

Statistical aspects of discrete dislocation plasticity

A. Needleman^{a,*}, E. Van der Giessen^b, V.S. Deshpande^c

^a Division of Engineering, Brown University, Providence, RI 02912, USA

^b Department of Applied Physics, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

^c Engineering Department, University of Cambridge, Cambridge CB2 1PZ, UK

Received 15 July 2005; received in revised form 14 October 2005; accepted 24 October 2005

Available online 21 November 2005

Abstract

Discrete dislocation calculations suggest that statistical effects are important in the modeling of crystal plasticity. These include: (i) effects of source limited plasticity; (ii) statistical variations of dislocation sources and obstacles in small volumes; and (iii) the sensitivity of the discrete dislocation predictions to small perturbations. Implications of these for phenomenological constitutive models and for statistical theories of the collective behavior of dislocations are discussed.

© 2005 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Dislocation; Theory; Micromechanical modeling

1. Introduction

In plastically deforming crystals, the accumulation, interaction, and motion of large numbers of dislocations give rise to complex spatiotemporal dynamics, which may lead to organized dislocation structures including, for example, walls, cells, subgrains, and persistent slip bands. The characteristic length scales that are associated with the dislocation patterns lead to the now well-appreciated size dependence of plastic response at the micron scale.

Conventional plasticity theories predict a size independent response. A variety of non-local plasticity theories (mainly strain gradient constitutive formulations) have been proposed to account for the observed size dependence of micro-scale plastic flow in crystalline solids, e.g. [1–6]. The physical motivation for these typically stems from accounting, in a phenomenological relation, for the effects of geometrically necessary dislocations [7,8]. Irrespective of the precise formulation, one or more material length scales (typically taken to be constant) are introduced that either need to be extracted from experimental measurements or

deduced from meso-scale simulations. Another approach, e.g. [9,10], is to characterize the dislocation dynamics in terms of the statistics of the dislocation distribution. Such a formulation naturally contains length scales through a coupled set of transport equations for dislocation density fields. A closure condition is needed in such statistical theories to truncate the number of dislocation densities; for example, in theories involving two dislocation densities one is the total dislocation density and the other is a net-Burgers vector density [6].

Discrete dislocation simulations of plastic flow can be used in a variety of ways to assist the development of such more coarse-grained theories of plastic flow of crystalline solids in small volumes, for example: (i) to identify plastic deformation mechanisms, such as a size-dependent hysteresis effects, that are not incorporated in current phenomenological theories; (ii) to discriminate between competing theories; (iii) to identify parameters and boundary conditions for various phenomenological frameworks; and (iv) to provide a basis for choosing a closure condition in a statistical theory.

At small scales, statistical effects play an important role in the behavior predicted by discrete dislocation simulations: (i) the finite number of possible dislocation sources

* Corresponding author.

E-mail address: needle@brown.edu (A. Needleman).

mean that even if the stress and deformation state are such that plastic flow could occur, no dislocation source may be available to provide the needed dislocations; (ii) because of the limited number of dislocations present, the overall behavior can depend on the location of dislocation sources and/or obstacles to dislocation glide; and (iii) dislocation dynamics is inherently chaotic in the sense that the evolution of the dislocation structures is sensitive to unavoidable (and uncontrollable) small perturbations.

Here, we provide examples illustrating these effects using plane strain two-dimensional discrete dislocation plasticity and discuss their implications for coarse-grained modeling plastic flow in crystalline solids. We note that there are aspects of dislocation plasticity that cannot be modeled within the two-dimensional framework used in the analyses discussed here. For example, the scaling of the flow strength with the square root of the dislocation density in stage II hardening is not found with the current framework, but requires additional constitutive rules that incorporate appropriate planar representations of three-dimensional physical processes [11]. Three-dimensional discrete dislocation analyses can be carried out but due to the large computational demands what can be calculated is still quite limited, e.g. [12–17]. Furthermore, in some circumstances, the three-dimensional effects neglected in two-dimensional discrete dislocation plasticity play a secondary role and rather complex phenomena can be represented qualitatively and, to a remarkable extent, even quantitatively [18,19]. This agreement suggests that qualitative features concerning the statistical aspects of discrete dislocation plasticity seen in two-dimensional calculations may also hold in three dimensions.

