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A Continuum Formulation of Stress Correlations of Dislocations in Two Dimensions

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The Continuum Dislocation Dynamics theory (CDD) of crystal plasticity, utilizing a second-order dislocation density tensor, is a powerful tool in understanding and modeling the dynamic behavior of dislocations on microscopic scales. Using this model, a number of benchmark systems have been tested. All results show excellent agreement with both analytic solutions, where available, as well as discrete simulations. While accurate solutions have been found for effectively one dimensional systems, fully two- and three-dimensional systems increase the complexity of the problem. In order to predict the behavior of the continuum density accurately, it must be properly understood as an ensemble average over discrete distributions. In this work, an overview of a simplified, integrated form of the CDD method is presented, along with an overview of one-dimensional results compared with both analytic solutions and discrete simulation. Then, the results from CDD for a distribution of one-dimensional glide planes in a two-dimensional elastic medium is presented. Using comparisons with Discrete Dislocation Dynamics (DDD) in a few simple systems, the multi-component stress field which must be considered for dislocation density motion is derived and demonstrated.

1 Introduction

A proper understanding of plastic deformation requires incorporation of the underlying dislocation behavior. While a dislocation based theory of plasticity has existed since the 1920's, recent works have led to a greater understanding of dislocation behavior, both at the discrete level (van der Giessen and Needleman (1995); Weygand et al. (2002); Arsenlis et al. (2004)) and the continuum (El-Azab (2000); Hochrainer et al. (2007)) level. Of particular interest, Continuum Dislocation Dynamics (CDD) theory, a generalization of the classical continuum formulation of dislocation dynamics based on the Kröner-Nye tensor, serves as a useful tool for bridging the gap between discrete dislocation simulations, and macroscopic phenomena. In this proceeding, we will briefly summarize the equations of CDD and implement them for a few model systems.

A derivation of the CDD method can be found in Hochrainer et al. (2007). Here we will only give a short overview of the derivation and the dynamic equations we will utilize. CDD is based on a second order dislocation density tensor, α^{II}. Following Hochrainer et al. (2007), equations for the evolution of α^{II} can be derived for a given velocity law. However, storing and modifying information about the dislocation density in this higher dimensional space is computationally expensive. Sandfeld et al. (2011) showed that by integrating α^{II} over the angle ϕ, the number of unknowns could be drastically reduced. Under this simplified theory (sCDD) the evolution equations are simplified to equations for the total dislocation density ρ at a point, and the geometrically necessary density κ, which will in general be a vector, indicating the net contribution of the dislocations at a point to the plastic slip. These equations can be further simplified if only systems of parallel edge dislocations are considered, confined to move in a single slip system, making the system two dimensional and dynamics essentially one dimensional. As has been shown in a number of works utilizing discrete dynamics (Ispanovity et al. (2010); Groma et al. (2003)) a number of interesting phenomena in crystal plasticity can be examined using this simplified two dimensional system. The evolution equations of sCDD in this case are as follows

$$\partial_t \rho = -\partial_x(\kappa v) + v\rho k \tag{1}$$
$$\partial_t \kappa = -\partial_x(\rho v) \tag{2}$$

where v is the scalar velocity of the dislocation density motion, k is the average curvature, and t is time. In the examples considered here, we will always have $k = 0$. In addition, the plastic slip can be determined by the Orowan equation

$$\partial_t \gamma = \rho b v \tag{3}$$

We mention here that the equations, by their nature, conserve the dislocation number, although source or annihilation terms could be introduced. As such, in a one dimensional system, where dislocation annihilation would be expected to play a role. This aspect has to be addressed. Here, for the one dimensional system the glide plane is represented, not as a single plane, but as a region with some finite height (fixed in this case by the discretization) over which the dislocations are distributed. Thus, we assume that dislocations can move past each other without annihilating.

In order to close our system dynamically, a velocity law needs to be introduced. Here, we assume overdamped dislocation motion, proportional to the total stress, which is composed of two components: the external stress τ^{ext} due to external loading and the interaction stress τ^{int} caused by the dislocations configuration:

$$v = \frac{b}{B}\tau \text{ with } \tau = \tau^{ext} + \tau^{int} \tag{4}$$

where B is the dislocation drag coefficient. With this information, the evolution of a dislocation density in a given elastic system can be determined.

