# Representation of Dislocation Dynamics Simulations

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## ABSTRACT

The dislocation content of each active slip system in a crystal is defined by its Dislocation Density Vector (DDV). Each DDV possesses signed screw and edge components having lengths equal to the length per unit volume of all dislocations of like sign lying in the slip plane, projected parallel and perpendicular, respectively, to the slip direction. The length of the DDV is proportional to the length/unit volume of dislocations of like sign and its orientation is a measure of the edge-screw character of the population. To demonstrate this representation, we analyze a simulation of a micropillar of single crystal Ni deformed in compression. Finally, we discuss possible extensions of the analysis to determine parameters characterizing the motion of the distribution.

## 1. Introduction

To provide input from DD simulations into crystal plasticity (CP) codes the discrete dislocation distributions produced by the former must be characterized by variables that capture the resultant length and character of the distributions on each operative slip system. Constitutive equations can then be constructed for CP codes that employ these variables in the description of deformation at larger length scales. In order to calculate the dislocation distortion and its rate associated with a DD simulation, an appropriate representation of the density of mobile dislocations on active slip systems is required. Quantities based on the edge-screw character of the population on a slip system [1] and on the rose of the direction of the dislocation structure [2] have been proposed. The dislocation density vector (DDV) description proposed by Hartley is directly related to the Nye tensor component [3] associated with dislocations on the relevant slip system. In addition, the DDV definition incorporates the concept of signed quantities [4] that represent the sense of the dislocation segments that contribute to the DDV representation. This work applies the DDV definition to the description of dislocation ensembles created by simulation of the deformation of a Ni single-crystal micro-pillar using the ParaDis DD code [5].

## 2. Dislocation Density Vector

The dislocation content of a volume element containing dislocations is described by the Nye tensor, $\alpha$, giving the net Burgers vector flux, $\mathbf{B}$, of dislocations intersecting a section plane with $\mathbf{n}$ as its unit outward normal: $\mathbf{B} = \alpha \cdot \mathbf{n}$. It is convenient to define signed quantities for each slip system employing a dislocation coordinate system based on $\eta$, a unit vector parallel to the Burgers vector, $\mathbf{b}$; the normal to the slip plane, $\mathbf{v}$; and the Taylor axis, $\xi$. Define the senses of the vectors such that $\mathbf{v} = (\xi \times \eta)$ points towards the extra half plane of a positive edge dislocation with unit tangent vector, $\mathbf{t} \parallel \xi$. The sign associated with a pure screw dislocation is + or − according to whether $\mathbf{t}$ is parallel or anti-parallel to $\eta$. The unit tangent

vector of the i$^{th}$ mixed dislocation is $\mathbf{t}^{(i)} = \boldsymbol{\eta}\cos\psi^{(i)} + \boldsymbol{\xi}\sin\psi^{(i)}$, where $\psi^{(i)}$ is the acute angle between $\mathbf{t}^{(i)}$ and $\boldsymbol{\eta}$. The contribution of this mixed dislocation to $\mathbf{B}$ is

$$\mathbf{B}^{(i)} = \left(\mathbf{b}\otimes\mathbf{t}^{(i)}\right)\cdot\mathbf{n} = \mathbf{b}\left[\left(\boldsymbol{\eta}\cdot\mathbf{n}\right)\cos\psi^{(i)} + \left(\boldsymbol{\xi}\cdot\mathbf{n}\right)\sin\psi^{(i)}\right], \tag{1}$$

illustrating the influences of the orientation of slip system relative to the section plane and the character of the intersecting dislocation. The value of $\mathbf{B}$ due to N dislocations crossing unit area normal to $\mathbf{n}$ follows from summing the contribution of each:

$$\mathbf{B} = \left[\mathbf{b}\otimes\sum_{i=1}^{N}\mathbf{t}^{(i)}\right]\cdot\mathbf{n} = \mathbf{b}\left(\boldsymbol{\eta}\sum_{i=1}^{N}\cos\psi^{(i)} + \boldsymbol{\xi}\sum_{i=1}^{N}\sin\psi^{(i)}\right)\cdot\mathbf{n} \tag{2}$$

whence it is evident that the individual terms in the sums will have signs determined by the sense of the screw or edge components. Signed values of these sums are defined by summing separately those containing like signs. Writing $N_{S\pm}$ and $N_{E\pm}$ for the number of unit tangent vectors with positive and negative screw (S) and edge (E) segments and replacing each sum of terms with like signs by its average value gives the definition of the signed components of the dislocation density vector:

$$\boldsymbol{\rho}^{\pm S} = \left(N_{\pm S}\cos\overline{\psi}^{\pm S}\right)\boldsymbol{\eta} \text{ and } \boldsymbol{\rho}^{\pm E} = \left(N_{\pm E}\sin\overline{\psi}^{\pm E}\right)\boldsymbol{\xi}. \tag{3}$$

