Discrete dislocation dynamics simulations in a cylinder

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Abstract. Mechanical properties of material are closely related to the motion of dislocations, and predicting the interactions and resulting collective motion of dislocations is a major task in understanding and modelling plastically deforming materials. A discrete dislocation dynamics model is used to describe the orientation substructure within the microstructure. Discrete dislocation dynamics simulations in three dimensions have been used to examine the role of dislocation multiplication and mobility on the plasticity in small samples under uniaxial compression. In this paper we describe the application of the dislocation dynamics simulations in a cylindrical geometry. The boundary conditions for the simulation were estimated from the distribution of the geometrically necessary dislocation density which was obtained from the orientation map. Numerical studies benchmark could validate the accuracy of the algorithms and the importance of handling the singularity correctly. The results of the simulation explain the formation of the experimentally observed substructure.

1. Introduction

Material mechanical properties, such as strength and deformation of crystalline materials, are largely determined by underlying mechanisms involving various crystal defects, such as vacancies, interstitials and impurity atoms, dislocations, grain boundaries, heterogeneous interfaces and micro-cracks, chemically heterogeneous precipitates, twins and other strain-inducing phase transformations. Among all of them, dislocations, which provide a useful link between crystal defects in atomic scales and the macroscopic response of crystals, are the most attractive form of defects for worthwhile study. Most often, dislocations define plastic yield and flow behaviour, either as the dominant plasticity carriers or through their interactions with the other strain-producing defects [1, 2].

Because of the multiplicity and complexity of the mechanisms of dislocation motion and interaction, it is nearly impossible to develop a quantitative analytical approach for understanding and mimicking these problems. The situation is further complicated by the need to trace the spatio-temporal evolution of a large number of interacting dislocations over long periods of time, as is required for the calculation of plastic response in a representative volume element. Such practical intractability of the dislocation-based approaches, together with the developing needs of material engineering at the nano- and micro-length scales, has created the current situation where the equations of crystal plasticity used for continuum modelling are phenomenological and largely disconnected from the physics of the underlying dislocation behaviour.

Fortunately, with the advancement in computational technology with bigger and faster computers, bridging the gap between dislocation physics and continuum crystal plasticity has become possible. In order to mimic the dislocation motions, various discrete dislocation dynamics models have been developed over the last two decades. In the 1990s, development of new computational approaches of
dislocation dynamics in three-dimensional space (3D) generated hope for a principal breakthrough in our current understanding of dislocation mechanisms and their connection to crystal plasticity [3-5], however, complications relate to dislocation multiplications, self-interactions and interactions with other defects, and keeping track of complex reactions and mechanisms have provided new challenges for developing efficient computational algorithms. To overcome these challenges, many researchers have been dedicated to devise the dislocation dynamics analysis and its computer simulation modelling over the past decade and they achieved significant progress in dealing with the problems [3, 6]. This progress has been further magnified by the idea to couple dislocation dynamics with continuum mechanics analysis in association with computational algorithms such as finite elements.

Our long term goal is to develop a physics-based multi-scale modelling hierarchy, validated and verified, to address outstanding questions regarding materials microstructure and mechanical properties. Small-scale structures offer opportunities for direct comparison between modelling and experiment at previously inaccessible scales. Discrete dislocation dynamics simulations in 3D have been used to examine the role of dislocation multiplication and mobility on the plasticity in small samples under uniaxial compression [5-8]. The experiments provide data for validation of models, and the models provide a path for new, physically based understanding and prediction of materials behaviour.

The focus of this article is on showing progress in simulation code development, and comparison of the simulation results with experiment to validate the code [9, 10]. In the following, we firstly present the principles of dislocation dynamics analysis and introduce the simulation procedure. Then we show some simulation results and compare to the experiments. Finally, in the conclusion section, evaluations and our long term project objectives are provided.