As a first test of our sCDD implementation, the simple double pileup for a single glide plane is used as a benchmark system. The use of sCDD on the double pileup and other sample one dimensional problems is explored more thoroughly in Schulz et al. Because of the existence of exact, analytic solutions, and the ability to easily compare results with discrete simulation (DDD), the double pileup provides an excellent test of the reliability of this method. In addition, by simply increasing the stress on the system, the model can be tested in a regime easily computable by DDD, but for which no analytic solution is known.

Second, we will extend our method to find the correlation function around a fixed dislocation (as dealt with, for example, in Groma et al. (2003); Ispanovity et al. (2008); Zaiser et al. (2001). This extension to a fully two dimensional system will show, first, the ability of our method to find solutions to a wide range of problems, and second, that the stress field in two dimensions must be augmented by statistical stress components.

2 Stress Correlations

The numerical implementation consists of a two scale system. The position and motion of dislocations is governed by a finite difference method (FD) using an explicit Euler scheme, forward difference in time and central difference in space. The motion of dislocations is halted at impenetrable boundaries at each end of the glide plane using zero-flux boundary conditions with the constraint $v = 0$ on the boundary node. The internal stress-field, and hence the force on the dislocations, is determined by solving the elastic eigenstrain problem, due to the plastic strains introduced by the dislocations, using the finite element method (FE). Details of this eigenstrain method can be found in Sandfeld (2010). The resulting stresses are applied to the FD grid to determine the velocity of the dislocations according to Eq. (4) which governs the evolution of the dislocation system. The new dislocation positions can then be used to determine new eigenstresses and in this way, the system as a whole evolves. The boundaries of the elastic problem are left traction free ($\sigma \cdot n = 0$ where n is the normal vector to the boundary and σ is the stress) and the size of the FE grid is several times larger than the FD system along which the dislocations move, in order to reduce the effect of spurious image stress.

In a completely continuous model, the interaction stress between dislocations could be applied in a straightforward way, as in Groma et al. (2003), following:

$$\tau^{int}(x) = \frac{\mu b}{2\pi(1-\nu)} \int \frac{\kappa}{x-x'} dx' \tag{5}$$

where μ is the shear modulus and ν is the Poisson's ratio. Here, the whole of the density exerts a stress on any single dislocation. However, it is advantageous computationally to allow the FE grid to remain coarser than the FD grid. If stresses are still correctly determined, this allows for high resolution of the dislocation motion at lower computational cost. However, the FD grid contains more information than can be used by the coarse FE grid, namely, the relative density of dislocations within a given FE cell. As a result, the stress solving the elastic eigenstrain problem, τ^{mf}, has a mean-field character which acts only as a long-range interaction term, neglecting the short-range interaction force. To compensate, we have introduced an additional, short-range, stress term, τ^{corr} which is proportional to the gradient of the geometrically necessary density:

$$\tau^{int} \approx \tau^{mf} + \tau^{corr} \tag{6}$$

$$\tau^{corr}(x) \approx \frac{\mu b}{2\pi(1-\nu)} \int_{-\Delta L}^{\Delta L} \frac{\kappa}{x-x'} dx' \tag{7}$$

$$\tau^{corr}(x) = \frac{\mu b}{2\pi(1-\nu)} \partial_x \kappa \Delta L \tag{8}$$

Here, ΔL is the length of the FE cell. τ^{corr} is calculated as follows: to first order, the mean-field stress will be the same as the interaction stress except for a length ΔL around the point where the stress is being determined. This difference can be approximated as a Taylor series, keeping only the lowest, non-zero term. For a one-dimensional system this is sufficient to determine the interations between the dislocations. For a two-dimensional system we have to account for further interactions among the slip planes. This interaction can be included through a back-stress, as is done in Groma et al. (2003).

