Size and boundary effects in discrete dislocation dynamics: coupling with continuum finite element

Hasan Yasin a, Hussein M. Zbib a, Moe A. Khaleel b,∗

a School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164, USA
b Pacific Northwest National Laboratory, Virtual Prototyping and Engineering Simulations Laboratory, MS# K2-18, Richland, WA 99352, USA

Abstract

In this work, we develop a framework coupling continuum elasto-viscoplasticity with three-dimensional discrete dislocation dynamics (micro3d). The main problem is to carry out rigorous analyses to simulate the deformation of single crystal metals (fcc and bcc) of finite domains. While the overall macroscopic response of the crystal is based on the continuum theory, the constitutive response is determined by discrete dislocation dynamics analyses using micro3d. Size effects are investigated by considering two boundary value problems: (1) uniaxial loading of a single crystal cube, and (2) bending of a single crystal micro-beam. It is shown that boundary conditions and the size of the computational cell have significant effect on the results due to image stresses from free-boundaries. The investigation shows that surface effects cannot be ignored regardless of the cell size, and may result in errors as much as 10%. Preliminary results pertaining to dislocation structures under bending conditions are also given. Published by Elsevier Science B.V.

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1. Introduction

Recently, there have been significant advances in modeling plasticity phenomena using discrete dislocations dynamics models [1–3]. These models are based on basic deformation mechanisms and aim at predicting strength properties of metals at small length scales. However, the main difficulty in these models, among other things, lies in connecting the observed macroscopic parameters (used in continuum models), such as stress and strain, to the collective behavior of dislocation groups, and their interaction with particles and interfaces. While, within the continuum mechanics framework, the governing equations of the material response are developed based on a representative volume element (RVE) over which the deformation field is assumed to be homogeneous, the dislocation dynamics models are presumably capable of describing the heterogeneous nature of the deformation field within the RVE. It is suggested that with a proper homogenization theory, or field averaging, one can couple the discrete dislocation dynamics models with continuum approaches, and provide a rigorous framework for analyzing deformations at small scales, where surfaces and interfaces are of great importance in determining materials response. The idea was advocated by Van der Giessen and Needleman [6] by coupling two-dimensional (2D) discrete dislocations with a continuum finite element model. In the present work, we develop a computational model coupling our (3D) three-dimensional discrete dislocations model (micro3d) with a continuum finite element model based on an elastic–plastic model. The main motivation is to develop a multi-scale model for investigating small-scale plasticity phenomena and deformation of small-scale structure.

2. The multi-scale elastic–plastic model

2.1. The continuum elastic–plastic model

Generally, the material response is measured in terms of the macroscopic strain rate tensor \(\dot{\varepsilon}\) and its relation to the stress tensor \(S\). We consider a computational cell of a size in the order of a few tens of micrometers containing many dislocations and point defects (microcracks, stacking fault tetrahedral, Frank sessile loops, rigid particles, etc.). On the macroscale level, we assume that the material obeys the basic law of continuum mechanics, i.e. equations of equilibrium

\[
\text{div} \ S = 0
\]  

(1)
For elasto-viscoplastic behavior, the strain rate tensor \( \dot{\varepsilon} \) is decomposed into an elastic part \( \dot{\varepsilon}^e \) and a plastic part \( \dot{\varepsilon}^p \) such that
\[
\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p, \quad \dot{\varepsilon} = \frac{1}{2}[\nabla \mathbf{v} + (\nabla \mathbf{v})^T]
\] (2)

For most metals the elastic response is linear and can be expressed by the incremental form of Hooke’s law, i.e.,
\[
\dot{\mathbf{S}} = [\mathbf{C}^e][\dot{\varepsilon} - \dot{\varepsilon}^p]
\] (3)

where \( \mathbf{C}^e \) is a fourth order tensor. The main difficulty in the plasticity theory is the development of proper constitutive law for \( \dot{\varepsilon}^p \). More importantly, this law should be based on the underlying microstructure, mainly dislocations. Nonetheless, this task is perhaps formidable, especially when bridging two scales orders of magnitude apart, i.e. the continuum scale and the discrete dislocation scale. Here, we emphasize that the “assumed” constitutive nature of \( \dot{\varepsilon}^p \) and flow stress, and their dependence upon internal variables and gradients of internal variables is very critical, since they dictate, among other things, the length scale of the problem and the phenomena that can be predicted by the model. In this respect, it goes without question that the most rigorous and physically based approach of computing the plastic strain and strain hardening in metals, with their interaction with other defects and particles. A complete description of micro3d is given in many articles by Zbib and co-workers [4,5]. The result is a set of nonlinear differential equations governing the motion of the dislocation segments. The governing equation of motion for each dislocation segment is given by equation of the form [7]
\[
F(v) + \frac{v}{M(T,p)} = F_i, \quad F = \frac{1}{v} \left( \frac{dW}{dv} \right) \frac{\partial v}{\partial t},
\]
\[
m^* = \frac{1}{v} \left( \frac{dW}{dv} \right)
\] (4)