1.1. Discrete dislocation formulation

We confine attention to a two-dimensional small strain discrete dislocation plasticity formulation with elastic isotropy. Plane strain conditions are assumed. Plastic deformation, when it occurs, is described by the nucleation and glide of discrete edge dislocations, represented as line singularities in an elastic medium, with Burgers vector b . Once dislocations nucleate, field quantities are computed using superposition. The singular (\sim) field associated with the N dislocations is calculated analytically from the infinite medium fields of the dislocations. The complete solution is obtained by adding an image (\sim) field that ensures that the boundary conditions are satisfied [20].

At the beginning of a calculation, the crystals are stress- and dislocation-free. New dislocation pairs are generated by simulating two-dimensional Frank–Read sources, randomly distributed on discrete slip planes, which generate a dislocation dipole when the magnitude of the Peach–Koehler force $f^{(I)}$ on source I exceeds a critical value $\tau_{\text{nuc}}b$ during a time period t_{nuc} . Each source is randomly assigned a nucleation strength, τ_{nuc} , from a Gaussian distribution with average $\bar{\tau}_{\text{nuc}}$ and standard deviation $\Delta\tau_{\text{nuc}}$. The sign of the dipole is determined by the sign of the resolved shear

stress along the slip plane while the distance between the two dislocations at nucleation, L_{nuc} , is taken such that the attractive stress field that the dislocations exert on each other is equilibrated by a shear stress of magnitude τ_{nuc} . Annihilation of two opposite signed dislocations on a slip plane occurs when they are within a material-dependent critical annihilation distance L_e . The magnitude of the glide velocity $V_{\text{gl}}^{(I)}$ along the slip direction of dislocation I is taken to be linearly related to the Peach–Koehler force $f^{(I)}$ through the drag relation $V_{\text{gl}}^{(I)} = f^{(I)}/B$, where B is the drag coefficient. Obstacles to dislocation motion are modeled as points associated with a slip plane, which pin dislocations as they try to pass until the Peach–Koehler force on the obstacle exceeds $\tau_{\text{obs}}b$.

2. Examples of statistical effects in plasticity

The following reference parameters are used in all the examples presented here: Young's modulus $E = 70$ GPa and Poisson's ratio $\nu = 0.33$; $b = 0.25$ nm; $\bar{\tau}_{\text{nuc}} = 50$ MPa; $\Delta\tau_{\text{nuc}} = 10$ MPa (except in the calculations of Section 2.2 where $\Delta\tau_{\text{nuc}} = 1.0$ MPa); $t_{\text{nuc}} = 10$ ns; $L_e = 6b$; $B = 10^{-4}$ Pa s; and $\tau_{\text{obs}} = 150$ MPa.

2.1. Source limited plasticity

All current continuum plasticity models assume that plasticity can occur at any point where the flow criterion is met. However, a necessary criterion for plasticity is that sufficient slip can be produced by the available dislocations. This in turn requires the presence of one or more dislocation sources close to the location where the flow criterion is met—this is not always the case. Here we give an example of source limited plasticity from discrete dislocation simulations of frictional sliding reported in [21].

The boundary value problem sketched in Fig. 1a represents the frictional sliding of a single crystal (three slip systems at $\phi = \pm 60^\circ$ and 0°) with respect to a rigid indenter of size a . The adhesive interaction between the crystal and indenter is modeled via the bi-linear shear traction T_t versus shear displacement Δ_t law (inset of Fig. 1a) with a maximum cohesive strength $\tau_{\text{max}} = 300$ MPa. The variation of the friction stress τ_{fr} (ratio of the frictional force to the contact area) is plotted in Fig. 1b as a function of the indenter size a for two choices of the source density $\rho_{\text{src}} = 72 \mu\text{m}^{-2}$ and $155 \mu\text{m}^{-2}$. For large contacts ($a \geq 10 \mu\text{m}$), τ_{fr} is approximately equal to the uniaxial tensile strength of the single crystals while $\tau_{\text{fr}} = \tau_{\text{max}}$ for small contacts. No dislocations are present in the crystal at small contact sizes even though $\tau_{\text{fr}} = \tau_{\text{max}} \gg \tau_{\text{nuc}}$. This is source limited behavior: in these small contacts no source is available in the high stress regions to nucleate dislocations. Of course, increasing the source density shifts this behavior with source limited behavior observed for $a \leq 0.5 \mu\text{m}$ and $0.2 \mu\text{m}$ for $\rho_{\text{src}} = 72 \mu\text{m}^{-2}$ and $155 \mu\text{m}^{-2}$, respectively.