3 Dislocation Pileup

To test the validity of the theory in one dimension, two comparisons are used for the double pileup. First, Hirth and Lothe (1982) solve the double pileup problems in an infinite medium analytically in a simplified continuum model. This model assumes a continuum density of dislocations with only the simple interaction stress between dislocations, and so is in principle only valid when the spacing between dislocations is small compared to the scale on which the solution is determined. In addition, it does not consider either the possibility of statistically stored dislocations or any dynamic evolution, examining only the steady state. While this model would be expected to break down for more complicated configurations or at scales where individual dislocations could be resolved, it serves to confirm that the sCDD method does reproduce the correct macro-scale behavior. The analytic solution for the GND density of the double pileup is:

$$\kappa(x) = \frac{2(1-\nu)\sigma}{\mu b} \frac{x}{\sqrt{((\frac{l}{2})^2 - x^2)}} \tag{9}$$

where $l = \frac{\mu N b}{\pi(1-\nu)\sigma}$ is the total length of the pileup, with N the total number of dislocations, and x is the distance from the middle of the pileup at $\frac{l}{2}$.

As a second means of comparison, discrete dislocation dynamic simulations were carried out on a 1D system and allowed to converge to their steady state. Because of the simplicity of the 1D system considered, multiple initial configurations of discrete dislocations all produce the same equilibrium configuration. As such, there was no need for averaging over multiple configurations.

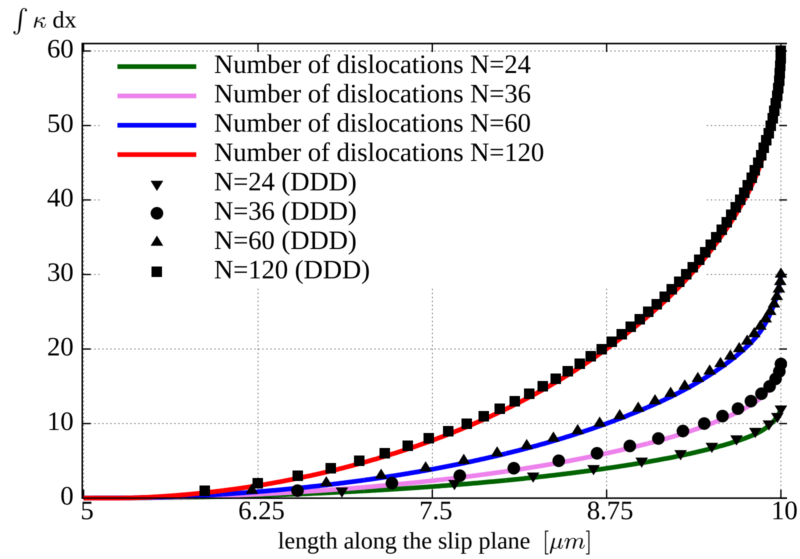

Figure 1: Continuum and discrete converged results for the right half of the double pileup system with different total numbers of dislocations, N. The stress is varied with the N so as to preserve the scaling.

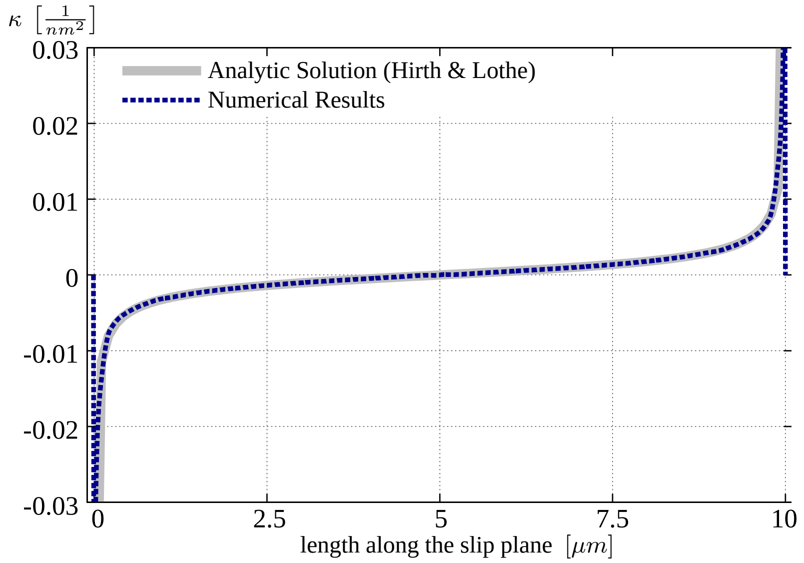

Figure 2: The converged numeric and analytic results for the stressed single pileup (left) and double pileup (right).

