SAND2020-3747J

Frontiers in the Simulation of Dislocations

Nicolas Bertin,[1] Ryan B. Sills,[2,3] and Wei Cai[4]

[1]Lawrence Livermore National Laboratory, Livermore, CA 94550, USA; email: bertin1@llnl.gov
[2]Department of Materials Science and Engineering, Rutgers University, Piscataway, NJ 08854, USA; email: ryan.sills@rutgers.edu
[3]Sandia National Laboratories, Livermore, CA 94551, USA
[4]Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA; email: caiwei@stanford.edu

Xxxx. Xxx. Xxx. Xxx. YYYY. AA:1–29

https://doi.org/10.1146/((please add article doi))

Keywords

dislocations, plasticity, multi-scale modeling, information passing, experimental validation, data science

Abstract

Dislocations play a vital role in the mechanical behavior of crystalline materials during deformation. To capture dislocation phenomenon across all relevant scales, a multiscale modeling framework of plasticity has emerged over the years, aimed at reaching a quantitative understanding of microstructure-property relations, such as to predict the strength and toughness of metals and alloys for engineering applications. This paper briefly describes the state-of-the-art for the major dislocation modeling techniques, and then discuss how recent progress can be leveraged to advance the frontiers in simulations of dislocations. The frontiers of dislocation modeling include opportunities to establish quantitative connections between the scales, validate models against experiments, and use data science methods (e.g., machine learning) to gain understanding and enhance the current predictive capabilities.

Contents

1. INTRODUCTION

The mechanics and dynamics of dislocations lies at the heart of many important engineering applications, including aerospace, automotive, aviation, energy, and semiconductors. The behaviors of dislocations, which are line defects in the crystal lattice whose motion generates plastic deformation, play a governing role in the strength, toughness, fatigue-life and creep-life of metallic materials. A comprehensive computational framework, capable of addressing dislocation phenomena across length and time scales, would therefore enable predictive tools to aid materials design, optimization of manufacturing processes, and design for extreme environments (1).

Dislocation physics spans a tremendous range of length and time scales—from the atomic structure of the dislocation core (~ 1 nm) up to the texture of polycrystals (~ 1 mm). Since no single computational tool is capable of capturing the physics across all these scales, a *multi-scale modeling* framework is needed, as shown in Fig. 1. In the context of the simulations of dislocations, the computational tools in this framework, in order from smallest to largest scale, are quantum mechanical models, classical molecular dynamics (MD), discrete dislocation dynamics (DDD), continuum dislocation dynamics (CDD), and crystal plasticity (CP). The essence of the multi-scale framework is that each modeling methodology is best suited to a particular time and length scale range. The higher scale models need inputs from lower scale models, however, on what physical features are most important and on how to faithfully represent those features in a coarse-grained (more approximate) description. For instance, CP models, which are at the top level of the multi-scale hierarchy, ideally should simultaneously account for, in a statistical manner, all phenomena and interactions that occur in lower scale models. This is indeed a very challenging task. Fortunately, the lower scale models are designed to provide such information. The overall thrust of the *information-passing* paradigm in multi-scale modeling is thus to study dislocations at the more fundamental (lower) scales, learn about the key features that govern their behaviors, and then pass that information up to higher scales. This process of upscaling information is repeated until the highest scale is reached, which can be used to make engineering predictions. In some sense, the overall goal of simulations of dislocations is to robustly

establish this multi-scale framework so that it can be applied pervasively across materials and applications.

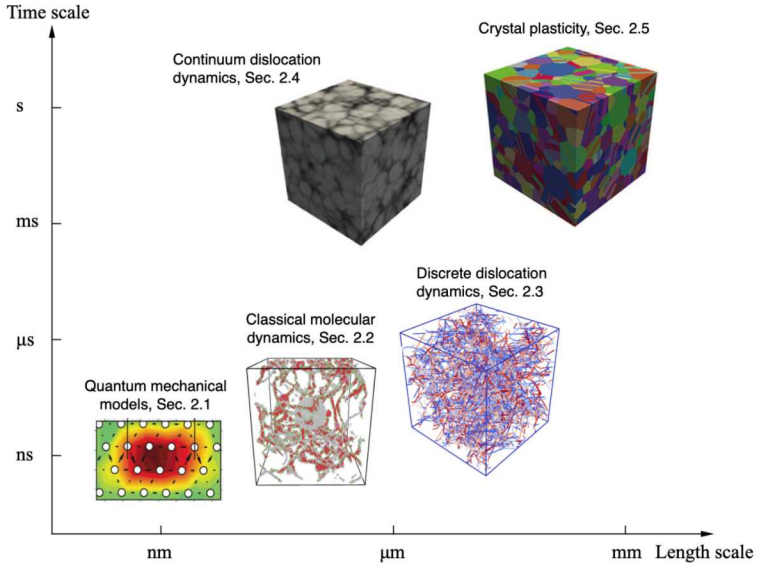

Figure 1

Multi-scale models of dislocations discussed in this review, showing the approximate length and time scales for each. Figure modified from (2). Graphics reproduced from (3, 4, 5, 6, 7) with permission.

There has been a lot of recent progress regarding simulations of dislocations at the various scales, see Table 1. However, the multi-scale framework of dislocation simulations presently still has a number of gaps that limit its predictive capabilities (1). The goal of this article is to highlight those gaps and discuss recent advances that present opportunities for addressing them. The largest issue is that, with a few exceptions, linkages between the various models are not well established. Some linkages are poorly established either because it is unclear how to meaningfully coarse-grain the information from the lower scale models, it is unclear how to make use of upscaled information in a higher scale model, or because performance of the lower scale model is too limited to simulate the necessary deformation processes. A consequence of the disjointed state of the multi-scale framework is that the higher scale models (CP) are still largely phenomenological, which often limits their accuracy and predictive power (8, 9). We believe another important aspect of the multi-scale modeling framework is that lower and higher scale models need to be directly compared in simulations with (nearly) identical conditions. Such comparisons serve as important validation steps for the large scale models, which are farther from fundamental physics than the small scale models. Similarly, comparisons must be made between models and experiments across as many of the scales as possible in order to establish that these models are accurate approximations of real material systems. In particular, comparisons between experiments and meso-scale models (DDD and CDD) are most lacking to date. Hence, the gaps in the multi-scale framework can be summarized in two words: *upscaling* and *validation*. These are the topics that need to be focused on to push multi-scale modeling

of plasticity forward in the coming years.

The frontiers of simulations of dislocations are areas where progress can be made to close these gaps by leveraging recent advances. These advances come in three areas: simulation techniques, experimental techniques, and data-science methods. Improved simulation techniques include: methods for extracting dislocation information from MD datasets; efficient time integrators, force computation routines, image solvers, and analysis tools for DDD; and new formulations for CDD. On the experimental side, new methods include: high strain rate small-scale testing methods; and techniques for extraction of 3D microstructure information in the transmission electron microscope and using X-ray diffraction. Finally, these improvements drive a need for advanced analysis techniques capable of making sense of increasingly complex data sets. Data science approaches, such as machine learning, are quickly filling this need, with a few examples in the area of dislocation modeling already. Likely, the frontier of dislocation simulations is the intersection of all three of these areas, where data science is concurrently applied to experimental and simulation data sets to advance understanding. In particular, we believe that because of DDD's maturity, affordable computational cost, and meso-scale position in the modeling hierarchy, it stands to advance the frontier of dislocation modeling substantially.

The remainder of this review seeks to quickly describe the state-of-the-art for the five major dislocation modeling techniques (Section 2), and then discuss how these methods can be leveraged to advance the frontiers (Section 3). The discussions are carried out in light of the recent advances in simulations of dislocations, whose representative publications are summarized in Table 1.

2. MULTI-SCALE FRAMEWORK OF DISLOCATION MODELS

2.1. Quantum mechanical models

Models based on quantum mechanics provide the most accurate physical description and are the most computationally expensive within the multi-scale framework of dislocation models. Most of these models take the Born-Oppenheimer (BO) approximation, in which the atomic nuclei follow classical mechanics, while the electrons are represented by quantum mechanical wave functions and are assumed to stay at the ground state given the instantaneous position of the nuclei. These models are often referred to as first-principles or *ab initio* models, for which the density functional theory (DFT) is the most widely used approximation for the quantum mechanical energy of the electrons (10).

The computational cost of DFT codes (e.g., VASP) often scales cubically with the number of atoms. Due to the high computational cost, DFT simulations are usually limited to a few hundred atoms. Hence DFT studies are most often focused on the structure and energy of the dislocation core (3, 11), through zero temperature energy minimization calculations. For example, DFT models have recently been used to study the stability and mobility of dislocations in the pyramidal and prismatic slip systems of hexagonal closed-packed (HCP) Ti and Zr, demonstrating that Ti exhibits a "locking" mechanism that limits overall mobility while Zr does not (13). DFT has also been used to study dislocation-solute interactions in Al (12) and Fe (11) alloys, showing in the latter case that interstitial solutes stabilize the so-called hard-core of a screw dislocation in body-centered cubic (BCC) metals. *Ab initio* models have also been widely used to generate material property databases for developing interatomic potentials (89) for classical molecular dynamics models (see Section 2.2). Recently, alternative implementations of the DFT method have been developed

Table 1 Recent advances in dislocation modeling and crystal plasticity.

	References
Quantum simulations	Review: (10)
Dislocation core structures	(3, 11)
Barrier to dislocation motion	(12, 13)
Dislocations in quantum crystals	(14, 15, 16)
Classical molecular simulations	Book: (17), Review: (18)
Dislocation core energies	(19, 20, 21)
Dislocation mobility	(22, 23, 24, 25)
Cross-slip	(26, 27)
Dislocation-obstacle interactions	(28, 29)
Dislocation nucleation	(30, 31)
Dislocation extraction algorithm (DXA)	(32, 33)
Ultra-scale MD simulations of plasticity	(34, 35)
Discrete dislocation dynamics	Book: (17), Review: (36)
Numerical integrators and parallelization	(37, 38, 39)
Long range stress calculations	(37, 40, 41, 42, 43, 44)
Image stress solvers for small samples	(45, 46, 47)
Latent hardening coefficients	(48, 49, 50, 51, 52)
Large-scale work-hardening	(53, 6, 54)
Grain boundaries and polycrystals	(55, 56, 43, 57)
Creep and dislocation climb at high temperature	(58, 59)
Irradiation-induced damage	(60, 61, 62, 63)
Obstacle bypass	(64, 21)
X-ray diffraction	(65, 66, 67, 68)
Continuum dislocation dynamics	Review: (69)
Field dislocation mechanics (FDM)	(70, 71, 72, 73, 74, 75, 76)
High-order continuum dislocation dynamics	(77, 78, 79, 80)
Dislocation patterning	(81, 4, 82)
Crystal plasticity models	Review: (83)
Dislocation-density based models	(84, 85, 86, 87, 88, 52)

that scale more favorably with system size (90, 91, 92), but they have yet to become widely adopted for dislocation studies.

While *ab initio* methods deal with the quantum mechanics of the electrons, it is also possible to account for the quantum effects of the atomic nucleii when modeling dislocations. For example, the effect of zero-point motion on the lattice resistance (i.e. Peierls stress) of screw dislocations in body-centered cubic (BCC) Fe has been investigated using the harmonic approximation (14) and ring-polymer molecular dynamics (RPMD) (15). The path-integral Monte Carlo (PIMC) method has been applied to study the dislocation core properties in hexagonal close packed (HCP) ^{4}He (16), which is a quantum solid due to the light mass and strong zero-point fluctuation of helium atoms.

