Advances in Discrete Dislocations Dynamics and Multiscale Modeling

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Discrete dislocation dynamics is a numerical tool developed to model the plasticity of crystalline materials at an intermediate length scale, between the atomistic modeling and the crystal plasticity theory. In this review we show, using examples from the literature, how a discrete dislocation model can be used either in a hierarchical or a concurrent multiscale framework. In the last section of this review, we show through the uniaxial compression of microcrystal application, how a concurrent multiscale model involving a discrete dislocation framework can be used for predictive purposes.
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1 Introduction

Almost all problems in science and engineering are multiscale in nature. Things are made up of electrons and atoms at the atomic scale, while at the same time they are characterized by their own geometric dimensions, which are usually several orders of magnitude larger. Therefore, to model the plasticity of a material, several length scales are involved. We need to find the scale of (i) the crystal lattice, (ii) the dislocation core, (iii) the mean distance between dislocations, and (iv) the grain size. The first two scales can be studied by either first principle calculations or molecular statics/dynamics calculations. However, when molecular statics/dynamics are considered, the interaction forces between neighboring atoms are calculated based on a semi-empirical potential. As first principle calculations are limited to a few hundred atoms, which give too small a representative volume element to study the plasticity, the semi-empirical potential constitutes the first bridge of a hierarchical multiscale framework. Depending on the accuracy of the potential [1], it can be used to model the mechanical behavior of a system containing several million atoms. For more information on semi-empirical potentials, the reader is referred to the review of Kim et al. [2] who presented a comparison between two potential frameworks: the embedded atoms method and the modified embedded atoms method. However, as the characteristic length (the smallest distance of the simulation cell) that is accessible using molecular statics/dynamics modeling is smaller than the mean free path of the dislocations (distance proportional to the inverse of dislocation density square root), the yield stress and hardening are not controlled by the dislocation interactions but by the nucleation of dislocations, and therefore a strong size effect is usually observed [3,4]. To model the mechanical behavior of a material at a length scale, where the hardening is controlled by the dislocation interactions (i.e., when the mean free path of the dislocations is smaller than the geometrical characteristic length scale), dislocations are modeled by lines of singularity in an elastic continuum and their dynamics are solved using a discrete dislocation framework [5,6]. Although other mechanisms, such as twinning deformation or grain boundary sliding, can accommodate the deformation, only dislocation motion and interaction are taken into account into the discrete dislocation framework. As it will be explained later, deformation twinning should be implemented in the framework for metals that crystallize in a hexagonal-close packed crystal structure, but the plasticity of a single-crystal crystallized with a cubic symmetry (fcc or bcc), can be investigated using only the notion of dislocation interactions. Therefore, the discrete dislocation framework was developed to model the plastic deformation of single crystals with dimensions in the order of micrometer. Discrete dislocation simulations give access to the evolution of dislocation density per slip systems and to the strain-strain curves. However, dislocation nucleation is not taking into account the framework, and the increase in dislocation density is a result of the multiplication of the initial dislocation microstructure. Another approach is to integrate the discrete dislocation dynamics within the viscoplasticity continuum mechanics framework. In this framework, typically one needs to develop a phenomenological constitutive equation for the plastic strain-rate tensor. However, Zbib and Diaz de la Rubia [7] proposed that the evolution of the plastic strain rate in the continuum theory could be determined explicitly from the discrete dislocation dynamics, thus coupling the continuum response directly to underlying discrete events. An alternative approach is to rely on the continuous field of eigenstrain, in which regions of high strain gradients reveal the locations of the dislocation lines. This representation leads to the phase field approach methods [8–10].

With respect to all other simulations, the discrete dislocation phase field method presents the enormous advantage of being able to treat the coupled evolution of concentration fields and elastic fields [11]. However, considering its present early stage of development, a few years will be needed before this method fully realizes its potential in the domain of plasticity. Crystal plasticity modeling [12,13] is the next scale level in investigating the plasticity of polycrystalline materials. The dislocation density, the hardening evolution, and the flow rule are described using functional forms, where parameters are characterized using experimental data [14,15] and/or numerical results from a lower length scale [16]. Finally, the design of structural components usually occurs at the macroscale using internal state variable model (see, for example, Ref. [17]). Shenoy et al. [18] proposed a hierarchical multiscale framework to link a crystal plasticity model to a macroscopic internal state variable model. With their approach, the microstructure dependence of the macroscale model parameters is identified at the crystal plasticity level.

Several surveys of the literature on multiscale modeling have been published, with our focus being on the particular articles of Liu et al. [19] and Curtin and Miller [20]. In the review of Liu et al. [19], it is asserted that multiscale methods can be naturally grouped into two categories: concurrent and hierarchical. Concurrent methods simultaneously solve a fine scale model in some local region of interest and a coarser scale model in the remainder of the domain. Hierarchical or serial coupling methods [21] use

results of a fine scale model simulation to acquire data for a coarser scale model that is used globally, e.g., to determine parameters for constitutive equations.

The aim of this review is to summarize the different multiscale frameworks involving 3D discrete dislocation dynamics. The general framework of the discrete dislocation simulations is recalled in Sec. 2.1. Hierarchical and concurrent frameworks involving discrete dislocations, available in the literature, are reviewed in Secs. 2.2 and 2.3, respectively. As an example of the robustness of the concurrent multiscale methods involving discrete dislocation dynamics, a review on the size-dependent flow stress in uniform loaded pillars is given in Sec. 3. Concluding remarks are given in Sec. 4.