The results obtained numerically are based on the sCDD method described above. For our system, we use one glide plane of length $L = 10\mu$m in an elastic medium with length $L* = 80\mu$m. The material is assumed to be isotropic with Young's modulus $E = 128.4$GPa, Poisson's ratio $\nu = 0.33$, shear modulus $\mu = 48.27$ GPa, Burgers vector $b = 0.256$nm, and dislocation drag coefficient $B = 5 \cdot 10^{-8}$GPa μs.

As can be seen in Fig. 1 and Fig. 2 our numerical simulation agrees excellently with both the analytic solution and the results from DDD. We can also extend our system beyond what is analytically solvable by increasing the applied external stress to a point where there are not enough dislocations available to quench it. Since the dynamic system used does not contain terms for dislocation creation, the pileups are pushed farther on to the boundary. Fig. 3 shows the converged results from a double pileup system with external stress up to five times greater than that which satisfies the analytical solution given in Hirth and Lothe (1982). Even in this more extreme stress regime, excellent agreement is found between sCDD and DDD.

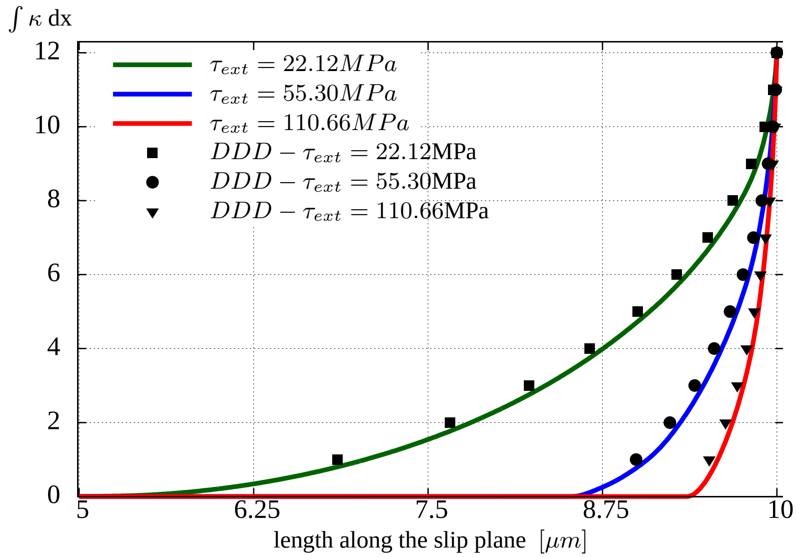

Figure 3: Continuum and discrete converged results for the right half of the double pileup system with different external stress, τ^{ext}. This system cannot be easily solved analytically.

4 Correlation Function

As mentioned above, the strength of the CDD method is its incorporation of statistically stored dislocations (SSDs) which, on average, do not affect the total plastic slip as their effect is canceled by dislocations of the opposite sign. Because of the tendency for adjacent dislocations of opposite sign to annihilate, SSDs can only be realized in an ensemble sense, where over several instance of a macroscopic system, a number of dislocations can be expected, on average, to occupy a given space, but with no net direction. As mentioned above, an ensemble understanding of our density parameters ρ and κ in one dimension is problematic in one dimension where annihilation should play a stronger role. In addition, even in the absence of dislocation annihilation, in one dimension, dislocations are able to move to their unique energy minimum, eliminating the possibility of a net SSD density existing “on average”.

It is therefore practical both to consider even our one dimension formulation as quasi-2D, with the glide plane occupying some small but finite height, and also to consider fully two dimensional systems. Here we will consider the average densities of both ρ and κ around a fixed dislocation in a given direction. This problem has been considered extensively in the discrete case in Groma et al. (2003); Ispanovity et al. (2008); Zaiser et al. (2001), as well as analytically in Groma et al. (2006). The averaged results from the discrete simulations can be compared with our continuum model. This dislocation correlation is useful to consider for a number of reasons. First, it is a 2D problem for which accurate discrete results are known. Second, it makes clear the role of our ensemble formulation of the dislocation density, as it must be compared to the ensemble average of discrete results. Finally, it is an interesting problem in its own right, as the form of the correlation function leads to the formulation of additional stress components which must be considered in the average result, and which, as will be seen, we must also consider.