2.2. Classical molecular simulations

In models based on classical mechanics, the fundamental degrees of freedom are the position of atoms, $\{\mathbf{r}_j\}$, $j = 1, \cdots, N$, where $\mathbf{r}_j$ is the position vector of atom j, and N is the total number of atoms. The atoms are assumed to interact with each other through a potential energy function, $U(\{\mathbf{r}_j\})$. In the classical molecular dynamics (MD) method, the atomic

trajectories are computed by integrating Newton's equation of motion,

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\nabla_{\mathbf{r}_i} U(\{\mathbf{r}_j\}), \quad i = 1....N \qquad 1.$$

under appropriate initial and boundary conditions, where m_i is the mass of atom i, and $\nabla_{\mathbf{r}_i}$ denotes the gradient with respect to the position of atom i. In the molecular statics (MS) method, the energy and structure of the dislocation can be obtained by minimizing the potential energy function $U(\{\mathbf{r}_j\})$. Classical MD and MS methods have been extensively used to study the properties of individual dislocations, e.g. such as line energies (19, 20), mobilities (22, 93, 23, 24, 25), cross-slip rates (26, 27), interactions between a few dislocations (94, 95), interactions between dislocations and other defects, such as twins and grain boundaries (96), precipitates (97, 98), and, more recently, the behavior of large collections of dislocations (34, 35).

While classical molecular simulation methods are well established (18), analyzing atomic trajectories to extract information on dislocations can be a labor intensive task. Although algorithms exist to identify atoms near defects (e.g., by coordination number or central symmetry analysis), it is not easy to identify the Burgers vector of dislocations from the atomic coordinates. Recently, the dislocation extraction algorithm (DXA) (32, 33) has been developed, which automatically detects, traces in space, and determines the Burgers vector of dislocations in an arbitrary atomic system. DXA is efficient enough that it can be employed on-the-fly during ultra-scale atomistic simulations ($> 10^9$ atoms) (34), enabling the complete time history of a dislocation network to be cataloged. We will discuss some of the opportunities enabled by DXA in Section 3.1.

Although the computational cost of classical MD scales linearly with the number of atoms, the cost of simulating large atomistic systems is still high. Today, MD simulations on dislocations are usually performed for systems containing up to $\sim 10^6$ atoms using $\sim$ 100 CPUs. Given that MD time steps are typically on the order of 1 fs, the time duration of MD simulations is on the order of $\sim$ 10 ns (assuming 10^7 steps), leading to very high strain rates ($\sim 10^7\,\mathrm{s}^{-1}$, assuming 10% strain over 10 ns). To overcome the timescale limitation, a number of advanced techniques for computing transition/activation rates have been applied to thermally activated dislocation processes such as nucleation (30, 31) and obstacle bypass (28, 29). Accelerated molecular dynamics methods (99) have shown promising results in the dynamics of point defects in crystals (100), but their applications to dislocations (being an extended defect) have been difficult.

2.3. Discrete dislocation dynamics

In discrete dislocation dynamics (DDD), the dislocation lines are often discretized into straight segments (17, 37) (although curved splines can also be used (101)), in which case the fundamental degrees of freedom are the position of a set of nodes $\{\mathbf{r}_j\}$, $j = 1, \cdots, N$, and the set of Burgers vectors $\{\mathbf{b}_{ij}\}$ for the segments connecting the nodes. A major distinction of DDD in the multi-scale hierarchy is that the total number of degrees of freedom do not stay constant. Instead, the number of nodes, N, often increases dramatically due to dislocation multiplication during straining.

Given the dislocation network (as specified by $\{\mathbf{r}_j\}$ and $\{\mathbf{b}_{ij}\}$), the stress field $\boldsymbol{\sigma}(\mathbf{x})$ can be computed based on continuum (usually isotropic) linear elasticity theory. The stress field produces Peach-Koehler force on the dislocation lines, leading to driving force $\mathbf{F}_i^{\mathrm{drive}}$ on every node i, and ultimately a nodal velocity based on a mobility law function $\mathbf{v}_i =$

$\mathbf{M}\left(\mathbf{F}_i^{\text{drive}}\right)$. Therefore, the equation of motion in DDD is a first-order over-damped equation that can be written as (102, 36),

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{g}_i\left(\{\mathbf{r}_j\}\right), \quad i = 1....N \qquad 2.$$

where the function $\mathbf{g}_i$ subsumes the calculation of nodal force followed by the nodal velocity using the mobility law. The mobility law encodes information about crystallographic constraints on dislocation motion and drag mechanisms and can be constructed from the predictions of molecular dynamics models (Section 2.2). Special algorithms have been developed to detect dislocation collisions and handle topological changes in the dislocation network (e.g., junction formation, annihilation, and insertion/deletion of discretization nodes as the lengths of the dislocation lines change).

Over the years, there have been significant performance improvements in DDD methods. These include the development of analytical expressions for short-range interaction forces (103, 104), efficient long-range force calculations with the fast multipole method (FMM) (37, 40), and full-field eigenstrain-based approaches using the finite element method (FEM) (105, 41) and the fast Fourier transform (FFT) method (42, 44).

Recently, Sills et al. (38) developed a subcycling time integrator based on a decomposition of the dislocation forces. This method showed a 100-fold performance gain compared to traditional integrators during serial computation, and fair scalability up to 64 cores during parallel computation. The subcycling integrator has further been extended for use with graphics processing units (GPUs), which provides an additional 40-fold improvement in performance compared to a single CPU (39). This gain in efficiency enables large-scale DDD simulations without the need for major computational resources.

Furthermore, several techniques have been introduced to perform DDD simulations beyond the traditional case of bulk single crystals. The developement of eigenstrain-based approaches (41, 42, 43) that are readily employable for anisotropic and heterogeneous media are paving the way to DDD simulations of polycrystals. In order to simulate small-scale experiments (106) (e.g., nano-indentation, micro-pillar compression, and micro-tension tests), image stress solvers capable of accounting for the free surfaces of the specimen have been developed. For example, fast spectral image stress solvers have been developed for simulating cylindrical (45) and thin film geometries (46), as well as nano-indentation (47). These methods exhibit exponential convergence in terms of the number of grid points used, making them significantly faster than FEM solvers.

2.4. Continuum dislocation dynamics

In continuum dislocation dynamics (CDD), the fundamental degrees of freedom are a set of fields defined over the simulation volume, $\{\rho_J(\mathbf{x})\}$, $J = 1, \cdots, N_{\text{f}}$, where N_{f} is the total number of fields. While the choice of field variables varies among different CDD formulations (see review in (69)), it is common for ρ_J to be a measure of some component of the dislocation density. For example, the Nye's tensor $\boldsymbol{\alpha}$ (107) is a commonly used field variable in CDD formulations. It measures the so called *geometrically-necessary* dislocation (GND) density and can be used to compute the internal stress field $\boldsymbol{\sigma}(\mathbf{x})$.

The equation of motion in CDD is a first-order (in time) partial differential equation (PDE) describing the rate of field evolution $\frac{\partial}{\partial t}\rho_I(\mathbf{x})$ given the current configuration of all fields $\{\rho_J(\mathbf{x})\}$. For example, in the field dislocation mechanics (FDM) formulation (70, 71),

the field evolution equation can be formally written as

$$\frac{\partial \boldsymbol{\alpha}(\mathbf{x})}{\partial t} = -\boldsymbol{\nabla} \times (\boldsymbol{\alpha}(\mathbf{x}) \times \mathbf{v}(\mathbf{x})) \tag{3.}$$

where $\mathbf{v}$ is a velocity vector describing the motion of dislocations subjected to the internal and applied stresses.

"Kinematic closure" is a frequently encountered challenge in CDD formulations. For example, the velocity field $\mathbf{v}(\mathbf{x})$ depends not only on the GND density $\boldsymbol{\alpha}$ but also the *statistically stored* dislocation (SSD) density, which was not captured in FDM. To address this problem, the phenomenological mesoscopic field dislocation mechanics (PMFDM) (72) was later introduced, in which the velocity field $\mathbf{v}(\mathbf{x})$ and the resulting plastic strain rate are prescribed phenomenologically. As another approach to achieve closure, Hochrainer et al. (77) proposed a new three-dimensional dislocation measure based on the dislocation density and the line curvature fields defined in the higher configurational space of the spatial position and the line direction. Simplified models (78, 79, 80, 81) were subsequently proposed to alleviate the computational cost of this higher-order CDD model, e.g., by using phenomenological relations to approximate the evolution of the average curvature (81).

Recently, Xia et al. (4) proposed a CDD model in which dislocations are represented as vector fields (representing the local dislocation line orientations) for every slip system. The kinetic evolution laws are then developed by assuming that dislocations on each slip system arrange into bundles with a unique line orientation at each material point. Much like in the higher-order CDD, this formulation has the advantage of preserving a direct connection between dislocation velocities and internal stresses through the Peach-Koehler force. Yet the decomposition into slip systems allows for explicit incorporation of fundamental unit mechanisms, such as cross-slip, in the transport evolution laws (108), offering a clearer path of calibrating CDD models against DDD simulations.

2.5. Constitutive laws in crystal plasticity models

Crystal plasticity (CP) models are at the top of the multi-scale hierarchy of plasticity models and allow for direct comparisons with experiments at the macro-scale. They have been used for a wide range of applications, including the prediction of the mechanical response of polycrystalline materials subjected to various loading types, texture evolution during forming, inter-granular and Hall-Petch behaviors, mechanical strength, failure and damage propagation, nanoindentation and micropillar plastic responses, to name a few; see (83) for a detailed review. CP models are often implemented using the finite-element method (FEM) (83), although other implementations such as the micro-mechanical self-consistent method (109) and the full-field Fourier-based method (110) have also been developed.

At the heart of CP models is a constitutive law, which, in the local formulation, prescribes the plastic strain rate at a material point given the current state of the material and the imposed loading at that point. For example, the fundamental degrees of freedom for a phenomenological CP model at a given material point can be the set of shear strain $\{\gamma_i\}$ and flow resistance $\{\tau_i^{\mathrm{c}}\}$ on slip system i, $i = 1, \cdots, N_{\mathrm{s}}$, where N_{s} is the total number of slip systems. A commonly used constitutive law can be written in the following form,

$$\dot{\gamma}_i = \dot{\gamma}_0 \left(\frac{\tau_i}{\tau_i^{\mathrm{c}}} \right)^n, \qquad \dot{\tau}_i^{\mathrm{c}} = \sum_{j=1}^{N_{\mathrm{s}}} h_{ij} \left| \dot{\gamma}_j \right| \tag{4.}$$

where the dot indicates time derivative, τ_i is the resolved shear stress on slip system i, $\dot{\gamma}_0$ and n are material constants accounting for the rate sensitivity of plastic flow, and h_{ij} is called the hardening matrix whose components are functions of τ_j^c.

While the phenomenological constitutive law as described above is not directly linked to lower scale dislocation models, dislocation-based constitutive laws have been developed, which incorporate more dislocation-specific variables, such as the dislocation densities $\{\rho_i\}$ on every slip system i, into the degrees of freedom and equations of motion. As a result, dislocation physics, such as Taylor and Orowan relations, can be naturally introduced, and the evolution of dislocation densities is quantitatively accounted for in the constitutive law (84, 85, 86, 87, 88). Further developments of CP models are aimed at making them more accurate and predictive. For this purpose, lower-scale dislocation models have an increasingly important role to play, both by determining the material parameters in CP models and, more importantly, by making CP models aware of dislocation microstructures (beyond density) and unit mechanisms (e.g., junction formation and cross slip) that control the microstructure evolution.

