XII International Conference on Computational Plasticity. Fundamentals and Applications
COMPLAS XII
E. Oñate, D.R.J. Owen, D. Peric and B. Suárez (Eds)

STRESS CORRELATIONS OF DISLOCATIONS IN A DOUBLE-PILEUP CONFIGURATION: A CONTINUUM DISLOCATION DENSITY APPROACH – COMPLAS XII

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Key words: Dislocation dynamics, Multi-Scale Modeling, Dislocation based Plasticity

Abstract. Dislocation motion in the crystal lattice of materials is the basis for macroscopic plasticity. While continuum models for describing the role of dislocations in plasticity have existed for decades, only recently have the mathematical tools become available to describe ensembles of moving, oriented lines. These tools have allowed for the creation of a Continuum Dislocation Dynamics (CDD) theory describing a second-order dislocation density tensor, a higher order analog of the classical dislocation density tensor, and its evolution in time.
In order to reduce the computational complexity of the theory, a simplified theory has also been developed, which more readily allows for a numerical implementation, useful for describing larger systems of dislocations. In order to construct a self-consistent implementation, several issues have to be resolved including calculation of the stress field of a system of dislocations, coarse graining, and boundary values.
The present work deals with the implementation including treatment of the near- and far-field stresses caused by the dislocation density tensor as well as boundary value considerations. The implementation is then applied to a few simple benchmark problems, notably the double pileup of dislocations in 1D. Applications to more general problems are considered, as well as comparisons with analytical solutions to classical dislocation problems. Focus is placed on problems where analytical solutions as well as simulations of discrete dislocations are known which act, along with experimental results, as the basis of comparison to determine the validity of the results.

1 INTRODUCTION

As microscale fabrication techniques have become more advanced and more commonplace, and the size of structures which can be fabricated becomes smaller, understanding material properties on the same scales has become a strong research focus. Of particular importance is a microscale theory of plastic deformation based on the motion of dislocations in the material. 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 [1, 2, 3] and continuum [4, 5] levels. 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, and shows promise as a method for accurately and efficiently modeling the dynamics of dislocation systems in a continuum setting.

A derivation of the CDD method can be found in [5]. Here we will briefly give an overview of the derivation and the dynamic equations which comprise the numerical formulation of a simplified method. CDD is based on a second order dislocation density tensor, α^{II}. This tensor stores information on the density of a particular dislocation orientation at a given point. Since the density depends on the orientation, no distinction is made in the CDD between statistically stored (SSDs) and geometrically necessary (GNDs) dislocations. CDD is also able to distinguish between straight and curved dislocations by containing information about the average curvature. Following [5], 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 every direction at every point is computationally expensive. [6] 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. The evolution equations of sCDD are as follows:

$$\partial_t\rho = -(\partial_x(\kappa_y v) - \partial_y(\kappa_x v)) + v\int_0^{2\pi} \rho k d\phi \tag{1}$$

$$\partial_t\kappa_x = -\partial_y(\rho v) \tag{2}$$

$$\partial_t\kappa_y = \partial_x(\rho v) \tag{3}$$

where κ_x and κ_y are the GND densities in the x, and y directions respectively, v is the scalar velocity of the dislocation density motion, k is the average curvature of the dislocation lines, and t is time. In order to focus solely on boundary effects and the stress components necessary to accurately predict dislocation density behavior, in this proceeding, only the simplified one dimensional case of a single glide plane (in the x direction) containing only straight edge dislocations will be considered. The burgers vector is taken to be in the x-direction, $\boldsymbol{b} = b_x$. In this case, Eqs. 1-3 reduce to

$$\partial_t \rho = -\partial_x(\kappa v) \tag{4}$$
$$\partial_t \kappa = \partial_x(\rho v) \tag{5}$$

where $\kappa = \kappa_x$. In addition, the plastic slip is determined by the Orowan equation:

$$\partial_t \gamma = \rho b v \tag{6}$$

Finally, for a closed dynamic system, a velocity law is required to determine the motion of dislocations for a given stress field. 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} among dislocations:

$$v = \frac{b}{B}\tau \tag{7}$$
$$\tau = \tau^{ext} + \tau^{int} \tag{8}$$

where B is the dislocation drag coefficient. Thus, for an initial dislocation configuration, the motion of the dislocation density can be determined.