The numerical system is constructed in an analogous way to the one dimensional case. Here, however, 63 separate, parallel glide planes are introduced. The finite element grid is refined such that each glide plane is separated by a single finite element cell width. A stress field is added which mimics the effect of a single dislocation located in the middle of the system. The dislocation density is allowed to relax in the presence of this field and the field generated by the mobile density. No other external stress is applied.

In order for the system under consideration to be properly compared to the ensemble average from a discrete system, additional stress terms must be considered. While a full description of the evolution of the system would additionally require some form of yield stress, in the zero external stress case considered here, it is sufficient only to introduce a backstress τ_b as derived in Groma et al. (2003)

$$\tau_b(x) = \frac{D\mu b}{2\pi(1-\nu)} \frac{\partial_x \kappa}{\rho} \tag{10}$$

Here, D is a parameter which can be determined from the properties of the correlation function. It is typically on the order of 0.1-1. Since we are here concerned only with the form of the correlation function we observe and not its scale, we can, without loss of generality, set $D = 1$ although carefully comparing the scale of the resulting distribution with discrete results can allow for an accurate determination of the parameter.

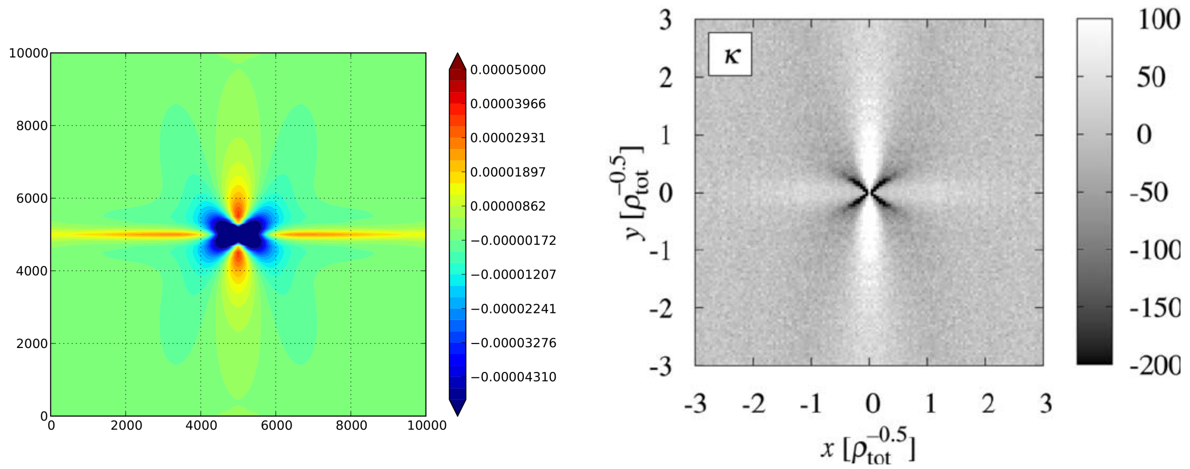

Figure 4: Density of geometrically necessary dislocations (κ [1/nm]) in the region around a fixed dislocation for the continuous system (left) and the discrete system (right). Axes for the continuum model are given in units of nm. Discrete results are from Ispanovity et al. (2008)

