A preliminary investigation of dislocation cell structure formation in metals using continuum dislocation dynamics

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Abstract. A continuum dislocation dynamics model capable of capturing the cellular arrangements of dislocations in deformed crystals is presented. A small strain formulation of the model is given, followed by sample results of stress-strain behaviour, dislocation density evolution, dislocation cell pattern, lattice rotation, and geometrically necessary dislocation density and strain energy density distributions. An important finding of the current work is that dislocations form patterns under all circumstances due to their long range interactions. It is found, however, that the famous cell structure pattern forms when cross slip is activated. It is also found that cells are 3D sub-regions surrounded by dislocations walls in all directions, and they form, disappear, and reappear as a result of the motion of cell walls and formation of new walls by cross slip. It is further found that the average cell size is connected with the applied resolved shear stress according to the similitude principle observed in related experiments. The importance of these results is briefly discussed in the context of recrystallization.

1. Introduction
Cellular dislocations patterns in deformed metals are important in understanding recrystallization because these patterns define the mesoscale energy and dislocation density distributions required to understand nucleation and crystal growth behaviour. In spite of many attempts to model cell structure formation in metals from the first principles of dislocation mechanics, capturing this structure remained a challenge to the mechanics and materials science communities for a long time. Early research on dislocation based plasticity was carried out from a continuum mechanics point of view, where dislocations were regarded as a measure of incompatibility of plastic distortion [1]. In this view, a tensor field called dislocation density tensor is proposed to characterize the dislocations ensembles in crystals [1,2]. Discrete Dislocation Dynamics (DDD) simulation [3] was introduced later as a means to model plasticity but it proved to be limited computationally. The ideas proposed earlier by Kröner [1] and Nye [2] regarding the representation of dislocations by a tensor density were later elaborated by Acharya and co-workers [4,5] into a field theory of dislocation mechanics in which the evolution equation for the dislocation density tensor is closed with constitutive specification of the velocity field. This work was adopted by Chen and co-workers [6] who captured a fractal dislocation structure in crystals relaxed after introducing random plastic distortions. Another approach to model dislocations from the perspective of statistics was carried out for 2D [7,8] and 3D [9,10] situations. In the 3D cases, the dislocation line orientation was an essential ingredient of the formulation because it defines cross slip processes and short range reactions such as annihilation [9,11].
In this paper, we summarize a newly developed 3D model of Continuum Dislocation Dynamics (CDD) [12] and report some results that are relevant to recrystallization. The model is based on a vector representation of the dislocation densities corresponding to individual Burgers vectors. The dislocation density evolution is governed by a set of kinetic equations, one for each Burgers vector. These equations are coupled to crystal mechanics via Orowan’s law for plastic shear strain, which is expressed in terms of the dislocation density and velocity, and the stress field driving the dislocation density evolution. The paper is organized as follows. The model is briefly summarized in Section 2 followed by a brief discussion of the numerical scheme in Section 3. Sample results are given in section 4, including dislocation density evolution, stress-strain behaviour, cell structure, and the lattice rotation and elastic energy distributions at the mesoscale. The paper ends with some remarks related to the importance of the current work in the context of recrystallization.

2. Continuum dislocation dynamics model
Consider a crystal undergoing small deformation where the kinematics of deformation is linearized. Consider also dislocations on a single slip system. The (partial) dislocation density tensor $\mathbf{\alpha}$ associated with dislocations on this slip system can be defined as the curl of the plastic distortion, $\mathbf{P}$, associated with these dislocations:

$$\mathbf{P} = -\nabla \times \mathbf{\alpha}.$$  

(1)

While this equation was originally derived for the overall dislocation density and plastic distortion tensors [1], it applies to individual slip systems in the case of linearized kinematics. The time derivative of the above equation gives the change of the dislocation density tensor:

$$\dot{\mathbf{P}} = -\nabla \times \dot{\mathbf{\alpha}}.$$  

(2)

Assuming that at a continuum point there are dislocations of the same line orientation, an assumption that is relaxed latter, the rate of plastic distortion can be obtained by Orowan’s law in tensor form:

$$\dot{\mathbf{P}} = -\mathbf{v} \times \mathbf{a},$$  

(3)

where $\mathbf{v}$ is the local dislocation velocity. Insertion of equation (3) into equation (2) generates the equation that governs the evolution of dislocation density tensor in terms of the velocity field:

$$\dot{\mathbf{\alpha}} = \nabla \times (\mathbf{v} \times \mathbf{a}).$$  

(4)