2. Theoretical Fundamentals of the Method

2.1. Dislocation Equation of Motion

A dislocation is a line defect in an otherwise perfect crystal described by its line sense vector $\xi$ and Burgers vector $b$. Under loading, dislocations glide and propagate on slip planes causing deformation and change of shape. When the local line direction becomes parallel to the Burgers vector, the dislocation may propagate into other slip planes. This switching of the slip plane, which makes the motion of dislocations three dimensional, is better known as “cross slip”, and is an important recovery phenomena to be dealt with in dislocation dynamics.

The dynamics of the dislocation is governed by a Newtonian equation of motion, consisting of an inertia term, damping term, and driving force arising from short-range and long-range interactions. The dislocation dynamics approach attempts to incorporate all of the kinematics and kinetics aspects into a computational traceable framework. It is possible to represent smooth dislocations with any desired degree of realism, provided that the discretization resolution is taken high enough for accuracy. In such a representation, the dynamics of dislocation lines is reduced to the dynamics of discrete degrees of freedom of the dislocation nodes connecting the dislocation segments.

The velocity $v$ of a dislocation segment $s$ is governed by a first order differential equation consisting of an inertia term, a drag term and a driving force vector [11, 12], such that

$$m_s \ddot{v} + \frac{1}{M_s(T,P)} v = F_s$$

with $m_s = \frac{1}{v} \left( \frac{dW}{dv} \right)$

$$F_s = F_{Peirel} + F_D + F_{Peirel} + F_{External} + F_{Obstacle} + F_{Image} + F_{Osmotic} + F_{Thermal}$$

In the above equation the subscript $s$ stands for the segment, $m_s$ is defined as the effective dislocation segment mass density, $M_s$ is the dislocation mobility which could depend both on the
temperature $T$ and the pressure $P$, and $W$ is the total energy per unit length of a moving dislocation (elastic energy plus kinetic energy). As implied by (1), the glide force vector $F$, per unit length arises from a variety of sources described in the previous paragraph.

2.2. Discrete Dislocation Equation of Motion

Equation (1) applies to every infinitesimal length along the dislocation line. In order to solve this equation for any arbitrary shape, the dislocation curve may be discretized into a set of dislocation segments. Then the velocity vector field over each segment may be assumed to be linear and, therefore, the problem is reduced to finding the velocity of the nodes connecting these segments. There are many numerical techniques to solve such a problem. For example, a straight dislocation segment $s$ is defined to be bounded by two nodes $j$ and $j+1$. Then within the finite element formulation, the velocity vector field is assumed to be linear over the dislocation segment length. This linear vector field $v$ can be expressed in terms of the velocities of the nodes such that $v = [N^D]^T V^D$, where $V^D$ is the nodal velocity vector and $[N^p]$ is the linear shape function vector [13].

Upon using the Galerkin method, equation (1) for each segment can be reduced to a set of six equations for the two discrete nodes (each node has three degrees of freedom). The result can be written in the following matrix-vector form,

$$[M^D] V^D + [C^D] V^D = F^D $$

(3)

where

$$[M^D] = m_s \int [N^D] [N^D]^T dl $$

is the dislocation segment 6x6 mass matrix,

$$[C^D] = (1/ M_s) \int [N^D] [N^D]^T dl $$

is the dislocation segment 6x6-damping matrix, and

$$F^D = \int [N^D] F dl $$

is the 6x1 nodal force vector.

2.3. Evaluation of Plastic Strains

The motion of each dislocation segment gives rise to plastic distortion, which is related to the macroscopic plastic strain rate tensor $\dot{\varepsilon}^P$, and the plastic spin tensor $W^P$ via the relations

$$\dot{\varepsilon}^P = \sum_{s=1}^{N_s} \frac{I_s V_{gs}}{2V} (n_s \otimes b_s + b_s \otimes n_s) $$

(4)

$$W^P = \sum_{s=1}^{N_s} \frac{I_s V_{gs}}{2V} (n_s \otimes b_s - b_s \otimes n_s) $$

(5)

where $n_s$ is a unit normal to the slip plane, $V_{gs}$ is the magnitude of the glide velocity of the segment, $V$ is the volume of the representative volume element and $N_s = N_t \times n^t$ is the total number of segments. Another microstructure quantity, the dislocation density tensor $\alpha$, can also be calculated according to

$$\alpha = \sum \frac{I_s}{V} b_s \otimes \xi_s$$

(6)
This quantity provides a direct measure for the net Burgers vector that gives rise to strain gradient relief.