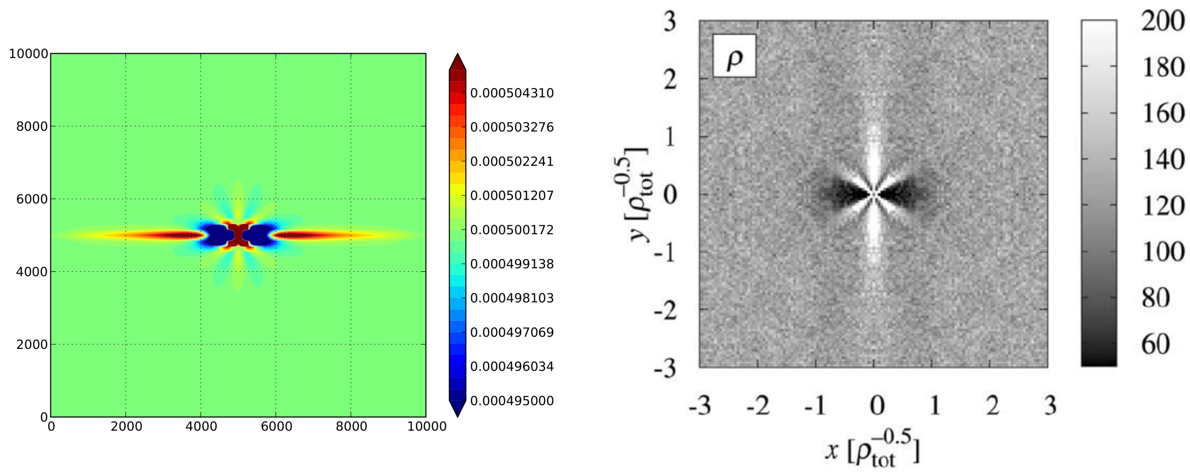

Figure 5: Total density dislocations (ρ [1/nm]) in the region around a fixed dislocation for the continuous system (left) and the discrete system (right). Axes for the continuum model are given in units of nm. Discrete results are from Ispanovity et al. (2008)

The results of the sCDD simulation for both ρ and κ as well as the discrete results, copied from Ispanovity et al. (2008) can be found in Figs. 4 and 5. By comparing our continuum model with discrete results, it can be seen that all of the relevant features of the correlation function are reproduced by our simulation. The discrete results represent a summation over more than 13,000 realizations of a system containing 128 dislocations, giving the total number of dislocations observed in each cell. The continuum model shows the line density of dislocations of a system with 63 glide planes each containing 5 dislocations. The maximum and minimum values for ρ and κ in the converged state are $\rho_{max} = 5.37 \cdot 10^{-4}$, $\kappa_{max} = 1.7 \cdot 10^{-5}$, $\rho_{min} = 4.82 \cdot 10^{-4}$, and $\kappa_{min} = -1.73 \cdot 10^{-4}$ respectively. In addition, it should be noted that this is the result of a single calculation, while the discrete results must be averaged over several thousand instances. Thus, the effective computational power of the continuum method in extending DDD results to larger systems can be seen.

5 Conclusion

Using a simplified form of the continuum dislocation dynamics theory, we were able to model the motion of dislocations in a single slip system for two benchmark problems in one and two dimensions. Through comparison with existing analytic results and discrete dislocation dynamic modeling, the accuracy of our numerical implementation was shown. Because the dislocation density was modeled at a higher resolution than the mean stress field, an additional stress component, τ^{corr} was introduced to reintroduce the density information not utilized by the finite element grid. This gradient dependent term is entirely of this coarse graining, and should not be confused with other gradient dependent terms such as the backstress utilized in the 2D system.

In one dimension, the double pileup, well known from classical continuum theory, was modeled, both using the continuum model presented, as well as discrete dynamics. The agreement between the two, as well as agreement with classical theory, shows that the sCDD method correctly determines the evolution of dislocations in 1D. In addition, it is also demonstrated that τ^{corr} is necessary to adequately model such systems, where the gradient of the GND distribution is significant.

Moving to the extended case of a fully two dimensional system, including a one dimensional slip system, the dislocation correlation function, the average density of both total and geometrically necessary dislocation in the area around a stationary dislocation, was also determined using the sCDD method. Because of the statistical nature of the problem, absent in the 1D case, τ_b had to be introduced to correctly model the ensemble average behavior observed in discrete simulation. However, with the introduction of this term, the continuum model was able to reproduce all the salient features of both ρ and κ in the vicinity of the stationary dislocation.

While many of the important features of crystal plasticity can be reproduced in two dimensions, a fully three dimensional continuum theory is ultimately desired. The CDD theory and its simplified form already contain the relevant kinematic equations, however, additional stress terms, such as the backstress which was introduced for the 2D system presented here, may be required. In order to move towards realizing a 3D implementation, the influence of curved dislocations must be considered. The motion of curved dislocations can first be considered in a single glide plane, analogous to the 1D problem considered here. From there, multiple glide planes and, additionally, multiple slip systems can be considered. The one and two dimensional results presented here, which already give accurate predictions for two important benchmark cases, are a first step towards the implementation of a continuum theory which can model the plastic behavior of crystals on a scale which is currently only poorly accessible.

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