Another type of source limited response is seen in the thin film simulations of Nicola et al. [22,23]. In this case,

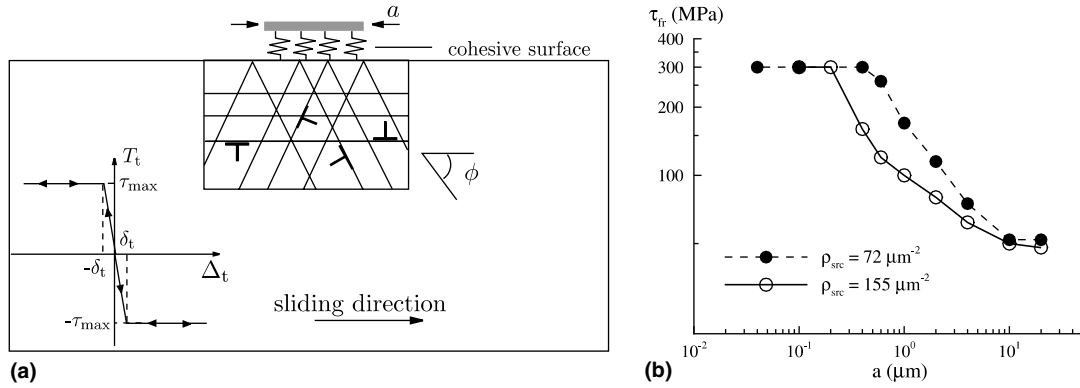


Fig. 1. (a) Sketch of the boundary value problem to investigate the static frictional resistance between a single crystal and a rigid indenter (the bi-linear adhesive relation employed in these simulations is shown in the inset) and (b) effect of source density on the friction stress versus contact size relation.

sources are available, but the dislocation structure that evolves gives rise to a back stress, which may become so large that it inhibits nucleation and an increased stress is required for nucleation. This back-stress-induced source limitation leads to enhanced size dependence in thin films and, in sufficiently small volumes, the effect on plastic flow is sensitive to the precise location of the dislocation sources.

2.2. Volume effects

Different realizations of initial distributions of dislocation sources and obstacles can have a significant effect on the plastic response of crystals, especially when the plastically deforming volume is small. We illustrated this effect via uniaxial tension calculations on single crystals with length to width ratios $L/W = 3$ and one active slip system at $\phi = 45^\circ$ (Fig. 2a), see [24] for further details. The flow strength σ_f of the crystals (defined as the average stress

between 4% and 5% nominal strain, $2U/L$) is plotted in Fig. 2b as a function of the specimen size W for crystals with initial source and obstacle densities equal to $56 \mu\text{m}^{-2}$. In an attempt to quantify the statistical variations, the calculations for each specimen size were performed for three spatial distributions of the sources and obstacles (all with the same overall source and obstacle densities). While the general trend that the flow strength decreases with specimen size remains unaffected, we observe that for large specimen sizes ($W = 4.0 \mu\text{m}$ and $8.0 \mu\text{m}$), σ_f values are nearly identical for the three realizations as there are approximately 10^4 dislocations in these specimens. On the other hand, there is about a 10% variation in σ_f for the $W < 0.4 \mu\text{m}$ specimens. In these specimens, two to ten dislocations are typically present at any stage of the deformation; the total number of dislocations nucleated scales approximately with the applied strain but the majority of dislocations have exited through the specimen sides. Thus, for a sufficiently small specimen, σ_f