3. FRONTIERS IN MULTI-SCALE MODELS OF DISLOCATIONS

We identify here five areas of research that we believe will be especially impactful to dislocation research in the next decade. As illustrated in Fig. 2, these represent exciting opportunities to establish quantitative connections between models at different scales, and between models and experiments, so that the multi-scale framework can be robust enough to allow dislocation physics to make a direct impact on the engineering calculations of crystal plasticity.

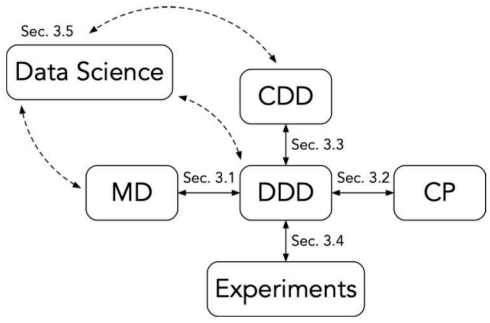

Figure 2

Layout of the frontier topics on dislocation research to be discussed in this section. They represent opportunities to strengthen the connections between models at different scales, and between models and experiments.

First, we discuss new opportunities for establishing meaningful connections between the various dislocation models. Quantitatively connecting the computational models across the different scales is one of the major challenges in obtaining and maintaining a successful, predictive framework for multi-scale modelling of plasticity. From a methodological standpoint, the purpose is to benchmark and calibrate an upper scale model against a more fundamental, lower scale model, while quantifying how much information is lost in the transfer. In the existing hierarchy of modelling approaches, we believe that DDD has a

central role to play in establishing links between the scales. By representing dislocations as line objects, DDD simultaneously retains key microstructural features of the dislocation network, while reducing the number of degrees of freedom by roughly ten orders of magnitude compared to an atomistic description. Therefore, when properly calibrated against atomistic models, the relatively affordable cost and high flexibility of DDD makes it an ideal platform for comparing and calibrating higher-scale models of dislocation-mediated plasticity. In Sections 3.1-3.3, we thus discuss new opportunities to connect DDD to MD, use DDD to inform constitutive laws, and connect CDD to DDD and continuum theories of plasticity. In Section 3.4, we then discuss how recent advances in experimental capabilities enable new direct comparisons between simulations and experimental observations. Finally, in Section 3.5, we discuss how data science and machine leaning tools can contribute to the development of physics-based models and theories of plasticity.

3.1. Connecting MD and DDD models

The key premise of the DDD method is that the response to straining of a statistically representative ensemble of dislocations can be assembled from the motion of its individual constituent dislocations. In going from an atomistic description to a line representation of dislocations, the connection between MD and DDD primarily lies in the core energies and mobility laws of individual dislocation lines. To establish this connection, the conventional workflow has consisted of simulations of isolated dislocations. Core energies of dislocation lines have been extracted by comparing the total energy of periodic arrays of straight, infinite dislocation dipoles calculated from *ab initio* (111, 112) or classical atomistic (19, 20, 21) simulations to their corresponding elastic energies obtained in continuum theories (113, 103). Similarly, mobility laws of individual, straight dislocations have been constructed by extracting force-velocity relations from classical MD simulations of dislocations with different character angles and temperatures in FCC metals (22, 25). For dislocations that experience a higher lattice resistance, atomistic simulations have focused on the kink-pair mechanism in BCC crystals (114, 115, 116, 23, 24), on the motion on different slip planes in HCP crystals (93), and phenomenological mobility laws have been proposed for DDD models (117, 118, 119, 120). Very recently, parametrization of line dynamics was also proposed by analyzing the spectrum of thermal fluctuations of the dislocations, here again extracted from atomistic simulations of dislocation dipoles (121).

While this conventional workflow has been widely adopted, the uncertainties associated with this approach of information passing are yet to be quantified. Specifically, it remains unclear if and how much is lost in transferring knowledge gained in atomistic simulations of individual dislocations to large-scale DDD simulations of crystal plasticity, and what are the effects of the atomistic mechanisms currently ignored in most DDD models, such as jog and point defect production from dislocation intersections. Here, the recent demonstration of the feasibility of ultra-scale MD simulations conducted by Zepada-Ruiz et al. (34, 35) now offers a way to address these questions and opens a new path to validate the DDD model. While such simulations have long been thought inaccessible, the authors in (34) performed MD simulations to probe the limits of dislocation-mediated plasticity in BCC Ta, using simulation cells as large as 0.3 μm, simulation times as long as 1 μs, and strain rates as low as 10^6 s^{-1}, see Fig. 3. Importantly, it was observed that after sufficient straining, the flow stress and dislocation density saturated to path-independent values that are only a function of the true strain rate. Similar simulations were also performed to investigate work

hardening in FCC Al crystals loaded in uniaxial tension along various orientations (35), where it was found that 3-stage hardening was solely a consequence of crystal rotation. Thanks to the DXA algorithm (32, 33), which extracts dislocation configurations from the atomistic trajectory in the form of discrete dislocation networks, the evolution of the dislocation networks in these works could be recorded and analysed. Thus, these simulations provide an unprecedented opportunity to compare and benchmark DDD to MD in terms of the collective dynamics and network structure of statistically representative dislocation ensembles, for which one-to-one correspondences can now be established.

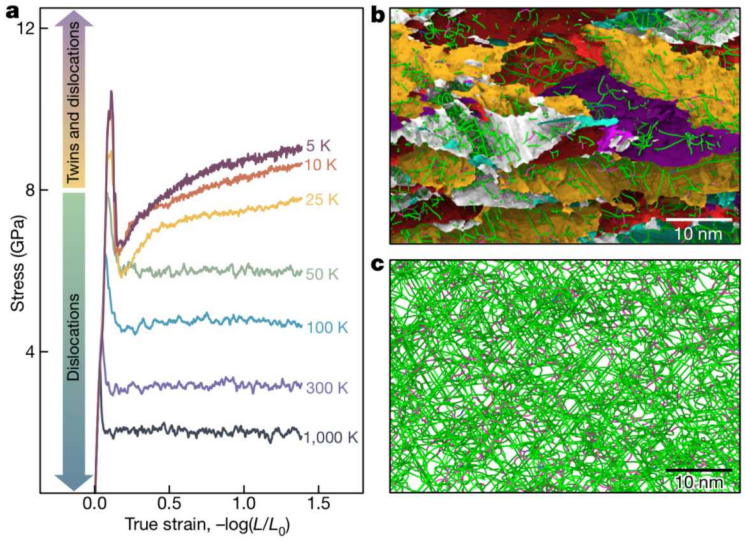

Figure 3

Results from molecular dynamics simulations of uniaxial compression of BCC Ta at a strain rate of 5.55×10^7 s^{-1}. (a) Stress-strain curves at different temperatures. Snapshots from (b) 25 K and (c) 50 K simulations showing twins and dislocations extracted from MD snapshots using DXA and the grain segmentation algorithm (GSA). Reproduced from Zepada-Ruiz et al. (34) with permission.

Achieving a quantitative agreement between MD and DDD simulations in terms of stress-strain response, dislocation multiplication, dislocation fluxes, and network structure evolution would constitute a major milestone for validating the coarse-graining approach from the atomistic scale to the meso-scale. In the future, ultra-scale MD simulations of the kind will become more common, and will be used to benchmark DDD models under more complex scenarios, e.g., in the presence of precipitates or grain-boundaries. Should the conventional approach based on knowledge transfer of individual dislocation properties and unit mechanisms be found insufficient, a new workflow will need to be established wherein key properties (dislocation core features, mobility laws, local rules, etc.) are extracted from direct observations of large-scale MD simulations.

Another way to connect MD and DDD models is through the so-called concurrent multi-scale approach, for which recent progress have been made through the development of the Coupled Atomistic / Discrete-Dislocation (CADD) method (122). In CADD, the simulation volume is decomposed into MD and DDD sub-domains that are evolved concurrently and

are coupled through an atomistic-to-continuum interface via displacement boundary conditions (122). With this approach, the dislocation behaviors can be accounted for in atomistic details in specific regions of interest (e.g., the crack tip), while the rest of the domain is simulated more efficiently with a DDD model. When core energies and mobility laws are well calibrated in the DDD model, the dynamics of dislocations in the CADD model has been demonstrated to be in very good agreement with fully atomistic simulations (123).

3.2. Using DDD to inform constitutive models

The recent performance enhancements for DDD (41, 42, 38, 44, 39) are enabling an increased role in constitutive theory development for plasticity. In this regard, DDD is a unique tool within the multi-scale hierarchy of methods because it is capable of linking the physics of individual dislocation lines with the stress-strain response of a material volume through the evolution of dislocation networks. Two recent studies have demonstrated this capability through large-scale DDD simulations ($> (10\,\mu\text{m})^3$) of strain hardening.

Sills et al. (6) performed DDD simulations of tensile deformation of bulk single crystalline Cu in a $(15\ \mu\text{m})^3$ simulation cell at the strain rates of $10^2\,\text{s}^{-1}$ and $10^3\,\text{s}^{-1}$ along the [001] direction, making use of the subcycling time integrator (38). Notice that the simulation volume is much bigger and the strain rates are many orders of magnitude lower than what can be afforded by even the ultra-scale MD simulations. The authors observed that the lengths of dislocation lines forming the dislocation network obeyed an exponential distribution, which can be described by two parameters, the total density ρ and a non-dimensional parameter ϕ. If the lengths of a dislocation network were scaled down uniformly by a factor λ, then the total density ρ would increase by a factor of λ^2, while the non-dimensional parameter ϕ would remain constant. In this sense, ϕ is a "true measure" of how the dislocation lines are arranged, independent of their concentration, in the material volume. The parameter ϕ is an example of how DDD simulations can identify key parameters and relations that may be worth considering in the coarse-grained description of dislocation-mediated plasticity such as CDD and CP.

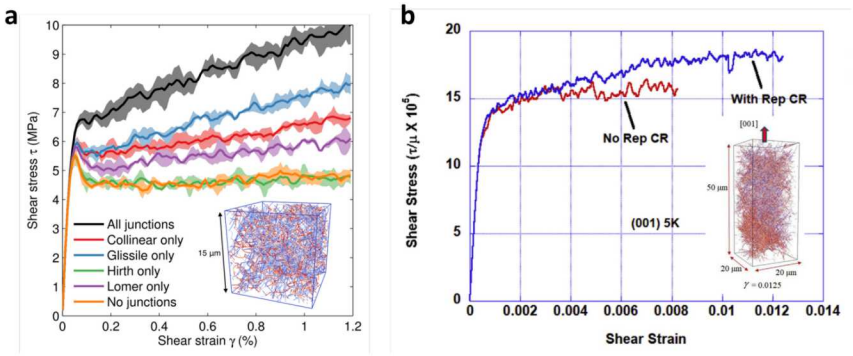

Figure 4

Shear stress-strain curves and simulation snapshots from DDD simulations of uniaxial deformation in pure FCC metals. (a) Results for Cu showing the influence of each junction type. (b) Results for Ni showing behavior with and without cross-slip. Reproduced from (a) Sills et al. (6) and (b) Rao et al. (54) with permission.

An interesting advantage of DDD compared to MD is that in DDD the dislocation physics can be altered by manipulating "local rules" to probe the significance of various mechanisms in the overall stress-strain behavior of the crystal. For example, by strategically suppressing the formation of certain types of junctions, the authors (6) found that junction formation was essential for strain hardening and ranked the relative contributions from the four types of junctions to the hardening rate in FCC crystals (Fig. 4(a)).