2 Stress Correlations

To confirm the accuracy of the sCDD method and the numerical implementation of it, the evolution of a number of simple, one dimensional systems have been modeled. In particular, focus is placed on the double pileup and the stressed single pileup systems of straight edge dislocation in a single glide plane. Because of the existence of exact, analytic solutions, and the ability to easily compare results with discrete simulation, a purely one dimensional system is used in this work. Extension to higher dimensions, both in the single glide plane and by incorporating additional glide planes is discussed in the conclusions.

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 ($\partial_x(\rho v) = \partial_x(\kappa v) = 0$). 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). A more complete discussion of this method can be found in [7]. For a very fine mesh, this

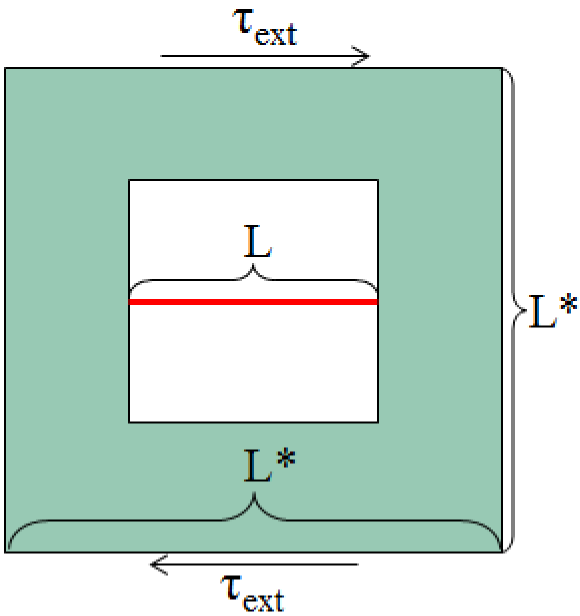

Figure 1: Schematic for the single glide plane system considered. The red line indicates the glide plane along which dislocations can move. The darker square shows the extent of the elastic problem considered. The large elastic area reduces the effects of images forces on the glide plane.

procedure leads to a correct determination of the internal stress. The resulting stresses are applied to the FD grid to determine the velocity of the dislocations according to (7) in addition to the external shear stress. In the simple system considered here, other stress components such as the yield stress are assumed to be zero.. The boundaries of the elastic problem are left traction free ($\sigma \cdot n = 0$ where n is the normal vector to the boundary) 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. Fig. 1 shows a schematic of the numerical implementation.

In a completely continuous model, the interaction stress between dislocations could be applied in a straight forward way, following:

$$\tau^{int}(x) = \frac{\mu b}{2\pi(1-\nu)} \int \frac{\kappa}{x - x'} dx' \tag{9}$$

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, because of the coarse nature of the FE grid (coarser than the FD grid on which the dislocation density is defined), dislocations within the the length of one FE cell do not exert a stress on one another through the interaction stress. 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 addition, short-range, stress term, τ^{corr} which is proportional to the gradient of the geometrically necessary density:

$$\tau^{int} = \tau^{mf} + \tau^{corr} \tag{10}$$

$$\tau^{corr}(x) \approx \frac{\mu b}{2\pi(1-\nu)} \int_{-\Delta L}^{\Delta L} \frac{\kappa}{x - x'} dx' \tag{11}$$

$$\tau^{corr}(x) = \frac{\mu b}{2\pi(1-\nu)} \partial_x \kappa \Delta L \tag{12}$$

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. Notice that even order terms in the Taylor expansion of $\kappa(x)$ vanish due to symmetry.