Here \( F = F(v) \) is the inertial force, \( M \) the mobility, \( F_i \) the force arising from interactions with other defects, from the Peierls barrier if present, and that produced by applied stresses, and \( W \) the total energy per unit length of a moving dislocation (elastic energy and kinetic energy). The driving force \( F_i \) is determined by first evaluating the total PK force which arises from all dislocation stress fields and the applied stress. The motion of each dislocation segment contributes to the overall macroscopic plastic strain rate tensor \( \dot{\varepsilon}^p \) and plastic spin \( \mathbf{W}^p \) via the relations
\[
\dot{\varepsilon}^p = \frac{1}{2V} \sum_{i=1}^{N} -l_i v_{gi} (n_i \otimes b_i + b_i \otimes n_i),
\]
\[
\mathbf{W}^p = \frac{1}{2V} \sum_{i=1}^{N} -l_i v_{gi} (n_i \otimes b_i - b_i \otimes n_i), \quad n_i = \hat{\nu}_i \times \xi_i
\] (5)

where \( l_i \) is the dislocation segment length, \( n_i \) a unit normal to the slip plane, \( V \) the volume of the simulated crystal or the RVE, \( b_i \) the Burgers vector, and \( N \) the total number of segments in the RVE.

2.3. The superposition principle — homogenous materials

The solution for the stress field of a dislocation segment is known for the case of infinite domain and homogeneous materials, which is used in DD codes. Therefore, the principle of superposition (developed by Van der Geisestein and Needleman [6] for the 2D case) is imposed to correct for the actual boundary conditions. Assuming that dislocation segments, dislocations loops and any other internal defects with self-induced stress, are situated in a finite domain \( \Omega \) bounded by \( \partial \Omega \), and subjected to arbitrary external traction and constraints. Then the stress, strain and displacement fields are given by the sum of two solutions, i.e. \( \mathbf{S} = \mathbf{S}^\infty + \mathbf{S}^* \), \( \mathbf{u} = \mathbf{u}^\infty + \mathbf{u}^* \), \( \varepsilon = \varepsilon^\infty + \varepsilon^* \), where \( \mathbf{S}^\infty \), \( \varepsilon^\infty \) and \( \mathbf{u}^\infty \) are the stress, strain and displacement fields, respectively, caused by the internal defects as if they were in an infinite domain, whereas \( \mathbf{S}^* \), \( \varepsilon^* \) and \( \mathbf{u}^* \) are the fields corresponding to the auxiliary problem satisfying certain displacement boundary conditions along with \( t = t^\infty \) on \( \partial \Omega \), where \( t^\infty \) is the externally applied traction, and \( t^\infty \) the traction induced on \( \partial \Omega \) by the defects (dislocations) in the infinite domain problem. The traction \( t^\infty \) on \( \partial \Omega \) results into an image stress which is superimposed onto the dislocations segments and, thus, accounting for surface-dislocation interaction. In passing, we note that the same method is extended to the case of dislocations in heterogeneous media [8].

2.4. Treatment of long-range stresses

Evaluation of the dislocations long-range stress field is computationally expensive (\( N^2 \) problem). A numerical technique termed as the superdislocation method, and based on the multipolar expansion method has been outlined by Zbib et al. (1998) which reduces the order of the problem to \( N \log N \). Here, we present another approach consistent with the finite element framework. The stress field induced by the dislocations contained within the RVE can be treated as
an internal stress $S^D$ (homogenized over the element with enough gauss points!). Then, the effective total stress within the RVE is the sum of the stress by all external agencies $S$ and the internal stress $S^D$. Hence, the constitutive equation in total form becomes

$$S + S^D = [C'][\varepsilon - \varepsilon^p]$$  \hspace{1cm} (6)

Since, the dislocation stress field varies as $1/r$, careful approximation of $S^D$ over the RVE is most important. One needs to consider high number of integration points to ensure high accuracy. The treatment of long-range stress using the internal stress concept results into a body-force vector in the finite element analysis (FEA) described in Section 2.5. This approximation works well for interaction among dislocations that do not reside in the same elements (in the FEA). The interaction of dislocations belonging to these elements must be computed one-to-one ($M^2$, $M$ = number of dislocation segments in a given element) as explained in this work.

