_{\rm eff}}{\dot\gamma_0}\right)^{N-1}\frac{\dot\gamma^{(\beta)}}{\dot\gamma_0}-L_\beta^2\tau_0\left[\left(\frac{\dot\gamma^{(\beta)}_{\rm eff}}{\dot\gamma_0}\right)^{N-1}\frac{\dot\gamma^{(\beta)\prime}}{\dot\gamma_0}\right]'}_{\text{dissipative hardening}}$$

$$\underbrace{-2\mu\ell^2\sin^2\theta_\beta\sum_{\kappa=1}^{B}\gamma^{(\kappa)\prime\prime}\sin^2\theta_\kappa}_{\text{energetic backstress}}=\mu\cos(2\theta_\beta)\Big[u'-2\sum_{\kappa=1}^{B}\gamma^{(\kappa)}\cos(2\theta_\kappa)\Big]\quad\forall\beta\,, \tag{7}$$

where $\dot\gamma^{(\beta)}$ is the slip rate of the system β and the standard part of the dissipative hardening involves the latent hardening of Pierce et al. [3]:

$$\dot H^{(\beta)}=\sum_{\kappa=1}^{B}H_{\beta\kappa}\dot\gamma^{(\kappa)}_{\rm eff}\,,\quad H^{(\beta)}(0)=\tau_0\,,\quad H_{\beta\kappa}=q\mathcal{H}(\lambda)+(1-q)\mathcal{H}(\lambda)\delta_{\beta\kappa} \tag{8}$$

$$\mathcal{H}(\lambda)=h_0\,\mathrm{sech}^2\,\frac{h_0\lambda}{\tau_s-\tau_0}\,,\quad \lambda=2\sum_{\beta=1}^{B}\int_{-\infty}^{t}\dot\gamma^{(\beta)}_{\rm eff}\,dt \tag{9}$$

with $\delta_{\beta\kappa}$ the Dirac delta, and τ_0, $\dot\gamma_0$, N, τ_s, h_0, q standard material parameters. For what concerns the higher-order terms, ℓ is an energetic length scale entering the defect energy for dimensional consistency, while two dissipative length scales, $L_\perp$ and L_N, are collected into

$$L_\beta=\sqrt{(L_\perp\sin\theta_\beta)^2+(L_N\cos\theta_\beta)^2} \tag{10}$$

entering the definition of effective slip rate:

$$\dot\gamma^{(\beta)}_{\rm eff}=\sqrt{(\dot\gamma^{(\beta)})^2+[L_\beta(\dot\gamma^{(\beta)})']^2} \tag{11}$$

The higher-order boundary conditions, essential to impose that dislocations are blocked when they reach the strip edges, in the case in which $L_\perp>0$ or $L_N>0$, are

$$\gamma^{(\beta)}(x_2=0)=0;\quad \gamma^{(\beta)}(x_2=H)=0\quad\forall\beta=1,\dots,B \tag{12}$$

For more details see [1].

Let us note that also Borg (see, e.g., [11]) extended the classical crystal model including latent hardening of Pierce et al. [3], but without including the energetic higher-order terms.

3.1 *Finite Element implementation*

The crystal model is implemented into a `uel` user subroutine for the commercial code ABAQUS [4]. We employ 2-noded isoparametric linear elements, both for the displacement u and the slips $\gamma^{(\beta)}$, $\beta=1,\dots,B$; hence, at each node there are $B+1$ independent variables. The time integration is based on the implicit Backward Euler scheme.

Many numerical issues have emerged from the implementation. For instance, the element size should decrease with the distance from the boundary, where dislocations pile-up and slip gradients

are maximum. For most analyses we have discretised the strip by means of 8000 elements (along its thickness).

The consistent jacobian turns out to be unsymmetric and diminishing the time increment is not necessarily beneficial, because the are terms of the jacobian components which go to infinity as the time step goes to zero. This unfavourable behaviour is emphasised as the exponent N governing the dissipation approaches to zero.

4 DISCUSSION AND CONCLUDING REMARKS

The DD results for the strips endowed with one sole couple of slip systems can be described by the strain gradient crystal plasticity model by appropriately setting the energetic length scale, which turns out to be $\ell \approx 0.6\mu$m. Dissipative higher-order terms seem to be unimportant in order to describe the DD results.

The parameter q governing the latent hardening is required to be set to values much higher than those established in conventional crystal plasticity, at sizes where dislocation pile-ups play a negligible role. Moreover, in order to have a latent hardening effect quantitatively similar to that observed in DD simulations by appropriately setting q, there is the need of choosing quite high values of N (e.g., $N = 0.5$), while for values of N lower than about 0.1 the effect of any q becomes unimportant for the description capability of the crystal model. In fact, at a given strain rate, in order to reproduce quite similar stress-strain curves, it is possible to change N if τ_0, τ_s, and h_0 are changed appropriately. However, values of N larger than 0.1 provide a relevant rate-dependence, which has been instead observed to be negligible in DD simulations.

Hence, our impression is that the strain gradient crystal plasticity model requires a further source of higher-order coupling between slips, as that provided by the defect energy set as quadratic function of Nye's dislocation density tensor seems to be too weak.

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