In understanding this model physically, the interpretation of the dislocation density is important. In real systems, dislocation densities are discrete, and appear as a continuum in this approximation either due to coarse graining or as the result of ensemble averaging. The derivation of τ^{corr} implies a coarse graining approach for the density used here. The interaction stress can also be understood as a mean-field stress, however, averaged over an ensemble of equivalent systems. In the one dimensional systems considered here, the distinction does not affect the results, as the equilibrium configurations are unique and thus there would be no deviation from the mean-field behavior. For more complex systems, however, corrections to the mean-field stress would have to be considered in the ensemble approach.

3 Dislocation Pileup

To test the validity of the theory, two comparisons are used. First, Hirth & Lothe [8] solve the single and double pileup problems in an infinite medium analytically in a simplified continuum model. This model assumes a true continuum density of dislocations (as opposed to an ensemble) 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 does serve confirm that the sCDD method does reproduce the correct macro-scale behavior. The analytic solutions for the stressed single pileup and double pileup respectively are:

$$\kappa(x) = \frac{2(1-\nu)\sigma}{\mu b}\sqrt{\frac{(\frac{l}{2})+x}{(\frac{l}{2})-x}} \text{ (Single Pileup)} \tag{13}$$

$$\kappa(x) = \frac{2(1-\nu)\sigma}{\mu b}\frac{x}{\sqrt{((\frac{l}{2})^2-x^2)}} \text{ (Double Pileup)} \tag{14}$$

where x is the distance from the middle of the pileup, and $l = \frac{\mu N b}{\pi(1-\nu)\sigma}$ is the total length of the pileup, with N the total number of dislocations. While in the case of the double pileup, l is artificially set by the boundary conditions, in the stressed single pileup it is determined by the other parameters, since the pileup does not approach the far boundary.

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.

The results obtained numerically are based on the sCDD method described above. In principle, size dependent terms, such as those proposed in [9] could be included as additional components to the total stress. In order to correctly analyze the behavior of a dislocation ensemble for more complicated systems, it is likely that similar terms would need to be included. However, because of the uniqueness of the solution for the pileup problem in one dimension, deviations from the mean-field approximation are minimal, and the total stress is well described by the external shear stress and the internal stress as presented in (10).

4 Results

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 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. For the pileup problems considered, N denotes the total number of dislocations and σ the externally applied shear stress.

In one dimension, the evolution of the system, starting with a single bundle of dislocations located in the center of the glide plane is observed. For the single pileup case, the bundle consists of dislocations all with the same orientation, so that $\kappa = \rho$, while for the double pileup, both orientations occur in equal amounts so that $\kappa = 0$. The converged