2.5. The finite element formulation

The equations described before are re-written in total form as in Eq. (6), and the system of equations is then cast into a finite element framework leading to the standard form

$$[\mathbf{K}][\mathbf{U}] = \{f^a\} + \{f^B\} + \{f^\infty\} + \{f^p\}$$  \hspace{1cm} (7)

where $[\mathbf{K}]$ is the stiffness matrix, $\{f^a\}$ the applied force vector, $\{f^\infty\} = \int_{\Omega} [\mathbf{N}] \mathbf{d}s$ a force vector arising from dislocation image stresses, $\{f^\infty\} = \int_{\Omega} S^\infty [\mathbf{B}] \mathbf{d}v$ a body force vector from dislocations long-range interaction, $\{f^\infty\} = \int_{\Omega} [C'][\varepsilon^p][\mathbf{B}] \mathbf{d}v$ a body-force like vector from plastic strain caused by dislocations, $[\mathbf{N}]$ a vector containing the shape functions, and the matrix $[\mathbf{B}]$ the gradient of $[\mathbf{N}]$. Dislocations are sorted out in each element, and they contribute to the plastic strain in Eq. (5).

The solution of Eq. (7) yields, among other things, the total stress field $S$ which includes the effect of applied loads, image stresses and the “homogenized” dislocation stresses. However, as mentioned above, dislocation–dislocation interaction is very strong for dislocations that are close to each other, and the homogeneous stress $S^D$ in this case is not accurate. Therefore, for a dislocation segment “$i$” residing in an element “$k$” which contains $M$ dislocation segments, the PK force is computed as follows:

$$F_i = \sum_{j=1}^{M} \left( \sigma^D_j \cdot \mathbf{b}_i \right) \times \xi_i + (S_k - S^D_k)$$

$$\times \xi_i + F_{i,i+1} + F_{i,i-1}$$  \hspace{1cm} (8)

where $\sigma^D_j$ is the stress field of dislocation “$j$”, $S_k$ the stress state in element $k$ as obtained from the FE analysis, $\xi_i$ the line sense vector, and $F_{i,i+1}$ and $F_{i,i-1}$ the interaction forces between segments $i$ and $i + 1$, and $i$ and $i - 1$, respectively. This way, the interaction among dislocations in the same element is treated explicitly (note that the homogeneous stress $S^D_k$ must be subtracted, otherwise there will be a double counting of the PK force!).

Fig. 1. Effect of free surfaces on dislocations: (a) initial configuration (dislocation loop); (b) stress contours of image stresses; (c) Peach–Kohler force on dislocation loop from self-force and image stresses.
2.6. The multi-scale plasticity model

The two models, DD model and the solid mechanics problem are coupled and the result is a multi-scale model which has the following features: (a) couples the continuum problem with the dislocation dynamics problem; (b) deals directly with boundary conditions, especially image stresses; (c) incorporates shape changes associated with dislocation motion and distortions; (d) incorporates directly dislocation long-range stresses, and (e) incorporates lattice distortion (elastic) that arise from dislocations.

3. Results and discussion

The effect of the free surface, i.e. the image stresses, on the behavior of a dislocation line, a square dislocation loop, a circular dislocation loop with different dimensions and parameters, and a random distribution of Frank–Read sources was thoroughly investigated [9]. Here, we give some representative results. We consider aluminum single crystal with the following properties (relevant to both the continuum model and the DD model): \( \mu = 26.6 \text{MPa} \); \( v = 0.334 \); \( \rho_m = 2800 \text{kg m}^{-3} \); \( b = 2.862 \times 10^{-10} \text{m} \), and \( M = 100.0 \text{Pa}^{-1} \text{s}^{-1} \) (dislocation mobility). The 3D box (various sizes were simulated ranging from 1000b to 10,000b) was divided into a finite element mesh using eight-node elements (mesh size ranged from 5\( \times \)5\( \times \)5 to 20\( \times \)20\( \times \)20), and was fixed at its lower four corners and constant extension rate was imposed on the upper surface.