Because the dislocation density tensor locally contains dislocations of the same line orientation, called here a dislocation bundle, it can be written following Nye [2]:

$$\mathbf{a} = \mathbf{\rho} \otimes \mathbf{b},$$  

(5)

where $\mathbf{b}$ is Burgers vector and the vector $\mathbf{\rho}$ is defined as:

$$\mathbf{\rho} = \rho \xi,$$  

(6)

where $\rho$ represents the number density of dislocation lines within the bundle and $\xi$ is the local line direction. Equation (4) and (5) can be combined to yield the kinetic equation in terms of the dislocation density vector $\mathbf{\rho}$,

$$\dot{\mathbf{\rho}} = \nabla \times (\mathbf{v} \times \mathbf{\rho}).$$  

(7)

Equation (7) preserves the form of equation (4) and serves as the main kinetic equation in the model. It is pointed again here that equation (7) only applies to one slip system under the assumption that at every point there exists only one line direction. The kinetic equation derived here tracks dislocation
bundles gliding on their slip planes. Cross-slip can be easily incorporated into this description by simply changing the direction of velocity field.

The plastic distortion \( \beta^p \) is the quantity that connects the dislocation kinetics with the crystal deformation. For a given slip system, it can be written as:

\[
\beta^p = \gamma S,
\]

where \( \gamma \) is the plastic shear strain and \( S = n \otimes b / b \), with \( b \) and \( n \) being Burgers vector (with magnitude \( b \)) and slip plane normal. The evolution law for plastic slip is given by Orowan’s relation:

\[
\dot{\gamma} = -v \times \rho.
\]

Equation (7) and equation (9) are used together in the model to evolve the dislocation density field and the corresponding plastic distortion tensor. The latter gives the eigenstrain [13] required to solve the elastic boundary value problem for stress.

In order to include cross-slip, \( \rho \) is separated into two parts: \( \rho^{CS} \) and \( \rho^G \) with the former corresponding to cross-slip density and the latter corresponding to the gliding density. For screw dislocations whose density vector is \( \rho \), the amount of dislocations that cross-slip in a time step \( \delta t \) can be written as:

\[
\delta \rho^{CS} = (\dot{\rho}^{CS}) \delta t = \delta \rho_{CS} \rho,
\]

where \( \dot{\rho}^{CS} \) is the cross-slip probability rate. Equation (7) can thus be rewritten into two parts:

\[
\dot{\rho}^G = \nabla \times (v^G \times \rho^G),
\]

\[
\dot{\rho}^{CS} = \nabla \times (v^{CS} \times \delta \rho^{CS}),
\]

where the velocity fields \( v^G \) and \( v^{CS} \) are dislocation velocities on slip plane and cross-slip plane, respectively. In a similar fashion, the plastic shear rate on glide and cross-slip planes are updated by the following equation:

\[
\dot{\gamma}^G n^G / b = -v^G \times \rho^G,
\]

\[
\dot{\gamma}^{CS} n^{CS} / b = -v^{CS} \times \delta \rho^{CS}.
\]

where \( \dot{\gamma}^G \) and \( \dot{\gamma}^{CS} \) represent the plastic shear strain on glide and cross-slip planes, respectively.

In both equation (11) and equation (12), \( \delta \rho^{CS} \) depends on the cross-slip probability, \( \delta \rho_{CS} \), which is based on a number of conditions. It is expressed in the form:

\[
\delta \rho_{CS} = l_0 l_1 l_2 \delta \dot{\rho}.
\]

The indicator functions \( l_0 \), \( l_1 \), and \( l_2 \) are used to check for the cross-slip conditions. An indicator is set to be 1 if the condition is satisfied and 0 otherwise. \( l_0 \) checks whether the dislocation orientation is within a small range of orientation deviation (15° [14]) from the screw orientation; \( l_1 \) checks whether the resolved shear stress (RSS) on the cross-slip plane is larger than its value on the glide plane; \( l_2 \) is evaluated by a Monte Carlo scheme, in which a random number between 0 and 1 is generated. If \( \delta \rho_{CS} \) is larger than the random number \( l_0 \), \( l_1 \), \( l_2 \) is set equal to 1.

During numerical solution of the hyperbolic equations (7) numerical errors accumulate and the density ceases to satisfy the divergence free condition,

\[
\nabla \cdot \rho = 0.
\]
One way to enforce this condition at all times during the solution is to enforce it numerically by adding it to the equations to be solved.