Similarly, the role of cross slip in strain hardening was investigated by Rao et al. (54) using DDD simulations of tensile deformation of single crystalline Ni micropillars with dimensions $20 \times 20 \times 50$ μm. These simulations used a detailed cross-slip formulation (53) based on atomistic calculations (26) considering cross-slip with a variety of dislocation geometries, such as from dislocation intersections. The study concluded that cross-slip was essential for strain hardening in micropillars; when the authors suppressed cross-slip the dislocation multiplication and hardening rate reduced significantly (Fig. 4(b)).

These studies give examples for how large-scale DDD simulations can be used to understand the physics of plasticity and give new insights into constitutive behaviors (e.g., hardening). Future studies can leverage the newly acquired DDD capabilities to improve constitutive laws used in crystal plasticity (CP) models.

At present, almost all CP models invoke phenomenological assumptions to enable closure of the governing equations (e.g., Eq. (4)). Accelerated DDD methods provide an opportunity for physics-based input into these equations. The difficult aspect of this process is determining what specific information to extract from the evolving dislocation network and how to then incorporate it into the governing equations. One example of successful transfer of information is the development of specialized DDD simulations to quantify latent hardening coefficients between different slip systems (48, 50, 51), which are now routinely used in dislocation density-based constitutive laws (49). Additional research is necessary to develop more general frameworks for upscaling information from DDD to CP.

Future studies can also leverage the ongoing research focused on simulating the deformation of polycrystalline geometries with DDD (55, 56, 57), renewed interest in the role of dislocation-like defects (e.g., disconnections) in grain boundary dynamics (124), as well as the incorporation of other complex physics (36), such as interaction with point defects (58, 59), precipitates (64, 21) and radiation-induced damage (60, 61, 62, 63).

3.3. Using CDD to understand dislocation patterning

Although CDD approaches are still in their nascency and their numerical implementation remains challenging, several applications have emerged in the recent years. FDM-based approaches have been applied to study thin-films (74) and dislocation pile-ups (76) in 2D, and to 3D settings by assuming particular forms for the velocity functional or imposing constant velocity fields (72, 73, 75). The first successful 3D implementation of higher-order CDD was reported in (78), where the model introduced in (77) was applied to simulate plasticity arising from two active slip systems in a micro-bending experiment.

Of particular interest in the development of CDD models is to predict the spontaneous emergence of dislocation patterning during plastic deformation, which has been observed consistently in experiments for several decades (125). Recent applications of CDD have indeed produced dislocation patterning in 2D (81, 82) and 3D (4). In (81), the authors adopted a simplified 2D version of the higher-order CDD framework introduced in (77), and used a Taylor-like relationship to describe short-range elastic interactions. By varying

the applied stress, they observed the formation of patterns that are consistent with the principle of similitude, i.e., whose wavelengths inversely scale with the applied shear stress (see Fig. 5(a-b)). Through linear stability analysis and simulation results, the authors attributed the origin of pattern formation to short-range interactions, while discarding the effect of long-range stresses. Surprisingly, however, the patterns obtained in this work consisted of cell-like structures with densely populated interior regions bounded by depleted walls. In another study, a CDD model based on slip systems (4) was used to study pattern formation in three-dimensional simulations. The model predicted the formation of dislocation patterning that is also consistent with the principle of similitude, see Fig. 5(c-d). Their observed pattern formation was seen to be contingent on the cross-slip mechanism, which is intrinsically a three-dimensional process. In contrast to the simplified 2D model (81), the resulting patterns exhibit high dislocation densities at narrow cell walls bounding lower-density cell interiors, consistent with experimental observations.

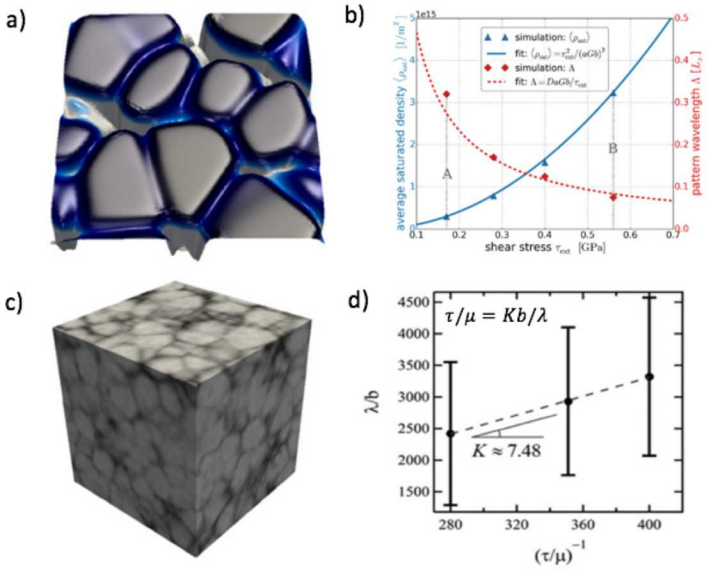

Figure 5

Examples of dislocation patterning and relation between patterns wavelength Λ and the applied shear stress τ using (a-b) the 2D CDD model in (81) and (c-d) the 3D CDD model developed in (4). Reproduced from Sandfeld and Zaiser (81)(a-b) and Xia et al. (4)(c-d) with permission.

In addition to these promising results, it is now also possible to benchmark CDD formulations against lower-scales simulations thanks to recent progress in their implementation. Such a comparison was for instance initiated in (126) where it was found that the kinematics of a CDD method is consistent with that of DDD under several different boundary conditions. So far, the comparison was carried out on relatively simple configurations made of non-intersecting circular dislocation loops subjected to a fixed velocity field, i.e., neglecting elastic interactions. Such comparisons are enabled by the recent development of techniques for converting discrete dislocations into continuum fields (126, 44). With these techniques, dynamic CDD fields that result from the motion of dislocation lines explicitly

computed with a DDD model can be generated, thereby offering a basis to compare and inform evolution laws to be incorporated in mesoscale CDD and FDM models at scales where individual dislocations are no longer resolved. The development of slip system based CDD approaches (e.g., (4)) in which the notion of crystallography is introduced explicitly also allows for direct connections between DDD and CDD. For instance, DDD simulations were used to inform the cross-slip mechanism implemented in the CDD model in (108). Direct comparisons between predictions of DDD and CDD simulations were recently made by Sudmanns et al. (127), where uniaxial tension of a 5 μm cube was simulated. Using guidance from DDD simulations, additional terms in the CDD governing equations were constructed to consider multiplication by glissile junction formation and cross-slip. The dislocation densities in the active and inactive slip systems from DDD and CDD were shown to be in strong agreement. This study shows how insight gained from a lower scale model can inform higher scale model development.

Once properly calibrated and validated, CDD appears as a promising technique for simulating dislocation-mediated plasticity with some unique advantages. First, as a mesoscale model CDD enjoys an advantage (compared to DDD) in that its number of degrees of freedom is independent of the strain level and dislocation density. Second, being the only model that has clearly shown dislocation patterning, it is in a unique position to investigate the fundamental mechanisms and resolve the controversy on the root cause of pattern formation (4, 81). Third, capturing patterning offers an opportunity to establish a direct comparison with experimental results, especially in the low strain rate regime (e.g. $< 1\,\mathrm{s}^{-1}$).

3.4. Opportunities to connect models to experiments

One of the keys to advancing our understanding of dislocation physics and dislocation-mediated plasticity is comparisons with experiments, which enable both validation of modeling assumptions and the establishment of mechanistic linkages (128). Such comparisons have been made at the atomic scale using high resolution transmission electron microscopy (HRTEM) (129) and at the continuum (polycrystalline) scale using digital image correlation (DIC) and electron backscatter diffraction (EBSD) (130, 131). Yet comparisons at the meso-scale between methods like DDD and observations of dislocation microstructures have been elusive. These comparisons have been difficult because of mismatches in time/length scales and because it is not always straightforward to relate experimental data sets to simulation data sets in an unambiguous way. We believe there are now three classes of experiments where direct comparisons with DDD are possible: high strain rate experiments, transmission electron tomography, and X-ray diffraction (see Fig. 6).

Due to time scale limitations, DDD simulations for pure FCC metals are limited to strain rates of $10^2\ \mathrm{s}^{-1}$ or greater, falling in the regime of high strain rate experiments. The Kolsky (split Hopkinson) bar is a widely used technique for testing materials at high strain rates (137). To our knowledge, direct comparisons between DDD simulations and Kolsky bar experiments have yet to be made. Recent DDD performance enhancements enable large enough strains ($\sim 5\%$) to be attained such that computed stress-strain curves can be meaningfully compared with experiments. Such comparisons could also leverage digital image correlation for full-field strain mapping (138) and pulse shaping methods (139) to increase test accuracy at the low strains which are attainable in DDD simulations. While the Kolsky bar can be applied to "bulk" samples ($\sim$ 0.1 to 1 cm), small-scale mechanical

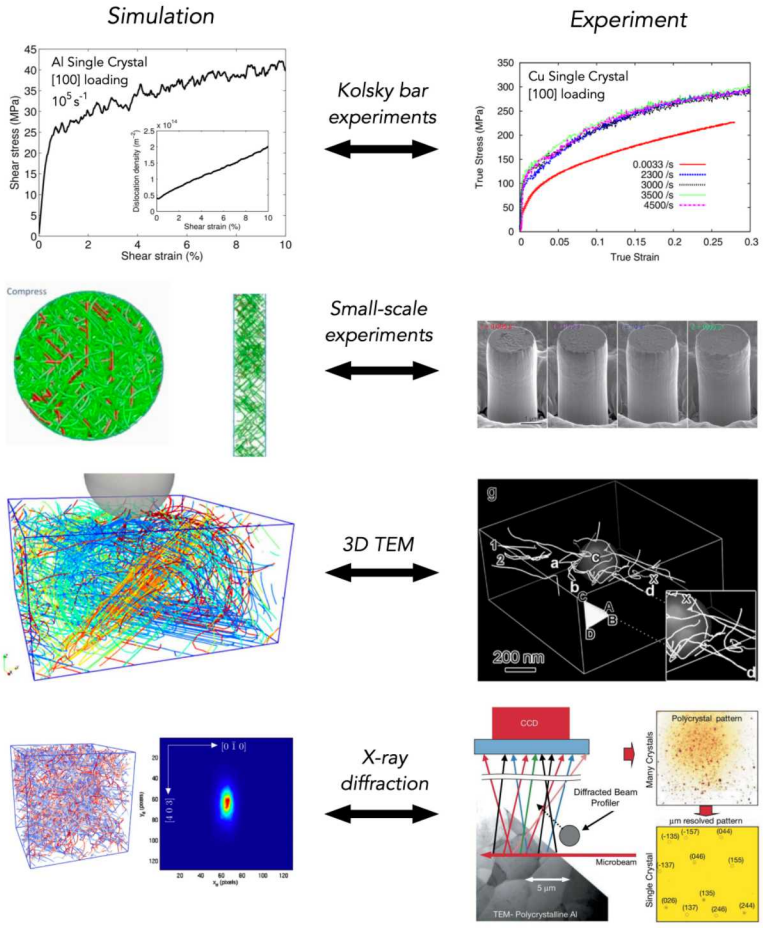

Figure 6

Opportunities for comparisons between DDD simulations and experiments. Kolsy bar experiments on single crystals (39, 132); Small scale experiments (133, 134); 3D TEM (47, 135) ; X-ray diffraction (68, 136). Reproduced with permission.

testing conducted in the scanning electron microscope (SEM) provides another valuable tool set for studying plasticity (106). These methods have traditionally been limited to low strain rates. Recently, Guillonneau et al. (134) developed a technique for performing nano-indentation and micro-compression with strain rates from 1 to 1000 s^{-1}. With this capability, direct comparisons can be made for the first time between small-scale mechanical experiments and DDD simulations. Efficient spectral image solvers (45, 46, 47) can be used to simulate the finite volumes of the small-scale specimens.