2.4. Modifications for Finite Domains
The solution for the stress field of a dislocation segment is true for a dislocation in an infinite domain and for homogeneous materials. While, in order to account for finite domain boundary conditions, the method for solving 3D problems involving free surfaces and interfaces developed by Zbib et al. is used [1, 14]. In this paper we perform discrete dislocation dynamics simulations of plasticity at small scales, with consideration of the influences from the free surfaces via a boundary-element method. Cross-slip motion of the dislocation was also included, and found to be critical to the modelling of the dislocation behaviour. Examination of details of the dislocation mechanism illuminates many features unique to small samples and points directly to the importance of both the surface forces and cross-slip in understanding small-scale plasticity.

3. Results and discussion
Recently, a study from Uchic et al. presented the size effects in compression of 1.0μm diameter metal samples [9, 10]. Cylindrical pillars with varying radii were machined with a focused ion beam (FIB) from single-crystal bulk samples and compressed by a blunted nano-indenter. This pioneering work spurred similar activities from several groups, with studies on a range of sample sizes, from sub-micron to tens micron. In the study reported here, we use our three dimensions dislocation code “Dis3D” to simulate the mechanical behaviour of Ni single crystals under uniform compression and compare our results to the results of experiments.

For the simulations in this work, the material properties of nickel used were: shear modulus $\mu = 76$ GPa, Poisson’s ratio $\nu = 0.31$ and lattice constant $a = 0.35$ nm. The dislocation mobility is taken to be $10^{-10}$ Pa$^{-1}$ s$^{-1}$ in the calculations, and other parameters were from references [5, 9, 10]. To investigate the effects of loading direction, as well as to make a direct comparison with the experimental results of Dimiduk et al. [10], we also prepared three 1.0 μm samples oriented in the [2 6 9] direction. For the single-slip case, only the $1/2[101](\overline{1}11)$ slip dislocation system has the maximum Schmid factor (equal to 0.48). For the multi-slip case, eight slip systems are active, each with the same Schmid factor of 0.41, whereas the other four slip systems have zero Schmid factors and are inactive.

![Figure 1](image.png)

**Figure 1.** Comparison of stress-strain curves of simulation (a) and experiment [10] (b).
The stress–strain behaviour for all simulations based on 1.0 \( \mu m \) samples is shown in Figure 1, while the equivalent experimental results for single-crystal nickel are shown. From Figure 1 we can see that the flow stress of the multi-slip simulations (from the [0 0 1] samples) and the single-slip simulations (from the [2 6 9] samples) are both similar to each other and agree well with the experimental results, which employed loading along the [2 6 9] single-slip direction.

In Figure 2 we show a series of stress-strain curves from samples with different diameters under uniaxial compression in the absence of loading gradients. These results illustrate pronounced dependence on size, smaller samples having higher strength.

4. Conclusions
The dislocation dynamics approach developed over the past decade has overcome many hurdles and established a useful framework for predictive simulations. In order to expand the range of engineering and scientific issues that can be addressed, the dislocation dynamics models should become more realistic and computationally efficient. There are still many unanswered questions regarding size-dependent strengthening in small volumes, such as the critical size for transition from bulk behaviour and the role that dislocation structures and mechanisms play in determining that critical size.

In this paper discrete dislocation dynamics simulations in three dimensions have been used to examine the role of dislocation multiplication and mobility on the plasticity in small samples under uniaxial compression. Numerical studies benchmark the accuracy of the algorithms and the importance of handling the singularity correctly. Further investigations are planned for larger samples based on our simulation framework to address these questions. As our research was just a start, we calculate some benchmark to validate the code and to understand the material evolvement procedure. Our goal is to develop a more sophisticated model to predict the mechanical behaviour of microcrystals over a wide range of sizes.

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