2 Methodology

In this section, a description of the discrete dislocation framework is presented in Sec. 2.1. How a discrete dislocation model can be used in a hierarchical or concurrent multiscale framework is presented in Secs. 2.2 and 2.3, respectively.

2.1 Discrete Dislocation. Brown [22], Bacon [23], and Foreman [24] gave the main idea for discrete dislocation simulations in the mid-1960s. These authors proposed the framework to characterize the curvature of a line of dislocation under an applied stress. In the beginning of the 1990s, Amadeo and Ghoniem [25] and Canova and Kubin [5] presented the first numerical tool based on linear elasticity that links the properties of a single dislocation to the collective behavior of dislocations (hardening). In 1992, Kubin et al. [26] presented the first numerical implementation of a 3D discrete dislocations (DD) simulations.

Discrete dislocation is a numerical technique where the plastic properties of a crystal are determined using the elastic theory of dislocations. Physically, plastic deformation in crystalline materials results from the collective interaction, motion, and reaction of a high density of dislocations. Since a dislocation is typically represented by a line singularity in an elastic solid [27,28], the evolution of the dislocation microstructure is governed by the elastic interactions between dislocations [29]. To model such evolution, the dislocation lines need to be represented and their dynamics solved. The methodology developed for three-dimensional dislocation dynamics can be categorized into two groups, according to the line discretization scheme and representation of a general curved dislocation segment. The first method is based on an edge-screw [26] or edge-mixed-screw [30,31] discretization of the dislocation lines. The basic idea of the approach is that the discrete segments move on a discrete lattice superimposed to the crystallographic lattice, but on the orders of a larger magnitude. The second category of methods simulates dislocations as smooth flexible lines discretized either by linear splines [6,32–34], cubic splines [35,36], or circular arcs [37,38]. It should be noted that in all of the aforementioned models, dislocation dynamics codes were developed for dislocations in isotropic media. This is mainly due to the fact that exact solutions for the strain field are readily available for this case. The effect elastic anisotropy was investigated by Rhee et al. [39], who developed a methodology for implementing strain fields, which are given in relatively complex integral forms, in their DD code (MICRO3D).

Once the dislocation lines are discretized, the formulation of the DD approach assumes that the dynamics of each dislocation segment is governed by a *Newtonian-type* equation of motion consisting of an inertia term, a drag term, and a driving force F [40], such that,

$$m^* \dot{v} + Bv = F^* \tag{1}$$

In the above equation, v is the dislocation velocity, m^* is the effective mass density, and B is the drag coefficient. The driving force itself consists of various components: dislocation-dislocation interaction force, self-force (or line tension), external force, osmotic force, dislocation-obstacle interaction force, and

thermal force (see, e.g., Ref. [41]), which can all be lumped together into one term F^{**}. In addition, there is a *Peirels* force F^P. This latter force acts like friction, and therefore if the magnitude of F^{**} is less than F^p, the right-hand side of Eq. (1) is set to zero. In most cases the inertia term can be neglected and the equation of motion can be rewritten in the following form [42]:

$$v = 0 \quad \text{if} \quad \tau^* \leq 0$$

$$v = \text{sign}(\tau^{**}) \frac{\tau^* b}{B} \quad \text{if} \quad \tau^* \geq 0$$

$$\tau^* = |\tau^{**}| - \tau^p \tag{2}$$

where τ^*, τ^{**}, and τ^p are the resolved shear stresses corresponding to F^*, F^{**}, and F^p, respectively. Note that the linear dependence of the dislocation velocity on the resolved shear stress given by Eq. (2) represents the velocity of a single gliding dislocation and not the average velocity calculated for the overall dislocation gliding on one slip system. Also, the above equation for viscous glide applies to dislocation motion in pure fcc crystals when no interaction of the gliding dislocation with localized obstacles, e.g., forest dislocations, is considered. Then, depending on the temperature, the coefficient B accounts for electron and phonon drag. This is either the case of the free flight dislocation mobility between the obstacles at "quasistatic" strain rates or the case of dislocation dynamics at high strain rates [43,44]. Physically, as the dislocation velocity cannot exceed the terminal velocity (i.e., the velocity of a transverse shear wave), a resolved shear stress cutoff value needs to be specified unless a complete dynamic analysis is used, which includes an inertia term, as in Eq. (1). When the resolved shear stress becomes larger than the cutoff value, the dislocation velocity saturates at the terminal speed.

Once the velocity of the dislocation i is known, a search algorithm is applied to check if there are any possible interactions with other dislocations within a virtual area of the gliding dislocation i. The length of the dislocation segment and the free flight distance define the virtual area gliding. The relation between the Burgers vector and the slip systems of the two intersecting dislocation segments define the type of interaction. When two dislocations intersect each other, one of the following interactions occurs.

- *Annihilation*. If the two dislocations have opposite Burgers vectors and glide in the same slip plane.
- *Collinear annihilation*. If the two dislocations have collinear Burgers vectors and glide in intersecting slip planes, each plane being the cross-slip plane of the other.
- *Hirth lock*. If the two dislocations have perpendicular Burgers vector and glide on different slip planes.
- *Glissile junction*. If the resulting Burgers vector is glissile on either of the planes.
- *Lomer Lock*. If the resulting Burgers vector is sessile on either of the planes.