Transmission electron microscopy (TEM) is perhaps the most important experimental technique for studying dislocations because it is historically the only technique which can unambiguously resolve the location of dislocation lines and determine their Burgers vectors. However, TEM images have always suffered from one major issue: each image only provides a two-dimensional representation of three-dimensional dislocation lines. Hence, directly

comparing TEM images with DDD simulations has been difficult because it is hard to tell how far dislocations are from each other and from free surfaces. For example, Drouet et al. (140) considered the interaction between a dislocation line with a small dislocation loop in an irradiated zirconium alloy. Because of the uncertainty in the TEM geometry, the authors used trial-and-error DDD simulations to deduce the position, habit plane, and Burgers vector of the dislocation loop.

A major drawback to TEM imaging is that samples must be very thin (several hundred nm or less) so that electrons are able to transmit through them. In contrast, imaging in the scanning electron microscope (SEM) examines only the surface region of samples and can accommodate much larger samples. A recent advance in SEM imaging provides another opportunity for comparisons with mesoscale simulations: accurate electron channeling contrast imaging (A-ECCI) (141). Using this technique, individual dislocations near the surface can be resolved and their Burgers vectors identified with a spatial resolution of 500 nm (142). This enables dislocation lines to be imaged during in situ mechanical testing of "bulk" samples in the SEM (143).

New advances in electron tomography enable fully three-dimensional reconstructions of dislocation networks, suitable for direct comparisons with DDD simulations. Using these methods, dislocation geometries extracted from TEM experiments could be directly imported into DDD codes. Stereo-pair imaging, wherein two TEM images are taken at different sample tilt angles, has been established as a technique for reconstructing dislocation line geometries in three-dimensions (144, 145). Wang et al. (144) used this technique to evaluate the influence of free surface image forces on dislocations in Cu. Recently, more general electron tomographic reconstruction methods based on Fourier analysis have been applied to dislocation lines as well (146, 135). In these methods, many images ($\sim$50 to 100) are taken in the TEM over a range of tilt angles and are assembled together to reconstruct the three-dimensional structure. The most widely used electron tomography method for dislocation geometries is the weighted back-projection method, which has been successfully applied to studies of dislocations at a crack tip, dislocation-precipitate interactions, and dislocation-grain boundary interactions, to name a few (135). These methods have also been used to evaluate how dislocations respond to increasing levels of stress, giving a four-dimensional picture of dislocation behavior (147). Finally, it is important to observe that all TEM observations require electron transparent samples (usually in the form of thin foils) with small thickness, typically on the order of 100 nm. Hence, an efficient image stress solver (46) is needed for DDD simulations of TEM-relevant geometries.

As another technique, X-ray diffraction has long been employed to study dislocation structures. With the recent increase in prominence of light source user-facilities, X-ray methods have become a backbone of experimental mechanics. Two X-ray diffraction methods have been used historically: powder diffraction and Laue diffraction (148). Powder diffraction provides bulk information about the state of a polycrystalline lattice in the form of intensity peaks; these peaks are known to shift and broaden as dislocation substructure forms. Laue diffraction provides detailed information about the orientation and state of deformation of local regions in a lattice. Recent advances in X-ray beam lines have enabled sub-micron beam resolution, with which Laue diffraction patterns can be analyzed to construct geometrically necessary dislocation density fields in three-dimensions (136). Furthermore, beam-line experiments have matured to enable *in situ* loading so that dislocation network evolution can be observed in real-time. In recent years, post-processing algorithms for DDD have been developed to predict powder (66, 67) and Laue (65, 68) diffraction

patterns from DDD simulations, enabling direct comparisons with experiments.

In both powder and Laue diffraction experiments, the obtained data sets are "averaged" representations of the dislocation network, i.e., discrete dislocation lines cannot be identified. Several promising X-ray imaging techniques have recently been developed which could be used to identify individual dislocation lines: Bragg coherent diffractive imaging (BCDI) and dark-field X-ray microscopy. BCDI uses coherent diffraction patterns from Bragg peaks obtained with X-ray nano-beams to provide a full three-dimensional displacement field at nanoscale resolution. BCDI has been used to image dislocation dynamics in nanoscale samples of Pd (149) and Au (150, 151). The primary drawback for BCDI at present is that the material size is limited by the X-ray beam coherence; current beamline technologies limit experiments to nanoscale samples (152). Dark-field X-ray microscopy utilizes an objective lens in the diffracted beam and is able to resolve crystallographic misorientations with a spatial resolution of $\sim$ 100 nm in specimens with $\sim$ 1 mm dimensions (153). Recently it was shown that individual dislocations could be mapped using dark-field X-ray microscopy in specimens with low dislocation densities (154).

While comparisons between computational models and experiments have been traditionally limited to typical experimental conditions (e.g., for macroscopic samples under low strain rates) or at the atomic scale, the recent progress in experimental testing and imaging techniques opens new paths for validating the models of dislocations, especially at the meso-scale. A promising approach to leverage these novel tools is to start establishing comparisons from the simplest scenarios (e.g., pure single crystals) and then progress towards more challenging cases (e.g., alloys then polycrystals) (1). In the future, we expect such comparisons to become part of a systematic validation workflow, e.g., whereby new complex physical mechanisms introduced in DDD models are benchmarked against small-scale experiments with *in situ* imaging.

3.5. Opportunities for data science approaches

The volume of available data from dislocation simulations is growing at an unprecedented rate thanks to recent algorithmic advances and the ever-increasing computational power at hand. This trend creates both challenges and opportunities. On the one hand, the amount of data that is being generated becomes so large and so detailed that it becomes difficult to analyze it and filter out relevant mechanisms from the uninteresting background. On the other hand, this vast amount of data, once appropriately reshaped, provides an excellent opportunity to apply machine learning (ML) techniques that can unravel and capture relationships within the data that could not have been easily identified, or simply missed, using traditional workflows and reasoning.

From a general perspective, the power of ML-based techniques resides in their demonstrated ability to learn the complex, highly non-linear mappings that may exist between well-chosen features describing the state of a system and the desired output that one wishes to predict with a given accuracy (e.g., mechanical response). Thus, it seems reasonable to expect that ML techniques could significantly help advance our understanding and predictive capabilities of dislocation-mediated plasticity, whose complex behavior that emerges from the collective effects of interacting dislocation ensembles has puzzled our scientific community for decades. More specifically, we believe that ML approaches could provide significant advances in the following key areas:

1. Developing inter-atomic potentials for metallic systems (especially multi-component

alloys) with superior accuracy-to-cost ratio, thereby enabling MD simulations with higher fidelity, getting us closer to simulating real material systems
2. Discovering new physics (correlations) potentially hidden in the vast, typically uninterpretable amounts of data generated by high-throughput calculations
3. Providing more direct connections between models across the scales, e.g., by identifying the optimal set of coarse-graining variables
4. Improving the predictive power of models, e.g. by replacing previously phenomenological models with ML models trained on already existing or new experimental or simulation data
5. Enabling more direct connections and comparisons between experimental data and model predictions

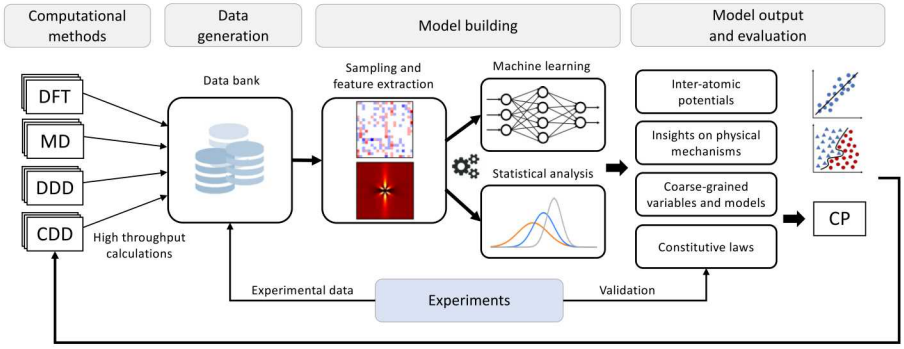

Figure 7

Workflow for applying data science techniques to simulations of dislocations.

Several recent works have already applied data-driven approaches in the context of continuum mechanics (e.g., see recent review in (155)), and general frameworks have been proposed to address the microstructure-property linkage (e.g., (156)). The development of ML-based inter-atomic potentials has become a very active subject of study, with well established methods (157) and applications that extend beyond the realm of materials science (158). In the following, we first draw attentions to recent applications of data-driven approaches in direct relation with dislocation microstructures before discussing the general directions which we believe would be beneficial for dislocation modeling.

One of the early applications of ML based techniques to dislocation microstructures was proposed by Yasser et al. (159). In this work, the GNDs dislocation density extracted from EBSD images was used to predict the flow-stress in Al alloys with various precipitate morphologies using artificial neural networks (ANN). More recently but in a similar spirit, convolutional neural networks (CNN) were employed as a way to predict the total density of dislocations from the density of GNDs alone (160). Since GND is a coarse-graining measure of the total density and both quantities are geometrically and physically related, the main idea relies on using a CNN to map the total density from small patches of GND neighborhoods. The CNN model was trained on synthetic, random discrete dislocation line configurations and then applied to extract total density from EBSD maps in α-Fe. Although the CNN model only led to a marginal increase in the accuracy of flow stress predictions

from the EBSD images compared to predictions based on the GNDs alone, such an approach presents an interesting perspective on how models trained on numerical simulation data can be used to infer hidden information from experimental measurements.

In (161), ML was used to assess whether sample to sample variability in stress-strain responses of small-scale crystals can be predicted from the initial microstructure. The authors used 2D DDD simulations in micron-sized volumes and employed both ANN and support vector machines (SVM) to train their models. It was found that larger systems (i.e., with more dislocations) are easier to predict, specifically because they exhibit smaller strain bursts resulting from avalanches-like processes. This led to the conclusion that such burst processes, which are stochastic in nature, pose fundamental limits on the predictability of plastic response of small crystalline systems. Among the various descriptors that were tested to encode the initial system state (dislocation microstructure), it was found that statistical measures of internal stresses as well as spatial densities of GNDs led to the most accurate predictions.

Another interesting ML application to DDD simulations data was recently proposed in (162). The authors ran hundreds of DDD simulations of different sizes with free-surfaces, and investigated whether a ML-based approach can classify the volume size based on dislocation microstructures sampled from a subvolume. More specifically, the focus was placed on examining what descriptors are best suited for performing such a classification task. To this end, several density fields that are commonly used in continuum models of dislocations were tested and compared; namely, the dislocation density, Nye's tensor, and higher-order fields measures introduced in the higher-order CDD models (77, 78). Using a Gaussian naive Bayes classifier, it was found that the set of descriptors used in higher-order CDD outperforms both the GNDs density and total dislocation density features, especially at coarse resolutions.

The methodology adopted in this last work (162) is particularly interesting because it leverages the power of ML techniques to identify the best sets of microstructural variables that need to be retained in coarse-grained models of plasticity. Thus, we believe that this type of approach is a promising direction for simulations of plasticity, because it provides a way to guide the development of higher-scale models. The use of ML techniques to construct constitutive laws from lower-scale simulations also appears as a promising path for extending the predictive capabilities of current models. An example of such an application was recently proposed in (52), where a data-driven approach was used to quantify slip systems interactions from a large set of DDD work-hardening simulations, instead of using specialized DDD simulations. Although significant challenges still remain, this work demonstrated the feasibility of constructing a ML-based crystal plasticity models directly trained on large-scale DDD simulation data.