The dislocation density vector components due to segments of like sign are the vector sums of the edge and screw components with like sign and their orientation is determined by the relative magnitudes:

$$\left|\boldsymbol{\rho}^{\pm}\right| = \sqrt{\left(\left|\boldsymbol{\rho}^{\pm E}\right|\right)^2 + \left(\left|\boldsymbol{\rho}^{\pm S}\right|\right)^2} \text{ and } \overline{\Psi}^{\pm} = \tan^{-1}\left(\left|\boldsymbol{\rho}^{\pm E}\right|/\left|\boldsymbol{\rho}^{\pm S}\right|\right) \tag{4}$$

Clearly for a dislocation population with no net Burgers vector the magnitudes of the positive and negative components of the DD vector will be equal and their orientations will be anti-parallel.

To analyze the results of DD simulations to obtain the dislocation density vector associated with each active slip system, it is necessary first to identify all dislocations present with respect to their slip system and sense. The DDV in each slip system is then determined by performing counts for each slip system separately as follows. First two sets of equally spaced section planes are generated normal to $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$. Since all dislocations in the slip system will lie in planes normal to $\mathbf{v}$, they will not intersect section planes in this orientation. The intercept densities of positive and negative dislocations with each section plane is then determined. The average positive and negative dislocation intercept density for planes normal $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$, are $N_{S\pm}$ and $N_{E\pm}$, respectively. Finally, the length and orientation of the dislocation density vector for each signed set on the slip system is calculated from from equation (4).

## 3. Simulation Results

We now apply the DDV definition to the description of dislocation ensembles developed from the DD simulation of a Ni single-crystal tetragonal micro-pillar having dimensions 2.8x2.8x11.3 μm and an initial dislocation density of $10^{13}$ m$^{-2}$. The initial dislocation structure was composed of Frank-Read sources having random sizes, randomly distributed on the 12 slip systems in the simulation cell. The average dislocation segment length used in discretizing dislocation lines was 170$b$. The micropillar simulations were performed under a compressive load with a constant uniaxial strain rate of 50 s$^{-1}$ along [41$\overline{3}$]. Complete description of the DD computations may be found in [6].

Calculations were performed on a snapshot of the dislocation microstructure after 16000 simulation time steps. Fig. 1 shows convergence of the computation for positive DDV

components as a function of Burgers vector magnitude, $|b|$, normalized by the spacing between the sectioning planes, $h$. Components of the negative DDV show similar behavior. It is clear that the positive DDV magnitudes and orientation converge quite fast as the number of sectioning planes increase. The maximum error is only about 5% when the spacing of section planes $h = 600b$, which is more than 3 times the average dislocation segment length used in the DD simulations.
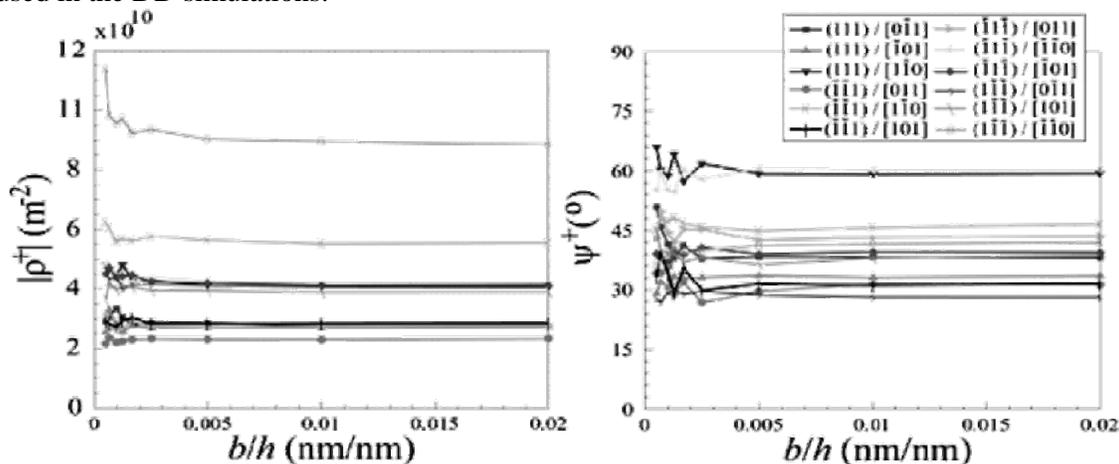


Figure 1. Convergence of the positive dislocation density vector components as a function of the Burgers vector magnitude normalized by the spacing between the section planes.