Finally, cross slipping of screw dislocations can relax internal stresses. A Monte Carlo method is used to check whether cross-slip is activated or not. The probability law of cross-slip is given by

$$P = \beta \frac{L}{L_0} \frac{\delta t}{\delta t_0} \exp\left[-V \frac{\tau_{\text{III}} - \tau}{kT} \right] \tag{3}$$

where β is a coefficient that ensures that the probability does not exceed 1.0; $\tau_{\text{III}} = 5$ MPa is the critical resolved shear stress at the onset of stage III work hardening for Al; $V_a = 300b^3$ is the activation volume; T is set to room temperature; $L_0 = 1$ μm and $\delta t_0 = 1$ s are reference values of length and time, respectively; L is the length for cross-slip of the screw dislocation segment; δt is the simulation time step; and τ is the resolved shear stress on the

cross-slip plane [26,45].

On the other hand, the increment of plastic shear is a consequence of the gliding of dislocation i of Burgers vector b_i, and it is given by Orowan's law.

$$\delta\gamma_i^p = \frac{b_i \delta A_i}{V} \tag{4}$$

where δA_i is the area swept during gliding, and V is the volume of the sheared body. Knowing the increment of plastic shear on slip system k, one can then compute the components of the plastic strain-rate tensor $\delta\varepsilon_{ij}$ using

$$\delta\varepsilon_{ij}^p = \sum_{k=1}^{12} \frac{1}{2}(n_i^{(k)} l_j^{(k)} + n_j^{(k)} l_i^{(k)}) \delta\dot{\gamma}^{(k)} \tag{5}$$

where $n_i^{(k)}$ and $l_i^{(k)}$ are the components of the unit vectors parallel to the slip plane normal and parallel to the Burgers vector, respectively. This framework associated with a set of periodic boundary conditions to equilibrate the flux of dislocations [46,47] can be used to model the hardening response of a representative cell extracted from a single crystal. Note that some authors (e.g., Bulatov et al. [46]) showed that even with heterogeneous dislocation motion, periodic boundary conditions can appropriately represent the physical phenomena.

Over the last decade, the previous framework has been applied to model different crystal structures. Moulin et al. [48] and Tang et al. [49] extended the edge-screw model to diamond cubic and bcc crystal structure, respectively. Kubin et al. [50] and Madec and Kubin [51] implemented the bcc crystal structure in the "edge-screw-mixed" model and investigated the strength of the junction in fcc and bcc crystal structures. Monnet et al. [52] extended the edge-mixed-screw model to hcp crystal structure with only $\langle\mathbf{a}\rangle$ dislocations. Additional work will be necessary to implement $\langle\mathbf{c+a}\rangle$ dislocations in the hcp crystal structure in order to have enough slip systems to accommodate the plastic deformation along the c-axis [53]. Durinck et al. [54] implemented the orthorhombic symmetry for olivine in a 3D discrete dislocation dynamics. They demonstrated that no junction formation results from the interaction between [55] and [001] dislocations in this crystal structure. Moreover, the collinear interaction [56] is thus the only mechanism for forest hardening in olivine. The linear spline models were developed for fcc crystal structure [32,57] and for bcc crystal structures [33]. The fcc crystal structure was implemented in the cubic splines models [35,37,38].

One of the main disadvantages of the discrete dislocation methodology arises from the long-range character of the dislocation stress field. Therefore, the computation of the dislocation elastic field and the treatment of dislocation core reactions increases like $O(N^2)$, where N represents the number of segments. Contrary to molecular dynamics where the number of atoms is constant, the number of segments used in the discrete dislocation methodology increases with plastic strain. To speedup the calculations, Hirth et al. [58] and Zbib et al. [6,32] developed a numerical technique based on the multipolar expansion method. They showed that this procedure leads to an efficient order N algorithm with 0.1% error and one order of magnitude reduction in CPU time. Later on, Verdier et al. [59] proposed to use the Greengard algorithm to transform the $O(N^2)$ in an $O(N)$ dependency. However, even with the Greengard algorithm, the calculations were still limited to less than 0.5% of plastic deformation [31,60].

The numerical limitations associated with three-dimensional DD may be overcome by the use of parallel algorithms. Rhee et al. [45] developed a parallel version of the DD code MICRO3D. They showed that speedup in CPU usage can be significant, but reaches a limit with an increasing number of processors. This is due mainly to short-range reactions, which necessitate communication among processors. Nevertheless, by using this parallel code, large-scale dislocation problems and dislocations-defect

Table 1 Summary of the input and output to use the DD methodology in a hierarchical multiscale modeling

Input
• Elastic properties
• Crystallographic properties
• Reaction between dislocations
• Dislocation mobility
• Cross-slip properties
• Dislocation sources
• Defects (SFTs, loops, particles, etc.)
• Loading conditions

Output
• Stress-strain curve
• Total dislocation density
• Dislocation density per slip systems
• Dislocation reactions: junction, jogs, dipoles
• Mobile dislocation
• Forest dislocation

problems were analyzed (see, e.g., Refs. [61,62]). Recently, Shin et al. [63] proposed a parallel algorithm to speedup the "edge-screw" model, while Wang et al. [64] and Arsenlis et al. [33] proposed a parallel algorithm to speedup the cubic and linear spline models, respectively. Using the parallel version of the DD code, Arsenlis et al. [33] was able to reach 1.7% of plastic deformation during the tensile test of a bcc molybdenum at an elevated temperature. The investigation of the cell organization and the similitude principle [65,66] are at the cost of a parallel discrete dislocation code. On the other hand, trends can be obtained using two-dimensional discrete dislocations framework where only edge dislocations are modeled. However, as our focus is mainly on three-dimensional DD, readers are referred to the studies of Needleman and co-workers [67–74] and Gomez-Garcia et al. [75].