The results given in Fig. 1 are for the interaction of a dislocation loop with free surfaces. Fig. 1(a) shows a contour plot of image stresses. The self-force of the loop is plotted in Fig. 1(c). Also, PK force caused by the image stresses on the dislocation loop is given in Fig. 1. These calculations show that the loop in the (1 \( \bar{1} \) 1) plane in a 1000b

![Fig. 2.](image) (a) Dislocation sources in the initial configuration; (b) dislocations start to move; (c) the difference in the yield strength when applying the free-boundaries effect and when ignoring it; (d) effect of box size.
(2.86 μm) aluminum single crystal with a Burgers vector of [110] propagates, if the initial configuration diameter of the loop is greater than 90.7% of the computational cell planer size. This ratio, of course, depends on the crystal structure, loop plane direction and Burgers vector direction. In all the simulations we performed, dislocation segments in the simulation cell near the free boundaries tend to move towards the boundary and annihilate. For example, a square dislocation loop on a (1̅11) plane 100b (28.6 nm) above the center of a 20,000b (5.72 μm) aluminum single crystal with a Burgers vector of [110], the numerical results show that when the loop size is greater than 86.5% of the
computational cell (crystal) size, the surface effect is greater than the self-force of the loop. Otherwise, the self-force effect is greater and the loop would collapse on itself as expected.

Next, we examine the effect of free surfaces on the predicted stress–strain curve. Frank–Read sources were distributed randomly with random length ranging from 4000b (1.144 μm) to 6000b (1.716 μm) in a cubic aluminum single crystal (Fig. 2(a)) with side dimension of 20,000b (5.72 μm). All the dislocation sources were placed on parallel (1 1 1) planes for a random distribution of three different Burgers directions of [1 1 0], [1 0 1] and [0 1 1]. The crystal was loaded under constant strain rate of 10 s\(^{-1}\) in the [0 0 1] direction, and the base was totally fixed in all directions.

Fig. 2(b) illustrates the behavior of the dislocations with time; the dislocation sources start operating when the resolved shear stress on the dislocation reaches the critical shear stress. Fig. 2(c) shows the difference between the strength of the crystal when the free-boundary effect is applied and when it is neglected. The percentage difference is 8% calculated at 0.05% yield strength. For the same dislocation source distribution, inside a 20,000b (5.72 μm) sub-domain cubic space, the size of the crystal was increased to 22,000b (6.29 μm), 30,000b (8.58 μm) and 40,000b (11.44 μm) to investigate the variation of the free-boundary effect with the crystal size. It is useful to define an aspect ratio ζ = B/A, where B is the size of the crystal and A the size of the sub-domain where all the dislocation sources are initially situated. In this study, A is taken to be fixed and equal to 20,000b (5.72 μm) while B is increased. Two methods were followed to investigate the size effect: (1) by evaluating the strain–strain curve based on the whole crystal size, and (2) by taking the properties based on the size of A. No significant difference in the result was found. The result summarized in Fig. 2(d) shows that the percentage difference in the 0.05% yield strength when the free surfaces are taken into account and when they are neglected. The difference decreases as the aspect ratio increases, implying that as far as the initial macroscopic yield stress is concerned, the effect of the free surface can be neglected when the initial sources are far enough from the free surfaces. But this is not true at large strain as can be deduced from Fig. 2(c). This leads to the conclusion that it does not matter how large the simulation cell B is with respect to the sub-domain A, one cannot simply neglect the effect of the boundaries of cell B on the dislocations in sub-domain A.

Finally, we give preliminary results pertaining to the dislocation behavior during the bending of a thin sheet single crystal Al oriented as shown in Fig. 3. The sheet is simply supported and loaded as shown in the figure (with load distribution of 120 MPa) (dimensions are given in the figure). Dislocations are initially situated on parallel (1 1 1) planes which are parallel to the loading plane as shown in the figure. Fig. 3(b) shows the distribution of shear stress. The shear stress is maximum at the edges of the sheet, and reduces towards zero at the center of the sheet. This results into a zone where the shear stress is not high enough to keep the dislocations moving, resulting in a zone where the dislocations pile-up.

In conclusion, a numerical model coupling 3D discrete dislocation dynamics with continuum finite element model based on elasto-plasticity has been developed. By using the super-position principle, dislocation-surface interaction is computed numerically. It is shown that one can’t simply neglect these surface effects regardless of the simulation cell size. Although, the interaction between dislocations and surfaces can be small when they are very far apart, there is a progressive surface effect that is transmitted to those dislocations through the dynamics of near-surface dislocations. Also, by using the finite element method, one can reduce the computation of dislocation long-range stress to that of an internal stress, provided an extreme care is taken with the homogenization of the dislocation stress field over the RVE.

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References