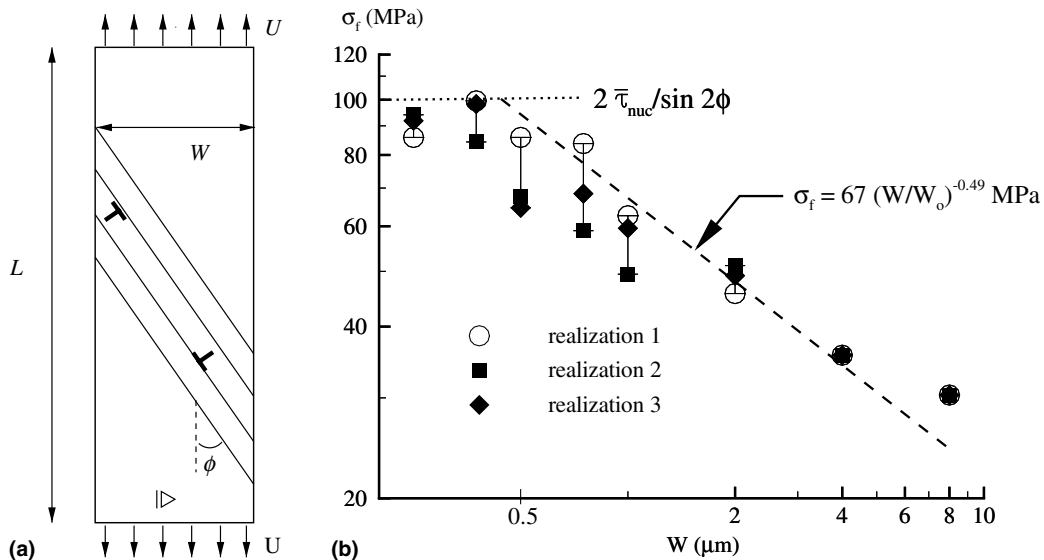


Fig. 2. (a) Sketch of the boundary value problem of the single crystal specimen subjected to uniaxial tension and (b) flow strength σ_f as a function of the specimen size W (W_0 is a reference size taken equal to $1.0 \mu\text{m}$).

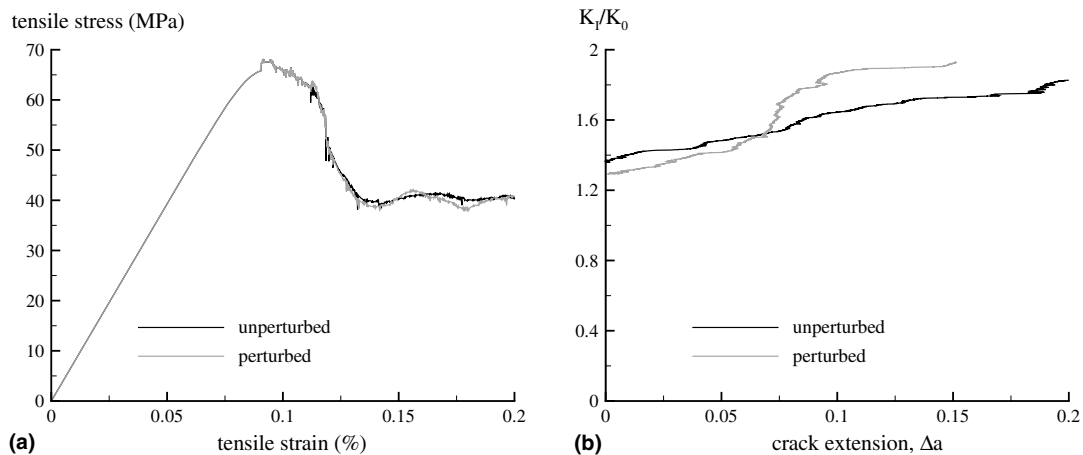


Fig. 3. (a) Uniaxial tensile stress versus strain response of a single crystal oriented for symmetric double slip and (b) applied normalized stress intensity factor K_I/K_0 versus crack extension Δa . Two calculations corresponding to (i) the unperturbed case and (ii) nucleation sites perturbed by $10^{-3}b$ are shown in each case.

is mainly governed by the nucleation stress τ_{nuc} and the variation in σ_f is due the variations in the minimum nucleation strengths in the different realizations. Variations in the values of σ_f are greatest for the intermediate size specimens with σ_f showing a 25% variation between the three realizations for the $W = 0.75 \mu\text{m}$ specimen. The strength of these specimens is governed by the structures formed by a relatively small number of dislocations and thus is sensitive to statistical variations.