2.2 Hierarchical Framework. To understand how a discrete dislocation code can be used in a hierarchical multiscale framework, the inputs as well as the outputs of the simulation are summarized in Table 1.

In a hierarchical multiscale framework, the lengths and time scales are not coupled. The input of the DD might be obtained by either first principle calculations or/and molecular dynamics/statics calculations. The outputs, on the other hand, are used to characterize material parameters at a higher length scale, such as the material parameters used in the hardening rule of a crystal plasticity model. Groh et al. [16] showed the feasibility of predicting numerically the mechanical behavior of an aluminum single crystal using a hierarchical multiscale framework, as illustrated in Fig. 1. The mobility properties of an individual dislocation were characterized at the atomistic scale and used as an input at the discrete dislocation level to model the hardening evolution of an aluminum single crystal under uniaxial compression. The hardening parameters of a Palm–Voce functional form [76,77] were correlated with the DD predictions and used at the crystal plasticity level to model the mechanical behavior and the change in shape of an aluminum single crystal under compression. However, such a method generates uncertainties related to scale bridging. A study to quantify the uncertainties related to scale bridging is currently under investigation.

2.2.1 From a Lower Length Scale to DD. Molecular dynamics calculations provide information concerning the mechanisms and/or the mobility of the dislocations that need to be implemented in the DD models. Bulatov et al. [78] used large-scale molecular dynamics calculations to establish the local rules for DD simulations. They characterized the force required to destroy a Lomer–Cottrell lock at the atomistic scale and then used this information to formulate the critical condition for junction de-
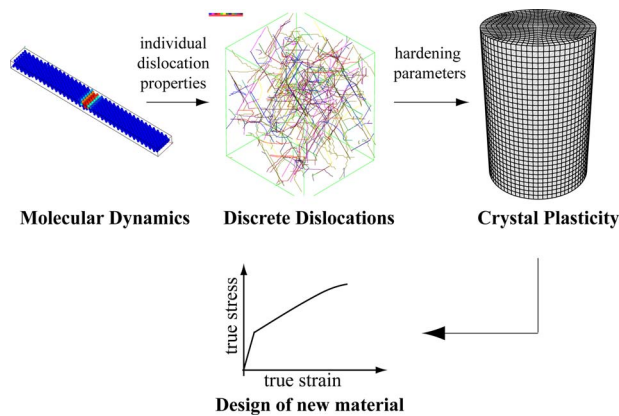
Fig. 1 Hierarchical multiscale modeling of the plasticity involving three characteristic length scales

struction in a dislocation dynamics simulations. Madec et al. [56] measured the interaction coefficients corresponding to the three junctions and their value, which agreed with the hierarchy of strength deduced from a latent hardening experiment. In addition, they performed molecular dynamics calculation to confirm their discrete dislocation calculations, showing that the collinear interaction was far from the strongest interaction in the fcc crystal structure. Marian at al. [79] presented a mechanism of dislocation motion in iron using atomistic calculations. In 2005, Olmsted et al. [80] calculated the drag coefficient of screw and edge dislocations in Al–Mg alloys using atomistic calculations, and the drag coefficient is needed in Eq. (2) to predict the dislocation velocity in the discrete dislocation framework. In 2006, Bulatov et al. [81] predicted the existence of multijunctions in bcc crystal structure using discrete dislocations and atomistic calculations before confirming their existence by transmission electron microscopy experiments. Martinez et al. [82] recently carried out large-scale three-dimensional molecular static and molecular dynamics calculations for Cu to calculate the value of the dislocation core energies and the value of the drag coefficient, respectively. Groh et al. [16] presented a hierarchical multiscale application from the atomistic up to the crystal plasticity to predict the mechanical behavior of an aluminum single crystal. The first bridge was the dislocation velocity calculated at the atomistic scale and was used as an input in the DD framework. Groh et al. [83] performed molecular statics and molecular dynamics simulations to characterize the anisotropy between slip systems in Mg single crystal.

2.2.2 From DD to a Higher Length Scale. Discrete dislocation simulations are usually used in a hierarchical multiscale modeling to measure the material parameters of the hardening rule used in the crystal plasticity modeling. Kocks and Mecking [84] introduced a dislocation-based hardening model, derived from the storage-recovery framework developed in scalar form by Mecking and co-workers [84–86]. This model assumes that all the slip systems harden at the same rate and, therefore, the interactions between different slip systems are averaged in a Taylor sense. Teodosiu et al. [87], or Kocks and Mecking [85], extended the scalar model to account for slip system interactions (matrix form). Within this extended storage-recovery framework, the hardening law was modified to predict the three stage behavior of a single crystal initially stretched in single slip [88,89]. The extended model predicted the main characteristics of single-crystal and polycrystal deformations during monotonic and sequential loading tests. Within the extended model, the interactions among the different slip systems were explicitly represented using an interaction coefficient matrix [90] and the value of the interaction coefficients were extracted using DD simulations. Such extractions have been performed for fcc materials by Fivel [91], Madec et al. [56], and Devincre et al. [92], while for bcc materials in the athermal re-