Finally, we conclude this section by highlighting several relevant considerations regarding the use of ML-based techniques for dislocation modeling. First, we stress the importance of the selection of the descriptor space. Choosing a good set of features for a given problem is a challenging task and is what usually distinguishes a successful ML-based model from the others. The selection of features can greatly benefit from prior knowledge of a system, whereby the machine is guided with physical insights, e.g., by imposing crystal symmetries. Conversely, training on a poor featurization of the input space can artificially increase the complexity of the relations between the input and output data, or worse, lead models to learn the "wrong" physics. More generally, while ML has shown promising results in a vast number of fields, the underlying structure of the discovered relations is often hidden within

the intricacy of the algorithm and cannot be easily interpreted. In other words, ML-based approaches are often used as black-box tools from which it becomes difficult to extract a clear understanding of the results or to generalize them. Even in this case, ML-based models, if adequately trained, can still be valuable as an efficient way to compute responses of systems whose unit mechanisms are well understood but whose emergent properties are expensive to predict from physical simulations. For instance, developing novel CP models that simultaneously (i) capture the complex interactions between microstructural features and (ii) embrace their statistical nature appears as a challenge for which ML-based techniques are promising.

4. CONCLUSION

We are in an exciting time regarding computational modeling of dislocations for the understanding and prediction of crystal plasticity. Several advances have been made for the models at the different scales, and individual models have been enjoying significant successes. At the lowest scale, the feasibility of direct MD simulations of metal plasticity has been demonstrated, and ultra-scale MD are expected to become more common. At higher scales, the DDD method has enjoyed several computational developments and is becoming a mature tool capable of providing significant physical insights, while recent formulations of the CDD method have led to the prediction of dislocation patterning.

Thanks to these advances, the multi-scale framework for dislocation based plasticity is starting to come together. Beyond successes at their individual scale, this recent progress now offers concrete opportunities to meaningfully connect the different methods together. Thanks to the DXA algorithm, a direct connection between MD and DDD is now possible, thereby allowing to go beyond the traditional workflow based on single dislocation matching. Similarly, connection between DDD and CDD is starting to happen, especially through the development of crystallographic-based CDD formulations. Large-scale DDD simulations will be increasingly used to construct sophisticated, physics-based constitutive models to be incorporated in CP frameworks. In the future, robust workflows will be established to link models across the scales and reduce the uncertainties associated with information passing. As a result, models at each scale will be better informed, and will be able to simulate microstructures of increasing complexity with higher fidelity.

Concurrently, experimental data are becoming more abundant and with higher fidelity, providing more opportunities to connect and benchmark computational models against experiments. Small-scale experiments coupled with novel, high resolution imaging techniques will allow for one-to-one comparisons between simulated and real material samples. These will provide direct ways to validate models—especially at the much needed mesoscale—and quantify their uncertainties both in terms of predictions of mechanical responses and dislocation microstructures.

Finally, as computational models are getting mature, high throughput calculations are becoming common and will generate ever increasing volumes of data. Application of data-driven and machine learning techniques will thus soon become key to analyze and extract information from simulation results and experimental data. Among the broad spectrum of possible applications, the identification of microstructural variables that are key to the development coarse-graining approaches, as well as the building of statistical constitutive models with enhanced predictive capabilities stand as promising avenues for future research.

ACKNOWLEDGMENTS

The work of NB was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. RBS was supported by Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. The work of WC was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0010412.

LITERATURE CITED

1. Sills RB, Bertin N, Bulatov VV, Cai W. 2019. Multiscale modelling of plasticity. In *Roadmap on Multiscale Materials Modelling*, eds. E Van der Giessen, P Schultz, vol. In Press. Modelling and Simulation in Materials Science and Engineering
2. Cai W, Ghosh S. 2018. Recent advances in crystal plasticity. In *Handbook of Materials Modeling*, eds. W Andreoni, S Yip. Cham: Springer
3. Woodward C, Trinkle DR, Jr. LGH, Olmsted DL. 2008. Prediction of dislocation cores in aluminum from density functional theory. *Physical Review Letters* 100:045507
4. Xia S, El-Azab A. 2015. Computational modelling of mesoscale dislocation patterning and plastic deformation of single crystals. *Modelling and Simulation in Materials Science and Engineering* 23:055009
5. Ghosh S, Groeber MA. 2018. Developing virtula microstructures and statistically equivalent representative volume elements for polycrystalline materials. In *Handbook of Materials Modeling*, eds. W Andreoni, S Yip. Cham: Springer
6. Sills RB, Bertin N, Aghaei A, Cai W. 2018. Dislocation networks and the microstructural origin of strain hardening. *Phys. Rev. Lett.* 121:085501
7. Sills RB, Boyce BL. 2019. Void growth by dislocation adsorption. *In-Preparation*
8. Pinna C, Lan Y, Kiu MF, Efthymiadis P, Lopez-Pedrosa M, Farrugia D. 2015. Assessment of crystal plasticity finite element simulations of the hot deformation of metals from local strain and orientation measurements. *International Journal of Plasticity* 73:24–38
9. Mello AW, Nicolas A, Lebensohn RA, Sangid MD. 2016. Effect of microstructure on strain localization in a 7050 aluminum alloy: Comparison of experiments and modeling for various textures. *Materials Science & Engineering A* 661:187–197
10. Rodney D, Ventelon L, Clouet E, Pizzagalli L, Willaime F. 2017. Ab initio modeling of dislocation core properties in metals and semiconductors. *Acta Materialia* 124:633–659
11. Lüthi B, Ventelon L, Rodney D, Willaime F. 2018. Attractive interaction between interstitial solutes and screw dislocations in bcc iron from first principles. *Computational Materials Science* 148:21–26
12. Leyson GPM, Curtin WA, Jr. LGH, Woodward CF. 2010. Quantitative prediction of solute strengthening in aluminum alloys. *Nature Materials* 9:750–755
13. Clouet E, Caillard D, Chaari N, Onimus F, Rodney D. 2015. Dislocation locking versus easy glide in titanium and zirconium. *Nature Materials* 14:931–937
14. Proville L, Rodney D, Marinica MC. 2012. Quantum effect on thermally activated glide of dislocations. *Nature Materials* 11:845–849
15. Freitas R, Asta M, Bulatov VV. 2018. Quantum effects on dislocation motion from ring-polymer molecular dynamics. *npj Computational Materials* 55:1–6
16. Borda EJL, Cai W, de Koning M. 2016. Dislocation structure and mobility in hcp ^{4}He. *Physical Review Letters* 117:045301
17. Bulatov V, Cai W. 2006. Computer simulations of dislocations, vol. 3. Oxford University Press

on Demand
18. Cai W, Li J, Yip S. 2012. Molecular dynamics. In *Comprehensive Nuclear Materials*, ed. RJM Konings. Amsterdam: Elsevier
19. Cai W, Bulatob VV, Chang J, Li J, Yip S. 2003. Periodic image effects in dislocation modelling. *Philosophical Magazine* 83:539–567
20. Zhou X, Sills R, Ward D, Karnesky R. 2017. Atomistic calculations of dislocation core energy in aluminium. *Physical Review B* 95:054112
21. Geslin PA, Gatti R, Devincre B, Rodney D. 2017. Implementation of the nudged elastic band method in a dislocation dynamics formalism: application to dislocation nucleation. *Journal of the Mechanics and Physics of Solids* 108:49–67
22. Olmsted DL, Hector Jr LG, Curtin W, Clifton R. 2005. Atomistic simulations of dislocation mobility in al, ni and al/mg alloys. *Modelling and Simulation in Materials Science and Engineering* 13:371
23. Kang K, Bulatov VV, Cai W. 2012. Singular orientations and faceted motion of dislocations in body-centered cubic crystals. *Proceedings of the National Academy of Sciences* 109:15174–15178
24. Cereceda D, Stukowski A, Gilbert M, Queyreau S, Ventelon L, et al. 2013. Assessment of interatomic potentials for atomistic analysis of static and dynamic properties of screw dislocations in w. *Journal of Physics: Condensed Matter* 25:085702
25. Cho J, Molinari JF, Anciaux G. 2017. Mobility law of dislocations with several character angles and temperatures in fcc aluminum. *International Journal of Plasticity* 90:66–75
26. Rao S, Dimiduk D, Parthasarathy T, El-Awady J, Woodward C, Uchic M. 2011. Calculations of intersection cross-slip activation energies in fcc metals using nudged elastic band method. *Acta Materialia* 59:7135–7144
27. Kang K, Yin J, Cai W. 2014. Stress dependence of cross slip energy barrier for face-centered cubic nickel. *Journal of the Mechanics and Physics of Solids* 62:181–193
28. Singh CV, Mateos AJ, Warner DH. 2011. Atomistic simulations of dislocation–precipitate interactions emphasize importance of cross-slip. *Scripta Materialia* 64:398–401
29. Saroukhani S, Nguyen LD, Leung KWK, Singh CV, Warner DH. 2016. Harnessing atomistic simulations to predict the rate at which dislocations overcome obstacles. *Journal of the Mechanics and Physics of Solids* 90:202–214
30. Ryu S, Kang K, Cai W. 2011. Entropic effect on the rate of dislocation nucleation. *Proceedings of the National Academy of Sciences* 108:5174–5178
31. Nguyen LD, Baker KL, Warner DH. 2011. Atomistic predictions of dislocation nucleation with transition state theory. *Physical Review B* 84
32. Stukowski A, Albe K. 2010. Extracting dislocations and non-dislocation crystal defects from atomistic simulation data. *Modelling and Simulation in Materials Science and Engineering* 18:085001
33. Stukowski A. 2014. A triangulation-based method to identify dislocations in atomistic models. *Journal of the Mechanics and Physics of Solids* 70:314–319
34. Zepeda-Ruiz LA, Stukowski A, Oppelstrup T, Bulatov VV. 2017. Probing the limits of metal plasticity with molecular dynamics simulations. *Nature* 550:492
35. Zepeda-Ruiz LA, Stukowski A, Oppelstrup T, Bertin N, Barton NR, et al. 2019. Metal hardening in atomistic detail. *arXiv e-prints* :arXiv:1909.02030
36. Sills RB, Aubry A. 2018. Line dislocation dynamics simulations with complex physics. In *Handbook of Materials Modeling*, eds. W Andreoni, S Yip. Cham: Springer
37. Arsenlis A, Cai W, Tang M, Rhee M, Oppelstrup T, et al. 2007. Enabling strain hardening simulations with dislocation dynamics. *Modelling and Simulation in Materials Science and Engineering* 15:553–595
38. Sills RB, Aghaei A, Cai W. 2016. Advanced time integration algorithms for dislocation dynamics simulations of work hardening. *Modelling and Simulation in Materials Science and*