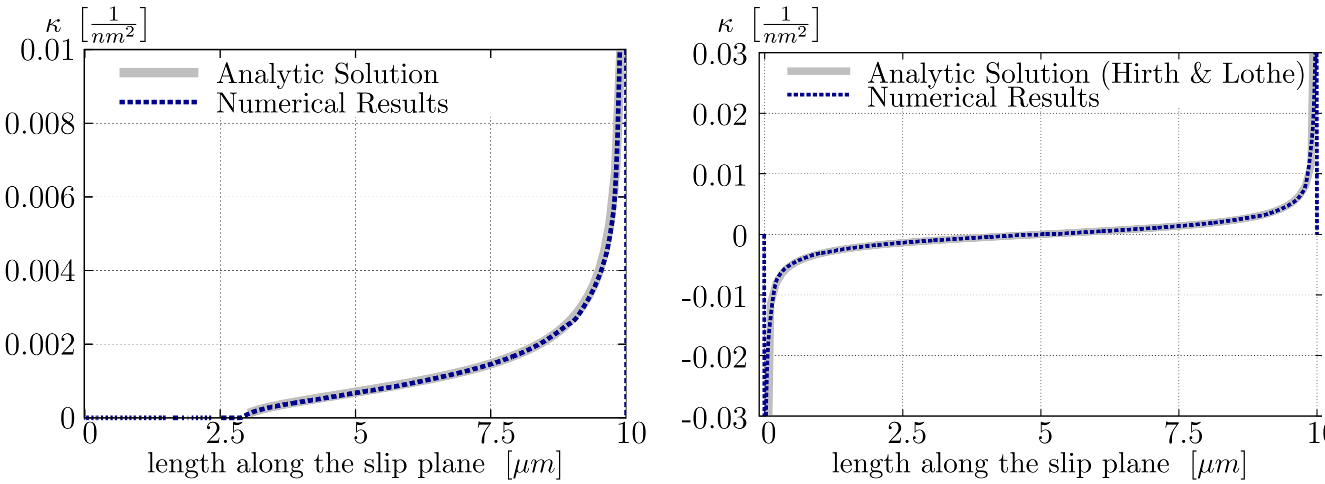

Figure 2: The converged numeric and analytic results for the stressed single pileup (left) and double pileup (right).

state both systems is shown in Fig. 2, along with the analytic solution given above. Excellent agreement is found between the converged numeric state and the analytic solution.

By varying the total number of dislocation (and the corresponding external stress), it can be seen in Fig. 3 that, as should be expected from the form of the constitutive equations, the total stress as modeled is fully scalable. This is an important realization with respect to τ^{corr}, as a corrective component to the stress need not scale linearly with density. In fact, it is expected that in higher dimensions, dislocation systems should scale with the average dislocation spacing, regardless of the dimension of the system. In addition, we see that our results are in good agreement with discrete simulation, even for the smallest dislocation density used. It is expected at some minimum density, the continuum approximation will break down, but even at $N = 24$ the sCDD method gives results which almost exactly match those from DDD.

Systems can also be considered for which analytical solutions are not readily available. In Fig. 4, 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 [8] are presented. As can be seen, with increasing external stress, the pileup is pushed farther against the boundary, with the density dropping to zero in the middle of the glide plane. Again, excellent agreement is found between sCDD and DDD results.

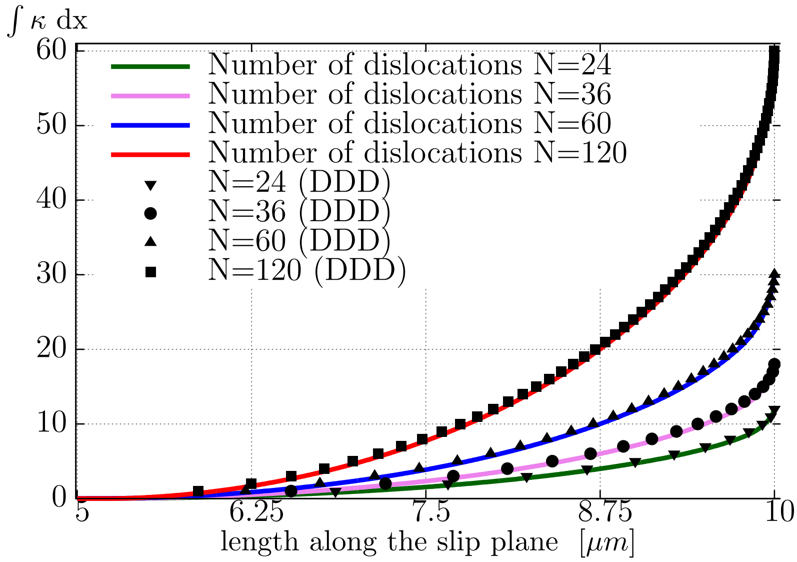

Figure 3: Continuum and Discrete converged results for the right half of the double pileup system with different total numbers of dislocations, N. The stress is varied with the N so as to preserve the scaling.