To close the kinetic equations (7) and (12) the velocities $v^G$ and $v^{CS}$ are required. The dislocation velocity vector takes on the form:

$$v^G = v^G \zeta^G$$

on the glide plane and:

$$v^{CS} = v^{CS} \zeta^{CS}$$

on the cross slip plane, with $v^G$ and $v^{CS}$ being the magnitude of the velocities and $\zeta^G$ and $\zeta^{CS}$ the velocity directions, which are perpendicular to the dislocation lines.

The stress field $\sigma$ that acts as a driving force for dislocations satisfies the equilibrium condition:

$$\nabla \cdot \sigma = 0 ,$$

where the stress tensor $\sigma$ is linearly related to the elastic strain tensor, which is the total strain minus the plastic strain. As such, the equilibrium equation can be rewritten in the form:

$$\nabla \cdot [C : (\varepsilon^{tot} - \varepsilon^p)] = 0 ,$$

where $C$ is the elastic tensor in Hooke’s law, $\varepsilon^{tot}$ the total strain, and $\varepsilon^p$ the plastic strain. Now by assuming that dislocations exist on all slip systems, the plastic distortion tensor, when summed over all slip systems, provides the desired plastic strain tensor in equation (18):

$$\varepsilon^p = \text{sym} \sum_{\phi=1}^{N_s} \beta^p_{\phi} = \text{sym} \sum_{\phi=1}^{N_s} \gamma^\phi S^\phi ,$$

where $N_s$ is the number of slip systems, and $\beta^p_{\phi}$, $\gamma^\phi$ and $S^\phi$ are the plastic distortion, plastic shear and Schmidt tensor on slip system $\phi$, respectively. In the current formulation, $\varepsilon^{tot}$ is decomposed into two parts, a perturbation $\hat{\varepsilon}$ superposed on an average field $\overline{\varepsilon}$. The latter is the control parameter for loading. These two strains correspond to displacement of different characteristics. The gradient of an average displacement $\overline{u}$ gives the average strain while the gradient of the perturbation displacement $\hat{u}$ is the perturbation strain. With this in mind, equation (18) is further rewritten as:

$$\nabla \cdot [C : (\text{sym}(\nabla \overline{u}) + \overline{\varepsilon} - \text{sym}(\beta^p))] = 0 ,$$

where the perturbation displacement $\hat{u}$ is the unknown fields to be solved for. The stress field obtained from the solution of equation (20) is used to determine the magnitude of velocity on each slip system via the resolved shear stress expression,

$$\tau_{\phi} = \sigma : S_{\phi} = (\sigma n_{\phi}) \cdot b_{\phi} ,$$

and the mobility law,

$$v_{\phi} = M \tau_{\phi} ,$$

with $M$ being the mobility coefficient. The numerical value of $M$ shown in table 1 includes $b$ already.

### 3. Numerical schemes

The solution proceeds as follows at a given time step: with a specified velocity field, equation (11) is solved to evolve dislocations on each slip system. The area swept by dislocations over their glide planes is integrated by Orowan’s law (12) giving the plastic distortion. Equation (19) gives the plastic strain, which is subsequently used in the equilibrium equation (20). The solution of equation (20)
provides the stress field which is resolved on each slip systems to generate a velocity field for the next times step. The kinetic equations (11) are hyperbolic and describe the evolution of the dislocation density field through the transport of dislocation lines. We choose a first order implicit time discretization to handle the time derivatives.

A least square finite element method (LSFEM), which suits well for the first order differential operators [15], is selected to solve the equation after time discretization. The equilibrium equation (20) is solved using a Galerkin finite element method [16]. During the simulation, the stiffness matrix of the final linear systems for equation (20) remains unchanged and only the loading vector varies. So an LU decomposition of the stiffness matrix can be implemented at the beginning of the simulation and reused afterwards. Equations (12) are ODEs which will be solved using a two-step Adam-Bashforth method. The finite element mesh used in the solution is customized to form a superlattice of the FCC crystal. The space is first partitioned into octahedral and tetrahedral elements and each octahedron is split into two pyramids. The faces of such an octahedron are parallel to slip planes and edges are parallel to Burgers vectors; see [12] for details. The mesh size in the current case is on the order of 20 nm, which is chosen in the range of annihilation distance of dislocations of opposite Burgers vectors. The time step for the simulation is adaptive and its value is determined according to the magnitude of the dislocation velocity. The average time step is around 6 ns which is about 10 times larger than the one used in discrete simulation [17].