Engineering 24:045019
39. Bertin N, Aubry S, Arsenlis A, Cai W. 2019. GPU-accelerated dislocation dynamics using subcycling time-integration. *Modelling and Simulation in Materials Science and Engineering* 27:075014
40. Chen C, Aubry S, Oppelstrup T, Arsenlis A, Darve E. 2018. Fast algorithms for evaluating the stress field of dislocation lines in anisotropic elastic media. *Modelling and Simulation in Materials Science and Engineering* 26:045007
41. Vattre A, Devincre B, Feyel F, Gatti R, Groh S, et al. 2014. Modelling crystal plasticity by 3d dislocation dynamics and the finite element method: The discrete-continuous model revisited. *Journal of the Mechanics and Physics of Solids* 63:491–505
42. Bertin N, Upadhyay MV, Pradalier C, Capolungo L. 2015. A FFT-based formulation for efficient mechanical fields computation in isotropic and anisotropic periodic discrete dislocation dynamics. *Modelling and Simulation in Materials Science and Engineering* 23:065009
43. Bertin N, Capolungo L. 2018. A FFT-based formulation for discrete dislocation dynamics in heterogeneous media. *Journal of Computational Physics* 355:366–384
44. Bertin N. 2019. Connecting discrete and continuum dislocation mechanics: A non-singular spectral framework. *International Journal of Plasticity* 122:268 – 284
45. Weinberger CR, Cai W. 2007. Computing image stress in an elastic cylinder. *Journal of the Mechanics and Physics of Solids* 55:2027–2054
46. Weinberger CR, Aubry S, Lee SW, Nix WD, Cai W. 2009. Modeling dislocaitons in a free-standing thin film. *Modelling and Simulation in Materials Science and Engineering* 17:075007
47. Bertin N, Glavas V, Datta D, Cai W. 2018. A spectral approach for discrete dislocation dynamics simulations of nanoindentation. *Modelling and Simulation in Materials Science and Engineering* 28:055004
48. Devincre B, Kubin L, Hoc T. 2006. Physical analyses of crystal plasticity by dd simulations. *Scripta Materialia* 54:741–746
49. Devincre B, Hoc T, Kubin L. 2008. Dislocation mean free paths and strain hardening of crystals. *Science* 320:1745–1748
50. Queyreau S, Monnet G, Devincre B. 2009. Slip systems interactions in α-iron determined by dislocation dynamics simulations. *International Journal of Plasticity* 25:361–377
51. Bertin N, Tomé C, Beyerlein I, Barnett M, Capolungo L. 2014. On the strength of dislocation interactions and their effect on latent hardening in pure magnesium. *International Journal of Plasticity* 62:72–92
52. Messner MC, Rhee M, Arsenlis A, Barton NR. 2017. A crystal plasticity model for slip in hexagonal close packed metals based on discrete dislocation simulations. *Modelling and Simulation in Materials Science and Engineering* 25:044001
53. Hussein AM, Rao SI, Uchic MD, Dimiduk DM, El-Awady JA. 2015. Microstructurally based cross-slip mechanisms and their effects on dislocation microstructure evolution in fcc crystals. *Acta Materialia* 85:180–190
54. Rao SI, Woodward C, Akdim B, Antillon E, Parthasarathy TA, et al. 2019. Large-scale dislocation dynamics simulations of strain hardening of ni microcrystals under tensile loading. *Acta Materialia* 164:171–183
55. Zhou C, LeSar R. 2012. Dislocation dynamics simulations of plasticity in polycrystalline thin films. *International Journal of Plasticity* 30:185–201
56. Fan H, Aubry S, Arsenlis A, El-Awady JA. 2015. The role of twinning deformation on the hardening response of polycrystalline magnesium from discrete dislocation dynamics simulations. *Acta Materialia* 92:126–139
57. Wei D, Zaiser M, Feng Z, Kang G, Fan H, Zhang X. 2019. Effects of twin boundary orientation on plasticity of bicrystalline copper micropillars: A discrete dislocation dynamics simulation study. *Acta Materialia* 176:289–296
58. Xiang YGY, Quek SS, Srolovitz DJ. 2015. Three-dimensional formulation of dislocation climb.

Journal of the Mechanics and Physics of Solids 83:319–337
59. Niu X, Luoa T, Xiang JLY. 2017. Dislocation climb models from atomistic scheme to dislocation dynamics. *Journal of the Mechanics and Physics of Solids* 99:242–258
60. Arsenlis A, Rhee M, Hommes G, Cook R, Marian J. 2012. A dislocation dynamics study of the transition from homogeneous to heterogeneous deformation in irradiated body-centered cubic iron. *Acta Materialia* 60:3748–3757
61. Sobie C, Bertin N, Capolungo L. 2015. Analysis of obstacle hardening models using dislocation dynamics: application to irradiation-induced defects. *Metallurgical and Materials Transactions A* 46:3761–3772
62. Cui Y, Po G, Ghoniem NM. 2018. A coupled dislocation dynamics-continuum barrier field model with application to irradiated materials. *International Journal of Plasticity* 104:54–67
63. Li Y, Robertson C. 2018. Irradiation defect dispersions and effective dislocation mobility in strained ferritic grains: a statistical analysis based on 3d dislocation dynamics simulations. *Journal of Nuclear Materials* 504:84–93
64. Sobie C, Capolungo L, McDowell DL, Martinez E. 2017. Scale transition using dislocation dynamics and the nudged elastic band method. *Journal of the Mechanics and Physics of Solids* 105:161–178
65. Hofmann F, Keegan S, Korsunskuy AM. 2012. Diffraction post-processing of 3d dislocation dynamics simulations for direct comparison with micro-beam laue experiments. *Materials Letters* 89:66–69
66. Balogh L, Capolungo L, Tomé CN. 2012. On the measure of dislocation densities from diffraction line profiles: A comparison with discrete dislocation methods. *Acta Materialia* 60:1467–1477
67. Upadhyay MV, Capolungo L, Balogh L. 2014. On the computation of diffraction peaks from discrete defects in continuous media: comparison of displacement and strain-based methods. *Journal of Applied Crystallography* 47:861–878
68. Bertin N, Cai W. 2018. Computation of virtual x-ray diffraction patterns from discrete dislocation structures. *Computational Materials Science* 146:268–277
69. El-Azab A, Po G. 2018. Continuum dislocation dynamics: Classical theory and contemporary models. *Handbook of Materials Modeling: Methods: Theory and Modeling* :1–25
70. Acharya A. 2001. A model of crystal plasticity based on the theory of continuously distributed dislocations. *Journal of the Mechanics and Physics of Solids* 49:761 – 784
71. Acharya A. 2004. Constitutive analysis of finite deformation field dislocation mechanics. *Journal of the Mechanics and Physics of Solids* 52:301 – 316
72. Acharya A, Roy A. 2006. Size effects and idealized dislocation microstructure at small scales: Predictions of a phenomenological model of mesoscopic field dislocation mechanics: Part i. *Journal of the Mechanics and Physics of Solids* 54:1687 – 1710
73. Varadhan S, Beaudoin A, Acharya A, Fressengeas C. 2006. Dislocation transport using an explicit galerkin/least-squares formulation. *Modelling and Simulation in Materials Science and Engineering* 14:1245
74. Puri S, Das A, Acharya A. 2011. Mechanical response of multicrystalline thin films in mesoscale field dislocation mechanics. *Journal of the Mechanics and Physics of Solids* 59:2400–2417
75. Djaka KS, Taupin V, Berbenni S, Fressengeas C. 2015. A numerical spectral approach to solve the dislocation density transport equation. *Modelling and Simulation in Materials Science and Engineering* 23:065008
76. Zhang X. 2017. A continuum model for dislocation pile-up problems. *Acta Materialia* 128:428 – 439
77. Hochrainer T, Zaiser M, Gumbsch P. 2007. A three-dimensional continuum theory of dislocation systems: kinematics and mean-field formulation. *Philosophical Magazine* 87:1261–1282
78. Sandfeld S, Hochrainer T, Gumbsch P, Zaiser M. 2010. Numerical implementation of a 3d continuum theory of dislocation dynamics and application to micro-bending. *Philosophical*

Magazine 90:3697–3728
79. Hochrainer T, Sandfeld S, Zaiser M, Gumbsch P. 2014. Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. *Journal of the Mechanics and Physics of Solids* 63:167 – 178
80. Hochrainer T. 2015. Multipole expansion of continuum dislocations dynamics in terms of alignment tensors. *Philosophical Magazine* 95:1321–1367
81. Sandfeld S, Zaiser M. 2015. Pattern formation in a minimal model of continuum dislocation plasticity. *Modelling and Simulation in Materials Science and Engineering* 23:065005
82. Arora R, Acharya A. 2019. Dislocation pattern formation in finite deformation crystal plasticity. *International Journal of Solids and Structures*
83. Roters F, Eisenlohr P, Hantcherli L, Tjahjanto DD, Bieler TR, Raabe D. 2010. Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications. *Acta Materialia* 58:1152–1211
84. Arsenlis A, Parks DM. 2002. Modeling the evolution of crystallographic dislocation density in crystal plasticity. *Journal of the Mechanics and Physics of Solids* 50:1979–2009
85. Ma A, Roters F. 2004. A constitutive model for fcc single crystals based on dislocation densities and its application to uniaxial compression of aluminium single crystals. *Acta materialia* 52:3603–3612
86. Beyerlein I, Tomé C. 2008. A dislocation-based constitutive law for pure zr including temperature effects. *International Journal of Plasticity* 24:867–895
87. Lee M, Lim H, Adams B, Hirth J, Wagoner R. 2010. A dislocation density-based single crystal constitutive equation. *International Journal of Plasticity* 26:925–938
88. Bertin N, Capolungo L, Beyerlein I. 2013. Hybrid dislocation dynamics based strain hardening constitutive model. *International Journal of Plasticity* 49:119–144
89. Payne MC, Robertson IJ, Thomson D, Heine V. 1996. Ab initio databases for fitting and testing interatomic potentials. *Philosophical Magazine B* 73:191–199
90. Motamarri P, Gavini V. 2014. Subquadratic-scaling subspace projection method for large-scale kohn-sham density functional theory calculations using spectral finite-element discretization. *Physical Review B* 90:115127
91. Mi W, Shao X, Su C, Zhou Y, Zhang S, et al. 2016. Atlas: A real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications* 200:87–95
92. Ponga M, Bhattacharya K, Ortiz M. 2016. A sublinear-scaling approach to density-functional-theory analysis of crystal defects. *Journal of the Mechanics and Physics of Solids* 95:530–556
93. Groh S, Marin E, Horstemeyer M, Bammann D. 2009. Dislocation motion in magnesium: a study by molecular statics and molecular dynamics. *Modelling and Simulation in Materials Science and Engineering* 17:075009
94. Zhou S, Preston D, Lomdahl P, Beazley D. 1998. Large-scale molecular dynamics simulations of dislocation intersection in copper. *Science* 279:1525–1527
95. Rodney D, Phillips R. 1999. Structure and strength of dislocation junctions: An atomic level analysis. *Physical Review Letters* 82:1704
96. Spearot DE, Sangid MD. 2014. Insights on slip transmission at grain boundaries from atomistic simulations. *Current Opinion in Solid State and Materials Science* 18:188–195
97. Terentyev D, Bonny G, Domain C, Pasianot R. 2010. Interaction of a 1 2¡ 111¿ screw dislocation with cr precipitates in bcc fe studied by molecular dynamics. *Physical Review B* 81:214106
98. Singh C, Mateos A, Warner D. 2011. Atomistic simulations of dislocation–precipitate interactions emphasize importance of cross-slip. *Scripta Materialia* 64:398–401
99. Perez D, Uberuaga BP, Shim Y, Amar JG, Voter AF. 2009. Accelerated molecular dynamics methods: Introduction and recent developments. In *Annual Reports on Computational Chemistry*, ed. RA Wheeler, vol. 5. Elsevier, 79 – 98
100. Uberuaga BP, Martínez E, Perez D, Voter AF. 2018. Discovering mechanisms relevant for