2.3. Sensitivity to small perturbations

Hamiltonian systems involving nonlinear many-body interactions are known to exhibit chaotic behavior: for example, gravitationally interacting point masses, molecular dynamics, and vortex dynamics. Dissipative systems such as those characterized by the Lorenz equations can also exhibit chaotic behavior (or extreme sensitivity to small perturbations) and such effects have been observed in dislocation dynamics simulations [25]. The effect of the sensitivity of the discrete dislocation predictions to small initial perturbations in the source positions is illustrated in Fig. 3. The overall tensile stress versus strain response of a crystal ($W = 4.0 \mu\text{m}$) with two slip systems at $\phi = \pm 30^\circ$ is shown in Fig. 3a for two cases: (i) a reference case and (ii) a case with the location of the nucleation sites perturbed by at most $10^{-3}b$. The difference in the overall macroscopic response in this case is negligible even though the separation of the trajectories in the two simulations (measured by evaluating a norm $\|\delta\|$ based on the positions of dislocations) grew exponentially with time, see [25] for details. This can be contrasted with the crack growth resistance of the crystal, which depends on local conditions. In Fig. 3b, the crack growth resistance of a crystal is shown by plotting the normalized applied remote mode I stress intensity factor K_I/K_0 against the crack advance Δa (see [26] for details). The crack growth resistance varies significantly with perturbations of $10^{-3}b$ in the positions of the nucle-

ation sites. Thus, while the sensitivity of the discrete dislocation calculations to extremely small variations in initial conditions did not appreciably influence the overall tensile stress versus strain response, it did affect the crack growth resistance: the conditions for crack growth are determined at a very small length scale and are much more sensitive to local variations.

3. Implications for modeling of crystal plasticity

Both discrete dislocation simulations and experiments (see e.g. [27]) indicate that statistical effects can have a significant effect on plasticity in small volumes. However, discrete dislocation plasticity is computationally intensive, even in two dimensions. Therefore, phenomenological plasticity constitutive relations and statistical theories of collective dislocation behavior have a potentially important role to play, particularly when statistical effects are involved and calculations need to be carried out for a variety of realizations. Schemes that average the response over many realizations (conditional upon limited information on the sources, obstacles, etc.) could be developed, e.g. following recent ideas of Luciano and Willis [28], making the numerical prediction of statistical variations much more efficient.

Current phenomenological plasticity constitutive relations, including those that aim to model size-dependent plastic flow, are deterministic. Non-deterministic behavior can be obtained, e.g. [29,30], in the context of a structural instability. Discrete dislocation plasticity indicates that statistical effects, arising for a variety of reasons as discussed in Section 2, can be significant even in the absence of a structural instability. These statistical effects can be important in a variety of circumstances of much technological relevance, e.g. the growth of small fatigue cracks involves small plastic zone sizes where the statistical effects come into play. The current non-local plasticity theories focus on the size dependence arising from geometrically necessary dislocations and do not model features of plastic flow

in small volumes, such as source limited plasticity, which give rise to the statistical dependence. Statistical theories seem promising in being able to directly account for these effects. However, most current statistical theories use only two-point statistics and it remains to be seen whether they are sufficient to capture the effects revealed by discrete dislocation plasticity. Comparisons between discrete dislocation plasticity predictions and solutions from these statistical theories may be useful in identifying appropriate closure conditions.