5 Conclusion

Through the numerical implementation of the simplified CDD method, the motion of a density of straight edge dislocations in a single glide plane under a constant shear stress was modeled. Depending on the relative orientation of the individual dislocations (either as GNDs or SSDs), the density relaxed to a stressed single pileup or a double pileup configuration. By comparing with both analytical results from classical continuum theory, as well as numerical results from DDD simulations, it was shown that the sCDD method accurately reproduces the pileup behavior. In addition, by examining the over stressed double pileup, the ability of this method to predict the behavior of dislocations in the absence of classical analytical results was demonstrated.

In order to accurately model the full interaction stress of the dislocation density, including interaction among dislocations within the same cell of the finite element grid, an integrated stress term τ^{corr} was introduced. This gradient dependent term arises entirely from the discretization. It should also be noted that this is not merely a fitting parameter, but one that is determined directly from the material parameters, the density, and the parameters of the discretization. Inclusion of this term in the velocity equation allows almost exact agreement between the numerical results and both theory and discrete methods.

The accuracy of numerical solutions obtained using τ^{corr} shows it to be a valuable tool in determining the behavior of dislocations at scales below the coarse resolution of finite element stresses. While solving the elastic eigenstrain problem at high resolution is

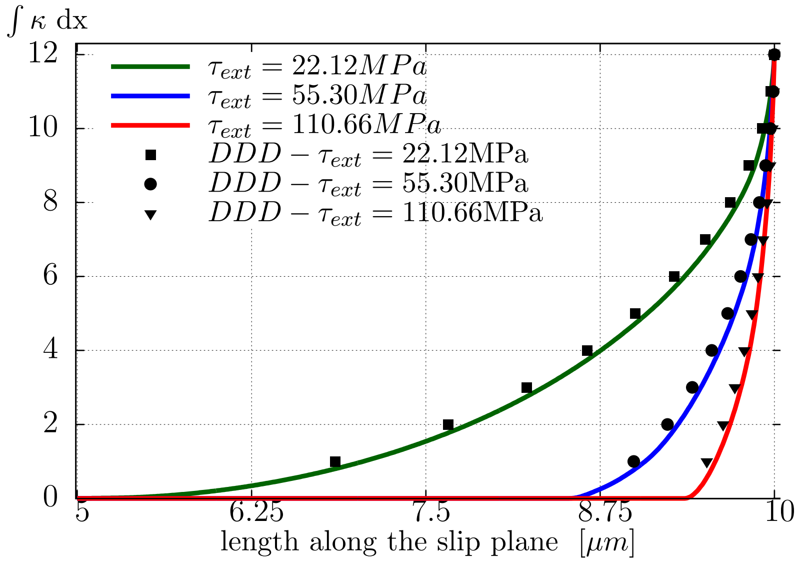

Figure 4: Continuum and Discrete converged results for the right half of the double pileup system with different external stress, τ^{ext}. This system cannot be easily solved analytically.

relatively expensive, the use of the short range, gradient dependent τ^{corr} can be efficiently and locally computed on the FD grid. If appropriate corrective terms can be generalized to three dimensional systems, such stress terms could drastically reduce the time of dislocation system computations, as stresses could be effectively calculated on a much coarser grid.

While these results demonstrate the applicability of this method to more general problems, the ultimate goal of modeling the evolution of fully three dimensional dislocation systems is still being pursued. The two most direct extensions of the work presented here are (1) the introduction of additional glide planes, both in parallel and cross-slip configurations, and discretely or continuously spaced, and (2) the evolution of densities in a single, fully two dimensional glide plane. While the computational framework for (1) is already in place, these more elaborate geometries will certainly require a more complex, fully statistical description of the stress field acting on our ensemble distribution, as described previously. (2) will also require an extension of the corrective stress to a higher order density tensor, including both edge and screw components, as well as, potentially, curvature. Implicit in the sCDD approximation is that the scalar velocity at a given point is the same regardless of dislocation orientation, and any corrective stress terms must take this restriction into account.

6 Acknowledgements

We gratefully acknowledge the financial support from the German Research Foundation (DFG) through the DFG Research Group 1650 "Dislocation-based plasticity", under contract gu374/30.

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