radiation damage evolution. *Computational Materials Science* 147:282 – 292
101. Ghoniem NM, Tong SH, Sun LZ. 2000. Parametric dislocation dynamics: A thermodynamics-based approach to investigations of mesoscopic plastic deformation. *Phys. Rev. B* 61:913–927
102. Sills RB, Kuykendall WP, Aghaei AA, Cai W. 2016. Fundamentals of dislocation dynamics simulations. In *Multiscale Materials Modeling for Nanomechanics*, eds. CR Weinberger, GJ Tucker, chap. 2. Switzerland: Springer, 53–87
103. Cai W, Arsenlis A, Weinberger CR, Bulatov VV. 2006. A non-singular continuum theory of dislocations. *Journal of the Mechanics and Physics of Solids* 54:561–587
104. Aubry S, Arsenlis A. 2013. Use of spherical harmonics for dislocation dynamics in anisotropic elastic media. *Modelling and Simulation in Materials Science and Engineering* 21
105. Lemarchand C, Devincre B, Kubin LP. 2001. Homogenization method for a discrete-continuum simulation of dislocation dynamics. *Journal of the Mechanics and Physics of Solids* 49:1969–1982
106. Dehm G, Jaya BN, Raghavan R, Kirchlechner C. 2018. Overview on micro- and naomechanical testing: New insights in interface plasticity and fracture at small length scales. *Acta Materialia* 142:248–282
107. Nye J. 1953. Some geometrical relations in dislocated crystals. *Acta metallurgica* 1:153–162
108. Xia S, Belak J, El-Azab A. 2016. The discrete-continuum connection in dislocation dynamics: I. time coarse graining of cross slip. *Modelling and Simulation in Materials Science and Engineering* 24:075007
109. Lebensohn RA, Tomé C. 1993. A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: application to zirconium alloys. *Acta metallurgica et materialia* 41:2611–2624
110. Lebensohn RA, Kanjarla AK, Eisenlohr P. 2012. An elasto-viscoplastic formulation based on fast fourier transforms for the prediction of micromechanical fields in polycrystalline materials. *International Journal of Plasticity* 32:59–69
111. Li J, Wang CZ, Chang JP, Cai W, Bulatov VV, et al. 2004. Core energy and peierls stress of a screw dislocation in bcc molybdenum: A periodic-cell tight-binding study. *Physical Review B* 70:104113
112. Clouet E, Ventelon L, Willaime F. 2009. Dislocation core energies and core fields from first principles. *Physical review letters* 102:055502
113. Anderson PM, Hirth JP, Lothe J. 2017. Theory of dislocations. Cambridge University Press
114. Domain C, Monnet G. 2005. Simulation of screw dislocation motion in iron by molecular dynamics simulations. *Physical review letters* 95:215506
115. Monnet G, Terentyev D. 2009. Structure and mobility of the 12¡ 111¿{112} edge dislocation in bcc iron studied by molecular dynamics. *Acta Materialia* 57:1416–1426
116. Queyreau S, Marian J, Gilbert M, Wirth B. 2011. Edge dislocation mobilities in bcc fe obtained by molecular dynamics. *Physical Review B* 84:064106
117. Monnet G, Devincre B, Kubin L. 2004. Dislocation study of prismatic slip systems and their interactions in hexagonal close packed metals: application to zirconium. *Acta materialia* 52:4317–4328
118. Wang Z, Beyerlein I. 2011. An atomistically-informed dislocation dynamics model for the plastic anisotropy and tension–compression asymmetry of bcc metals. *International Journal of Plasticity* 27:1471–1484
119. Srivastava K, Gröger R, Weygand D, Gumbsch P. 2013. Dislocation motion in tungsten: atomistic input to discrete dislocation simulations. *International Journal of Plasticity* 47:126–142
120. Po G, Cui Y, Rivera D, Cereceda D, Swinburne TD, et al. 2016. A phenomenological dislocation mobility law for bcc metals. *Acta Materialia* 119:123–135
121. Geslin PA, Rodney D. 2018. Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity. *Physical Review B* 98:174115
122. Anciaux G, Junge T, Hodapp M, Cho J, Molinari JF, Curtin W. 2018. The coupled

atomistic/discrete-dislocation method in 3d part i: Concept and algorithms. *Journal of the Mechanics and Physics of Solids* 118:152–171

123. Cho J, Molinari JF, Curtin WA, Anciaux G. 2018. The coupled atomistic/discrete-dislocation method in 3d. part iii: Dynamics of hybrid dislocations. *Journal of the Mechanics and Physics of Solids* 118:1–14
124. Han J, Thomas SL, Srolovitz DJ. 2018. Grain-boundary kinetics: A unified approach. *Progress in Materials Science* 98:386–476
125. Mughrabi H, Ungar T, Kienle W, Wilkens M. 1986. Long-range internal stresses and asymmetric x-ray line-broadening in tensile-deformed [001]-orientated copper single crystals. *Philosophical magazine A* 53:793–813
126. Sandfeld S, Po G. 2015. Microstructural comparison of the kinematics of discrete and continuum dislocations models. *Modelling and Simulation in Materials Science and Engineering* 23:085003
127. Sudmanns M, Stricker M, Weygand D, Hochrainer T, Shulz K. 2019. Dislocation multiplication by cross-slip and glissile reactions in a dislocation based continuum formulation of crystal plasticity. *Journal of the Mechanics and Physics of Solids* 132:103695
128. Pollock TM, LeSar R. 2013. The feedback loop between theory, simulation and experiment for plasticity and property modeling. *Current Opinion in Solid State and Materials Science* 17:10–18
129. Mills MJ, Miracle DB. 1993. The structure of a¡ 100¿ and a¡ 110¿ dislocation cores in nial. *Acta metallurgica et materialia* 41:85–95
130. Gioacchnio FD, de Fonseca JQ. 2015. An experimental study of the polycrystalline plasticity of austenitic stainless steel. *International Journal of Plasticity* 74:92–109
131. Chen Z, Daly SH. 2017. Active slip system identification in polycrystalline metals by digital image correlation (dic). *Experimental Mechanics* 57:115–127
132. Rawat S, Chandra S, Chavan VM, Sharma S, Warrier M, et al. 2014. Integrated experimental and computational studies of deformation of single crystal copper at high strain rates. *Journal of Applied Physics* 116:213507
133. Ryu I, Nix WD, Cai W. 2013. Plasticity of bcc micropillars controlled by competition between dislocation multiplication and depletion. *Acta Materialia* 61:3233–3241
134. Guillonneau G, Mieszala M, Wehrs J, Schwiedrzik J, Grop S, et al. 2018. Nanomechanical testing at high strain rates: New instrumentation for nanoindentation and microcompression. *Materials and Design* 148:39–48
135. Liu GS, House SD, Kacher J, Tanaka M, Higashida K, Robertson IM. 2014. Electron tomography of dislocation structures. *Materials Characterization* 87:1–11
136. Larson BC, Levine LE. 2013. Submicrometre-resolution polychromatic three-dimensional x-ray microscopy. *Journal of Applied Crystallography* 46:153–164
137. Ramesh KT. 2008. High rates and impact experiments. In *Springer Handbook of Experimental Solid Mechanics*, ed. J William N. Sharpe. Boston: Springer, 929–960
138. Gilat A, Schmidt TE, Walker AL. 2009. Full field strain measurement in compression and tensile split hopkinson bar experiments. *Experimental Mechanics* 49:291–302
139. Chen W, Song B, Few DJ, Forrestal MJ. 2003. Dynamic small strain measurements of a metal specimen with a split hopkinson pressure bar. *Experimental Mechanics* 43:20–23
140. Drouet J, Dupuy L, Onimus F, Mompiou F. 2016. A direct comparison between in-situ transmission electron microscopy observations and dislocation dynamics simulations of interaction between dislocation and irradiation induced loop in a zirconium alloy. *Scripta Materialia* 119:71–75
141. Guyon J, Mansour H, Gey N, Crimp M, Chalal S, Maloufi N. 2015. Sub-micron resolution selected area electron channeling patterns. *Ultramicroscopy* 149:34–44
142. Kriaa H, Guitton A, Maloufi N. 2019. Modeling Dislocation Contrasts Obtained by Accurate-Electron Channeling Contrast Imaging for Characterizing Deformation Mechanisms in Bulk

Materials. *Materials* 12:1587
143. Ben Haj Slama M, Maloufi N, Guyon J, Bahi S, Weiss L, Guitton A. 2019. In Situ Macroscopic Tensile Testing in SEM and Electron Channeling Contrast Imaging: Pencil Glide Evidenced in a Bulk β-Ti21S Polycrystal. *Materials* 12:2479
144. Wang Z, McCabe RJ, Ghoniem NM, LeSar R, Misra A, Mitchell TE. 2013. Dislocation motion in thin cu foils: a comparison between computer simulations and experiment. *Acta Materialia* 52:1535–1542
145. Hong C, Huang X, Winther G. 2013. Dislocation content of geometrically necessary boundaries aligned with slip planes in rolled aluminum. *Philosophical Magazine* 93:3118–3141
146. Saghi Z, Midgley PA. 2012. Electron tomography in the (s)tem: From nanoscale morphological analysis to 3d atomic imaging. *Annual Review of Materials Research* 42:59–79
147. Kacher J, Robertson IM. 2012. Quasi-four-dimensional analysis of dislocation interactions with grain boundaries in 304 stainless steel. *Acta Materialia* 60:6657–6672
148. Swygenhoven HV, Petegem SV. 2013. In-situ mechanical testing during x-ray diffraction. *Materials Characterization* 78:47–59
149. Ulvestad A, Welland MJ, Cha W, Liu Y, Kim JW, et al. 2017. Three-dimensional imaging of dislocation dynamics during the hydriding phase transformation. *Nature Materials* 16:565–573
150. Dupraz M, Beutier G, Cornelius TW, Parry G, Ren Z, et al. 2017. 3d imaging of a dislocation loop at the onset of plasticity in an indented nanocrystal. *Nanoletters* 17:6696–6701
151. Yau A, Cha W, Kanan MW, Stephenson GB, Ulvestad A. 2017. Bragg coherent diffractive imaging of single-grain defect dynamics in polycrystalline films. *Science* 356:739–742
152. Schülli TU, Leake SJ. 2018. X-ray nanobeam diffraction imaging of materials. *Current Opinion in Solid State & Materials Science* 22:188–201
153. Simons H, King A, Ludwig W, Detlefs C, Pantleon W, et al. 2015. Dark-field x-ray microscopy for multiscale structural characterization. *Nature Communications* 6:1–6
154. Jakobsen AC, Simons H, Ludwig W, Yildirim C, Leemreize H, et al. 2019. Mapping of individual dislocations with dark-field x-ray microscopy. *Journal of Applied Crystallography* 52:122–132
155. Bock FE, Aydin RC, Cyron CJ, Huber N, Kalidindi SR, Klusemann B. 2019. A review of the application of machine learning and data mining approaches in continuum materials mechanics. *Frontiers in Materials* 6:110
156. Kalidindi SR. 2015. Hierarchical materials informatics: novel analytics for materials data. Elsevier
157. Behler J, Parrinello M. 2007. Generalized neural-network representation of high-dimensional potential-energy surfaces. *Physical review letters* 98:146401
158. Behler J. 2016. Perspective: Machine learning potentials for atomistic simulations. *The Journal of chemical physics* 145:170901
159. Yassar RS, AbuOmar O, Hansen E, Horstemeyer MF. 2010. On dislocation-based artificial neural network modeling of flow stress. *Materials & design* 31:3683–3689
160. Zhang Y, Ngan AH. 2019. Extracting dislocation microstructures by deep learning. *International Journal of Plasticity* 115:18–28
161. Salmenjoki H, Alava MJ, Laurson L. 2018. Machine learning plastic deformation of crystals. *Nature communications* 9:5307
162. Steinberger D, Song H, Sandfeld S. 2019. Machine learning-based classification of dislocation microstructures. *Frontiers in Materials* 6:141