gime extractions have been performed by Queyreau et al. [93]. Preußner et al. [94] proposed a physics-based constitutive law, which allows the describing of the creep behavior of single-crystal alloys by mutual interaction of dislocations on different slip systems, with an emphasis on the evolution of the dislocation density. Their model described well the first two stages of creep. A study related to the multiscale modeling of metals is presented by Ohashi et al. [95], who used a multiscale modeling approach to model the scale-dependent characteristics of mechanical properties of metallic polycrystals. These authors proposed to modify the hardening law of a dislocation-based crystal plasticity model [96], according to the minimum shear stress needed to emit a dislocation loop into a confined system calculated by DD simulations [97]. Using such a multiscale approach, Ohashi et al. [95] was able to reproduce a variation in the macroscopic yield stress as a function of the grain size. Using DD predictions on Al single crystal, Groh et al. [16] measured the hardening parameters of the model of Kocks and Mecking [84] and then simulated the mechanical response of an Al single crystal under compression. These authors found a good agreement with the experimental data.

2.3 Concurrent Framework. To study the plasticity of structural materials made of interfaces and free surfaces, the conventional DD framework presented above needs to be extended to solve a heterogeneous stress field. Most of the solutions proposed in the literature are based on the superposition method proposed by Van der Giessen and Needleman [67]. The solutions are obtained as the sum of two contributions. The first represents the solution for dislocations in an unbounded crystal and the other is the complementary elastic solution needed to satisfy equilibrium at external and internal boundaries. The second solution can be solved in a continuum mechanics way, such as finite element methods (FEM) [55,97–100] or boundary element method (BEM) [101,102]. Although this approach works well when all dislocation segments are away from the internal or/and external boundaries, it becomes inefficient when one or more dislocation segments intersect the surface. When standard FEM is applied to solve the image stress due to such singular traction forces, the result is found to strongly depend on the mesh size [100]. A possible solution is to use adaptive meshes with multiple resolutions that follow the intersection points [103]. However, adaptive meshing is a cumbersome and challenging problem in itself, especially for massive DD simulations where many dislocations intersect the surfaces. Another solution is to remove the singularity from the FEM calculations.

Khraishi and Zbib [104,105] developed a rigorous method to handle the issue of image stresses. The method is semi-analytical/numerical in nature, in which they enforce either traction or displacement boundary conditions at collocation points on a surface. In their method, the image stress field of a subsurface dislocation segment near a free surface is obtained by an image segment and by a distribution of prismatic rectangular dislocation loops padding the surface. The method derives from crack theory and falls under "generalized image stress analysis," whereby a distribution of dislocation geometries or entities and not *just* simple mirror images, are used to satisfy the problem's boundary conditions. For the special case of a dislocation interesting the surface, Tang et al. [106] developed a method to treat the singularity at the point of intersection by superimposing two solutions: (i) image stress field of a semi-infinite straight dislocation intersecting the free surface of a half-space, for which analytic expressions exist, and (ii) the difference between these two image stress fields. By construction, the difference between the two image stress fields is a nonsingular function of space and is solved numerically, such as by FEM. A faster convergence than the conventional superposition method and the possibility to use a coarser mesh are the two advantages of this decomposition, compared with the conventional superposition method proposed by van der Giessen and Needleman [107]. Diverse applications were solved with the model developed based on the superposition methods. Depres et al. [108,109] analyzed the

Table 2 Summary of additional inputs and outputs in a concurrent DD-FEA multiscale modeling

Input
• Finite element data
• Boundary conditions

Output
• Stress, strain, and temperature fields
• Deformed configuration
• Lattice rotation

early stages of the formation of persistent slip markings in fatigue and the authors proposed a detailed scheme for persistent slip marking formation and morphology in relation to the persistent slip-band dislocation arrangements present within the grain. Shin et al. [110,111] investigated the interaction between dislocation of different characters and particles. In the case of spherical particle, these authors found that an increase in the particle elastic modulus favored the cross-slip mechanism, leading to a possible bypass of the particle by double cross-slip [110]. The shape of the particle appeared to be a critical parameter in the design of new materials and Shin et al. [111] concluded that a cubic particle is more resistant to dislocation climb than a spherical or cylindrical particle.

In addition to addressing issues related to image stress when dislocations are in finite volumes, the multiscale model developed by Zbib et al. [7,97] also integrates dislocation dynamics with continuum plasticity in such a way that the dislocation dynamics part replaces the "constitutive equations," which are typically postulated in the continuum theory. In this approach, the coupling is based on a framework in which the material obeys the basic laws of continuum mechanics, i.e., the linear momentum balance.