Discrete dislocation calculations predict extreme sensitivity to small perturbations. While this has a negligible effect on the material behavior averaged over relatively large volumes (uniaxial tension), it may have a significant effect on behavior, such as crack initiation and growth, that depends on local fields. Understanding this sensitivity is key for differentiating between controllable experimental scatter and the inherent variability of material responses. Phenomenological reaction–diffusion representations of plastic flow [29,30] can exhibit chaotic behavior in certain circumstances due to the competition between dislocation nucleation and annihilation. Such effects have not yet been investigated using the more recently developed statistical models: the implications of these models for this type of behavior merit exploration.

Acknowledgement

A. Needleman is grateful for support from the Materials Research Science and Engineering Center on Micro-and-Nano-Mechanics of Electronic and Structural Materials at Brown University (NSF Grant DMR-0079964).

References

- [1] Hutchinson JW. *Int J Solid Struct* 2000;37:225.
- [2] Acharya A, Bassani JL. *J Mech Phys Solids* 2000;48:1565.
- [3] Fleck NA, Hutchinson JW. *J Mech Phys Solids* 2001;49:2245.
- [4] Gurtin ME. *J Mech Phys Solids* 2002;50:5.
- [5] Gao H, Huang Y, Nix WD, Hutchinson JW. *J Mech Phys Solids* 1999;47:1239.
- [6] Yefimov S, Groma I, Van der Giessen E. *J Mech Phys Solids* 2004;52:279.
- [7] Nye JF. *Acta Metall* 1953;1:153.
- [8] Ashby MF. *Philos Mag* 1970;21:399.
- [9] Groma I. *Phys Rev B* 1997;56:5807.
- [10] El-Azab A. *Phys Rev B* 2000;61:11956.
- [11] Benzerga AA, Bréchet Y, Needleman A, Van der Giessen E. *Modell Simul Mater Sci Eng* 2004;12:159.
- [12] Devincre B, Kubin LP. *Modell Simul Mater Sci Eng* 1994;2:559.
- [13] Schwarz KW. *J Appl Phys* 1999;85:108.
- [14] Zbib HM, de la Rubia TD, Rhee M, Hirth JP. *J Nucl Mater* 2000;276:154.
- [15] Weygand D, Friedman LH, Van der Giessen E, Needleman A. *Modell Simul Mater Sci Eng* 2002;10:437.
- [16] Han X, Ghoniem NM, Wang Z. *Philos Mag* 2003;83:3705.
- [17] Cai W, Bulatov VV. *Mater Sci Eng A* 2004;387:277.
- [18] Nicola L, Xiang Y, Vlassak JJ, Van der Giessen E, Needleman A, submitted for publication.
- [19] Chng AC, O'Day MP, Curtin WA, Tay AAO, Lim KM, *Acta Mat*, to be published.
- [20] Van der Giessen E, Needleman A. *Modell Simul Mater Sci Eng* 1995;3:689.
- [21] Deshpande VS, Needleman A, Van der Giessen E. *Acta Mater* 2004;52:3135.
- [22] Nicola L, Van der Giessen E, Needleman A. *J Appl Phys* 2003;93:5920.
- [23] Nicola L, Van der Giessen E, Needleman A. *Philos Mag A* 2005;85:1507.
- [24] Deshpande VS, Needleman A, Van der Giessen E. *J Mech Phys Solids* 2005;53:2661.
- [25] Deshpande VS, Needleman A, Van der Giessen E. *Scripta Mater* 2001;45:1047; see also Ananthakrishna G, Fressengeas C. *Scripta Mater* 2005;52:425; Deshpande VS, Needleman A, Van der Giessen E. *Scripta Mater* 2005;52:429.
- [26] Cleveringa HHM, Van der Giessen E, Needleman A. *J Mech Phys Solids* 2000;48:1133.
- [27] Espinosa HD, Prorok BC, Peng B. *J Mech Phys Solids* 2004;52:667.
- [28] Luciano R, Willis JR. *J Mech Phys Solids* 2005;53:1505.
- [29] Walgraef D, Aifantis EC. *J Appl Phys* 1985;58:688.
- [30] Kok S, Bharathi MS, Beaudoin A, Fressengeas C, Ananthakrishna G, Kubin LP. *Acta Mater* 2003;51:365.