4. Results and discussions
In this section some sample results from the simulation of a bulk of copper single crystal under tensile loading in the [001] direction are presented. The crystal is first populated with random dislocation loops and relaxed. The loops size is on the order of the simulation box or larger and so they appear as large curved segments arranged so as to conserve the Burgers vector for each slip system. Periodic boundary conditions are enforced. The loading is applied on the crystal by updating the applied strain \( \varepsilon \) in the [001] direction at a strain rate of 30/s. All of the 12 slip systems are activated. The parameters used in the simulation are listed on table 1. We note that the cross slip probability value is relatively high so as to accelerate the effect of cross slip. This value can be calibrated using DDD simulations of cross slip and analysing the resulting rates in a continuous fashion [18].

![Table 1. Simulation parameters.](image)

The total dislocation density \( \rho_{\text{tot}} \) at a point is given by:

\[
\rho_{\text{tot}} = \sum_{\nu} \| \rho^\nu \| ,
\]

where \( \rho^\nu \) is the dislocation density vector corresponding to a given Burgers vector and the total number of Burgers vector is \( N_{\text{BV}} = 6 \). The volumetric average of \( \rho_{\text{tot}} \), denoted here by \( < \rho_{\text{tot}} > \), defines the average dislocation density at a given strain. The average dislocation density for various
Burgers vectors is denoted by $\rho_{\alpha i}$ ($i=1,2,...,6$). Using a similar notation, the average stress along the loading direction, $\sigma_{33}$, is obtained by the volumetric average of stress component $\sigma_{33}$.

The stress-strain curve and average dislocation density are plotted in figure 1(a). The characteristic hardening regime starts right after yielding which happens at about 100 MPa. The value of the yield strength is sensitive to the details of cross slip and short range reactions. Not all such reactions are included in the model at this point. Glissile junction formation, for example, is still missing in the model. The flow stress, both the initial yield point value and the instantaneous values in the hardening regime, is above the experimental values. Several factors might contribute to this difference. For example, the strain rate implemented here is much higher than that in the real experiment, which is usually less than or close to $10^{-3}$/s. Secondly, the material is treated as isotropic in the simulation, which is not true for single FCC crystal. An investigation shows that the anisotropic treatment causes the yielding point to drop about one third of the value calculated by the isotropic treatment [19]. In addition, the value of cross slip probability is high, which leads to frequent cross slip events that lead to rapid dislocation density multiplication. Lastly, glissile junction formation, which provide alternate paths for crystal shearing, is absent in the model.

Figure 1. (a) Applied stress and average dislocation density versus strain. (b) Cell structure at 1% strain. The dislocation density on the colour bar is in units of m$^{-2}$.

The dislocation density evolution shown in figure 1(a) indicates that the density evolves mainly on the 8 slip systems oriented for slip. On the other hand, the density does not evolve on the slip systems with Burgers vectors normal to the loading axis. This result is consistent with the DDD simulation of copper. It has been observed that the dislocation density distribution in the crystal gradually changes from the initial random distribution to a cell structure following the initial yielding of the crystal. Figure 1(b) shows the spatial distribution of the dislocation density in the crystal at 1% strain. The cell pattern is already obvious at this level. As mentioned earlier, 3D cells form once cross slip is activated. The partial density patterns corresponding to different Burgers vectors look different from the one shown in figure 1(b). Namely, the cells associated with dislocations of a given Burgers vector do not appear to be completely surrounded by dense dislocation walls. This implies that cells form by cooperation of dislocations on multiple slip systems.

Several deformation factors are important in the context of recrystallization [20,21]. These include the local lattice misorientation, the distribution of the dislocation density shown above and its geometrically necessary density (GND) distribution, and the distribution of elastic strain energy in the crystal. Misorientation determines the likelihood of a subgrain becoming a nucleus and influences the speed of its boundary during growth – it is known that the stored elastic energy, which is relieved by
recrystallization, is a part of the thermodynamic driving force. A robust simulation of crystallization should thus start from the end of the deformation stage with a 3D map of the deformed state of the crystal with the stored energy distribution. One of the goals of the current work is to demonstrate that such deformed state maps are possible to obtain once the deformation itself is properly modelled. As such, some of the relevant fields are shown here.