$$\sigma_{ij,j} = \tilde{n}\dot{v}_i \qquad (6)$$

and the energy equation,

$$\tilde{n}c_v\dot{T} = k\nabla^2 T + \sigma_{ij}a_{ij}^P \qquad (7)$$

where $v = \dot{u}$ is the particle velocity, and $\boldsymbol{u}$, ρ, c_v, and k are the displacement vector field, mass density, specific heat, and thermal conductivity, respectively. In DD, the representative volume cell is further discretized into subcells or finite elements, each representing a representative volume element (RVE). Then the internal stresses field induced by the dislocations (and other defects) and

the plastic strain field within each RVE can be calculated at any point within each element. Furthermore, the plastic strain increment results from only the mobile dislocations that exit the RVE (or subcell) and is computed as in Eq. (5), but with V being the volume of the element (or subcell). The dislocations that are immobile (zero velocity) do not contribute to the plastic strain increment. Therefore, the dislocations within an element induce an internal stress due to their elastic distortion. When some of these dislocations (or all) move and exit the element, they leave behind plastic distortion in the element and the internal stress field should be recomputed by summing the stress from the remaining dislocations in the element. With this homogenization procedure the rate Hooke's law for the RVE becomes

$$\dot{\sigma}_{ij} = C^e_{ijkl}(\dot{\varepsilon}_{kl} - \dot{\varepsilon}^P_{kl}) \qquad (8)$$

where C^e_{ijkl} is the fourth-order elastic tensor. In the continuum plasticity theory, one would need to develop a phenomenological constitutive law for plastic stress-strain behavior. Zbib and coworkers avoid this ambiguity by using the explicit expressions given by Eq. (5) for the plastic strain-rate tensor, as computed in the dislocation dynamics. So in addition to the inputs and outputs one gets from DD, as summarized in Table 1, one also now has a second set of inputs and outputs, as summarized in Table 2, when a concurrent multiscale modeling involving discrete dislocations and finite elements analysis.

The way the two scales, the DD scale and the continuum scale, communicate and pass information to one another is illustrated in Fig. 2.

With the multiscale method described above, Zbib and coworkers were able to address a number of boundary value problems in small-scale crystal plasticity with a wide range of loading and boundary conditions and internal dislocation structures. Here we give only a few examples. Hughes et al. [112] and Khan et al. [113] examined the role of the various dislocation structures, such as geometrically necessary boundaries in hardening phenomena. They showed that by correctly modeling the boundary conditions of dislocations in a finite domain, such as grain, the finite dislocation walls are stabilized, but still result into long-range stress, yielding hardening as well as size effects. Shehadeh et al. [114] studied shock wave propagation and interaction with dislocations in copper single crystals. These authors have shown that avalanche of dislocation density is a natural consequence of shock wave dislocations interaction and the dislocation density followed power law dependence on the pressure. Moreover, the inclusion of pressure-dependent elastic properties for isotropic media leads to
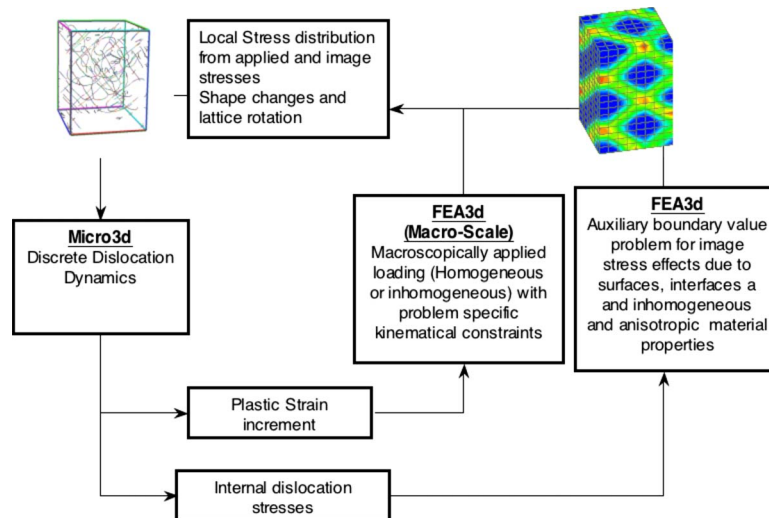
Fig. 2 Multiscale dislocation dynamics plasticity model: coupling of dislocation dynamics with continuum elastovisoplasticty

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faster wave propagation speed and incorporating the effect of crystal anisotropy in the elastic properties results in an orientation dependent wave speed and peak pressure. Moreover, Shehadeh et al. [115] also studied shock-induced dislocation nucleation in single-crystal copper. They developed a model for homogenous nucleation of dislocation based on large-scale molecular dynamics (MD) simulations and nucleation theory and implemented the model in the multiscale dislocation dynamics model described above. They showed that at extremely high pressures, plastic deformation is driven by dislocation nucleation, resulting in a prodigious rate of dislocation production that takes the uniaxially compressed material to a hydrostatically compressed state after a few tens of picoseconds. Akasheh et al. [116,117] used a concurrent multiscale method involving a discrete dislocation model to study the strength of nanoscale metallic multilayered composites. Like in the bulk material, interactions between dislocations (between the threading dislocations and the intersecting interfacial dislocations) predict strength in agreement with experimental trends, which are higher than the predictions obtained with a simple capped layer model. Yashiro et al. [118] used the multiscale model to simulate dislocations cutting into a γ' precipitate and interfacial dislocation network in Ni-based superalloys. They showed that a superdislocation nucleates after two dislocations pile up at the interface and that the width of dislocations is balanced by the antiphase boundary (APB) energy and repulsion of dislocations.