Fig. 2 shows the evolution of the magnitude and orientation of the positive and negative dislocation density vectors as a function of simulation time step. These calculations employ a sectioning plane spacing of $h = 400b$. and were made on dislocation structure snapshots after 1, 100, 1000, 10000, 15000 and 16000 time steps, respectively.
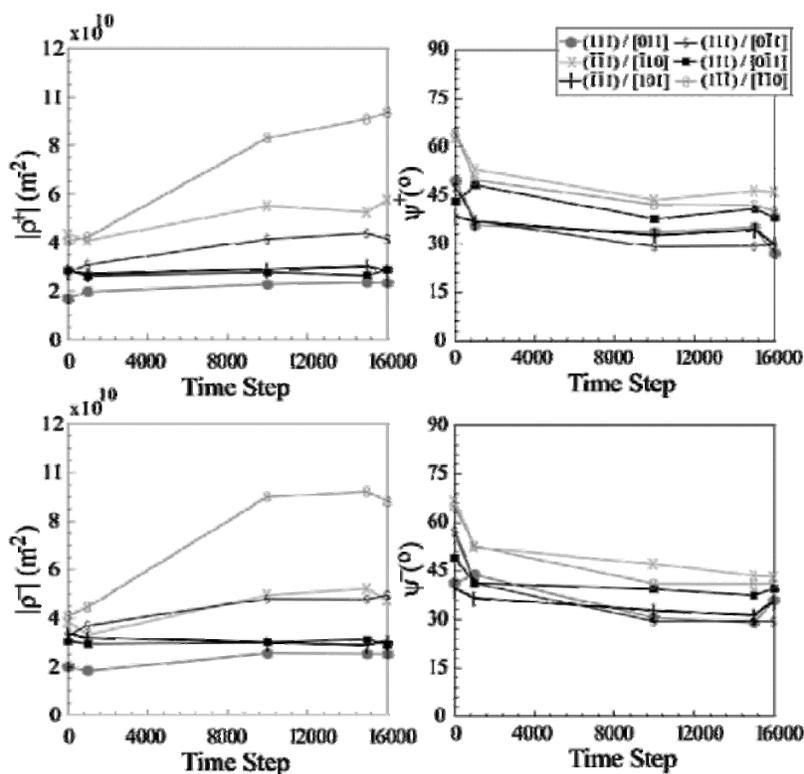


Figure 2. The evolution of the magnitude and orientation of positive and negative dislocation density vectors as a function of simulation time step.

## 4. Discussion and Conclusions

It should be noted that continuous fluctuations in the dislocation density are not captured in Fig. 2 since the current computations have been only computed at specific time steps. The fluctuations can be calculated if the current analysis were performed at each simulation time step. In addition, since the crystal is oriented for single slip most dislocation activities are observed on the slip plane with the highest Schmid factor, the $(1\bar{1}\bar{1})/[\bar{1}10]$ slip system. This can be observed in Figure 2 from the continuous increase in the magnitude of the positive and negative dislocation densities. In addition, we can observe that the orientations of the DDVs do not change significantly with the extent of deformation in these calculations.

The DDVs calculated in this work apply to the entire dislocation content of the micro-pillar. The origin of the DDVs should be placed at the centroid of the sample. Subdividing the simulation volume into sub-regions affords the possibility of determining the variation in dislocation content throughout the specimen. In that case the DDVs calculated should be placed at the centroid of the volume from which they were obtained. Further resolution of the characteristics of the distribution can be obtained by calculating the centroid of the intersections of positive and negative dislocations with section planes and locating the associated DDVs for the volume sampled at the appropriate centroid.

The DDV provides a convenient and compact means of describing the evolution of dislocation structure in dislocation dynamics simulations. It provides information on the relative content of positive and negative segments and on the edge-screw character of the dislocation population. Experiments that follow the evolution of the DDV for various simulation conditions should be useful to provide quantitative information that can be used in constructing constitutive relations for crystal plasticity calculations based on these simulations. Experiments based on this premise are currently under way.

## Acknowledgements

## References

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