The elastic lattice rotation under deformation fixes the lattice misorientation. The lattice rotation vector, $\Omega_k$, is defined by

$$\Omega_k = (e_{ikl} \omega_{kl}) / 2 ,$$

where $\omega_{kl}$ is the rotation tensor. The latter is the skew symmetric part of the elastic distortion. The direction of vector $\Omega_k$ is the axis about which a lattice point rotates. In order to visualize this vector, each component of it is linearly mapped to the RGB value which ranges from 0 to 255. A colour map is formed based on the final RGB values for all components of $\Omega_k$. In this scheme, if the rotational axis of a point is mostly toward $+x$ direction, the colour at the point is purely red. Likewise, purely green colour and blue colour represent $+y$ and $+z$ directions, respectively.

The colour map of lattice rotation is plotted in figure 2 both for the 3D body (figure 2 (a) and for the top surface of the crystal (figure 2(b)). In figure 2(b), the norm of the dislocation density tensor, which measures the geometrically necessary dislocations (GND) density, is superposed in black and white on the RGB map. It is seen that, by crossing the GND wall, the lattice rotation changes its direction (the gradual transition of colour around dark lines in figure 2) and that, within GND cells, the lattice rotation is almost the same. It is also noted that the GND density is mostly concentrated in the cell walls. The current preliminary analysis thus shows that it is the GND distribution that is tied with the lattice misorientation [22], and that capturing the GND distribution is an important mesoscale aspect of both deformation and recrystallization.

It is to be noted here that GND is responsible for the elastic strain energy distribution in crystals. The elastic strain energy density is plotted in figure 3. In doing so, the applied stress is first subtracted from the stress tensor with the remaining part referred to as internal stress tensor, $\sigma^I_{ij}$. The internal elastic energy density, $E^I$, is then estimated from:

$$E^I = \frac{1 + \nu}{2E} \sigma^I_{ij} \sigma^I_{ij} - \frac{\nu}{2E} \sigma^I_{ij} \sigma^I_{ij} ,$$

Just as the distribution of total dislocations, the internal energy distribution is highly inhomogeneous, which can be seen clearly from figure 3 (a). Although the pattern of $E^I$ differs from that of $\rho_{tot}$, the former quantity tends to be at high values around dislocation walls (figure 3 (b)). The reason for this is obvious – the dislocation walls represent the regions where the GND density is significant and the elastic strain (stress) is highest where GND is highest. The stress (elastic strain) state of the walls is thus important if we are to use this information in the context of post-deformation behaviour of metals. A distinctive difference between $E^I$ and $\rho_{tot}$ patterns is that the elastic energy decays much slower away from dislocation-dense area, which is due to the long range nature of dislocation elastic fields.

5. Conclusions

A continuum dislocation dynamics model capable of capturing dislocation cell structure has been presented. The model is based on coupled dislocation kinetics and crystal mechanics equations, and it is able to capture the dislocation density evolution, cell structure formation, stress-strain behaviour, and all other internal fields required to understand, say, recrystallization of deformed metals. The preliminary results show that cross slip is a necessary mechanism for cell structure formation and that the cells form and become smaller in size according to the empirical similitude rule. It is also shown that the GND distribution in the crystal is concentrated in the dislocation walls and that the GND
density clearly marks the lattice misorientation in the crystal. The elastic strain energy distribution in the crystal is found to be highest within and near the cell walls.

**Figure 2.** RGB colour representation of lattice rotation. A red colour means the lattice rotation vector along the $x$ direction, green in the direction of $y$, and blue in the direction of $z$. A body visualization is shown in (a) and a (001) plane cross section in (b). The latter is plotted together with the GND pattern represented by the norm of the dislocation density tensor. It is clear that the non-trivial values of GND are associated with the points of significant lattice misorientation.

**Figure 3.** Internal elastic energy distribution at strain = 0.5% plotted in 3D cube (a) and on (001) plane (b). The pattern of total dislocation density $\rho_{\text{tot}}$ is shown along with the energy distribution in figure (b). It is seen that the elastic energy distribution is highly inhomogeneous and tends to take on larger values near dislocation walls.

We remark here that unloading simulations should be performed to estimate the residual stress tensor in order to come up with the right value of elastic energy density. For now thus, expression (25) should be considered an approximate, albeit reasonably accurate, estimate of the residual elastic energy density. We further remark that the model currently applies to small deformation cases (few %
strain), and that an extension of the model to finite deformation situations is required to simulate realistic deformation conditions encountered in real experiments. Finally, the model still requires a calibration of parameters used to represent cross slip and short range reaction rates, which can be accomplished using discrete dislocation dynamics simulations.

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