Lemarchand et al. [119] proposed an alternative framework to the superposition method. With this approach, the DD code serves as a material constitutive model and the dislocations are represented in the continuum by continuous fields of eigenstrain. The plastic strains induced by the slip propagating dislocation are calculated by the discrete dislocation method, instead of phenomenological equations used in conventional crystal plasticity. The discrete dislocation methodology was implemented in a finite element code as a material constitutive model using the small strain formulation. The superposition method and the framework used by Lemarchand et al. solve the same system of equations as presented by Devincre et al. [120]. Using the framework of Lemarchand et al., Groh et al. [121] studied the influence of the elastic anisotropy on the critical thickness for the plastic relaxation of thin films. They found that elastic anisotropy induces a significant increase in the critical thickness, with respect to the values predicted by a classical isotropic model. In addition, as the model of Lemarchand et al. includes two lengths scales, the mean distance between dislocations and the geometrical distance, this model is well adapted to study size effect in structural components. With this regards, Groh et al. [122,123] investigated the mechanical properties of a metal matrix composite reinforced by long and unidirectional fibers, Al/Al_2O_3, with dimensions in the micron-meters range. They concluded that the variations in the yield stress, as a function of fiber volume fraction, might be predicted from Orowan's law. Moreover, the dependence of internal stresses on fiber volume fraction leads to a size effect resulting from a virtual decrease in the channel width between fibers. Recently, Liu et al. [124] extended the work of Lemarchand et al. [119], based on the finite deformation theory of crystal plasticity. The major improvement proposed by Liu et al. [124], compared with the original work of Lemarchand et al., is concerning the pre-existing stationary dislocations. To be visible in the continuum, dislocations have to be introduced from the free surfaces in the formulation of Lemarchand et al., while Liu et al. represented pre-existing stationary dislocations by an internal stress field. With the new formation, discrete dislocation plasticity is completely handled under a continuum mechanics framework. Liu et al. applied this new framework to uniaxial compression test for micropillars of Cu to investigate the dislocation starvation hardening observed experimentally. The main results of their compression tests are reviewed in Sec. 3.

As describe above, implementing a dislocation dynamics model

to either a FEM or BEM codes has been proposed many times over the last decade. On the other hand, coupling a 3D discrete dislocations model with a lower length scale is still missing in the literature. However, Shilkrot et al. [125,126] proposed a computational method for multiscale modeling of plasticity, wherein each dislocation is treated as either an atomistic or continuum entity within a single computational framework. The method divides space into atomistic and continuum regions that communicate across a coherent boundary, detects dislocations as they approach the boundary, and seamlessly converts them from one description to another. The method permits the study of problems that are too large for fully atomistic simulation, while preserving accurate atomistic details where necessary, but is currently limited to a 2D implementation.

3 Multiscale Modeling of Micropillars Under Compression

The origin of the length scale effect observed in metals depends on the distribution of the macroscopic deformation. If the macroscopic deformation is not uniform, storage of geometrically necessary dislocations to accommodate the plastic strain gradient is usually considered to explain the origin of the length scale effect [127]. On the other hand, if uniform macroscopic deformation is considered, the storage of dislocation is not significant in a material free of internal interfaces, and length scale effects can be attributed to (i) dislocation cells, (ii) dislocation structures, or (iii) dislocation-obstacle distribution [107].

Uchic et al. [128,129], Greer et al. [130,131], and Shan et al. [132] conducted uniaxial compression tests using a nano-indenter with a flat-ended tip on focused-ion-beam fabricated Ni, Ni_3Al, and Au micropillars. These authors reported two main observations from such compression tests: (i) a dependency in strength scaling with the inverse of the square root of the sample and (ii) the plastic deformation proceeds intermittently as serial bursts. To explain the increase in the yield strength when the size of the pillars is decreased, Parthasarathy et al. [133] proposed a model considering only the statistical variation in the dislocation source length imposed by finite dimensions of the pillars. They have shown that such a model was accurate enough to rationalize the experimental trend. Greer et al. [130,131] proposed a dislocation starvation model to explain the strain bursts.

This problem of size effect in micropillars is well adapted to multiscale discrete dislocations modeling [124,134–137], because (i) the presence of large strain gradients is limited [138] and (ii) the effect of the free surfaces is crucial when the diameter of the sample decreases to the submicron range [102]. Tang et al. [134] performed 3D discrete dislocation simulations to model the mechanical properties of the micropillars orientated for multislips, without solving the boundary value problems [103]. Based on their results, these authors demonstrated that the escape of mobile dislocations in smaller pillars is faster than in larger ones. The decrease in the mobile dislocation density in decreasing the specimen size leads to an increase in the resistance to the plastic flow, and therefore, the scale-dependency yield strength effect was related to the escape of the dislocation through the surfaces. Starting with an initial dislocation Frank net structure, Tang et al. [139] showed that the observed plastic deformation from their simulation is caused by the operation of single junction-stabilized spiral sources and is followed by intervals of purely elastic straining when the sources are shut down. Although the initial dislocation density used by Tang et al. [139] are two orders of magnitude higher than the experimental value [130,140], their simulation results are in qualitative agreement with the experimentally observed behavior with that of Dimiduk et al. [140] and Greer et al. [130]. Using superposition method with the FEM, Weygand et al. [136] used their simulation results to fit the exponent of a power law linking the flow stress to the diameter of the pillar. They found an exponent in the order of −0.6, which is in the range of the experimental findings [140,141]. Senger et al. [137] found

similar results than Weygand et al. [136] by using more statistics. Note that the size effect modeled by Weygand et al. and by Senger et al. is weaker than the size effect reported experimentally by Greer et al. [130,131], who oriented their single crystals for multislips, while it was oriented for single slip for the numerical experiment of Senger et al. [137] and Weygand et al. [136]. El-Awady et al. [102] investigated the mechanical behavior of a cylindrical microcrystal oriented for single slip under compression using the superposition method implemented with the BEM. In addition to presenting data in agreement with experiments, these authors concluded, in agreement with the theoretical model of Parthasarathy et al. [133], which the mean length of dislocations trapped at the surface, was the dominant factor in determining the size effects on hardening of single crystals. Using a micropillar oriented for multislips, El-Awady et al. [137] tested a number of parameters and mechanisms, such as the micropillar size, the average length of activated single-pinned dislocation, and the cross-slip properties, in an effort to identify the size scaling aspects of plastic flow and work hardening. Although the flow stress versus the diameter of the pillars followed a power law with an exponent of −0.69, in good agreement with the data of Dimiduk et al. [140] and Volkert and Lilleodden [141], a stronger size effect was observed between the flow stress and the average length of the activated dislocations (flow stress versus the average length of the activated dislocations followed a power law with an exponent of −0.85). Moreover, the activation of the cross-slip leads to an increase in the dislocation density as well as a reduction in the average length of activated dislocations. Such a reduction in the average length of the activated dislocation leads to an increase in the yield strength. This result is in agreement with the effect of dislocation cross-slip in bulk material [142,143]. Liu et al. [144] studied the stress-strain response of Cu single-crystal micropillars containing initial dislocation networks. They showed that when such networks were loaded, the stress-strain curve can be divided into three distinct stages: (i) a linear elastic stage, (ii) a normal strain hardening stage, and (iii) a "dislocation starvation hardening" stage accompanying a rather high stress level.

More recently, Akarupa et al. [145] and Zbib et al. [146] reexamined the results obtained for micropillars and noted that in all the aforementioned DD simulations of the micropillar experiment, the stress and strain fields were assumed to be homogeneous and no surface effects were accounted for. They noted, however, that the deformation field in submicron scale specimens is far from being homogenous and becomes highly heterogeneous and localized with increased strain as all experiments have shown. Moreover, surface effects in such small dimensions are very important and cannot be neglected. To capture the heterogeneity of the macroscopic deformation and its influence on the microscopic mechanisms, Akarupa et al. [145] and Zbib et al. [145] employed the multiscale model described in Fig. 2. They investigated the deformation of micropillars under compression with constrained loading axis. They showed that the yield stress has strong inverse-power relationship with specimen size when the dimensions are in the submicrometer range. Dislocation arm operation on different glide planes were identified as the primary mechanism for plastic deformation in these microsize specimens. The jerky behavior in the plastic deformation was attributed to the intermittent operation of the dislocation arms. Due to the absence of storage of dislocations, it was concluded that the observed hardening is not because of the conventional work hardening, but because of pinning of dislocation segments due to the formation of junctions and entangled dislocation structures, as well as due to surface effects such as formation of ledges and stress concentration sites. Their results led to the hypotheses that jerky flow and hardening is mainly caused by dislocation stagnation (also noted in the literature as exhaustion), due to the formation of pinning sites resulting in an effective reduction in the mean free length of dislocation and not from a starvation and renuclation mechanism. These predictions were made possible by the use of a multiscale technique, which enables the rigorous analysis of nonuniform deformation of small-scale specimens with realistic treatment of loading and boundary conditions.

4 Concluding Remarks

In this article, we discussed, using examples from the literature, how a discrete dislocation model can be used either in a hierarchical or a concurrent multiscale modeling framework and introduced newcomers to the essential features and limitations of such approaches. As a summary of the methodologies, concurrent techniques were developed to solve a rigorous boundary value problem under complex loading conditions for specimens in the submicron range, while hierarchical techniques were developed to solve problems under homogeneous deformation with periodic boundary conditions.

However, in order to be useable as a predictive tool for the design of engineering materials and structural components, several breakthroughs on multiscale modeling techniques based on discrete dislocation simulations are needed. For example, since the first three-dimensional study on crack growth using homogeneous deformation discrete dislocation model carried out by Devincre and Roberts [147], most of the studies on crack growth were performed at two dimensions using the superposition framework [69,148,149]. Two-dimensional methodology can be used as a qualitative tool to characterize a trend, but cannot be used as a quantitative tool for predictive design. How can a two-dimensional methodology developed to keep track of the crack growth be implemented efficiently to a three-dimensional methodology? In addition, deformation twinning [150,151] is another mode of deformation that complements slip deformation. This mode of deformation is particularly important to model the mechanical behavior of magnesium alloys. Twinning deformation is usually taken into account through an internal state variable in a crystal plasticity model based on a Taylor assumption [152]. Is there a way to implement such a mode of deformation in a concurrent multiscale methodology in order to quantify the interaction between twin systems and dislocation slip systems? Furthermore, Shan et al. [132] reported inhomogeneous dislocation nucleation under the surface during compressive testing of Ni micropillar. Such a question of dislocation nucleation is of extreme importance for engineering materials where void growth occurs by nucleation of dislocation loops at the void surfaces [153–156]. The model developed by Shehadeh et al. [115] for the nucleation of dislocation glide loops provides a pathway to treat dislocation nucleation in a concurrent multiscale modeling technique based on discrete dislocations simulations.

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