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Situating the Vector Density Approach Among Contemporary Continuum Theories of Dislocation Dynamics

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Abstract

For the past century, dislocations have been understood to be the carriers of plastic deformation in crystalline solids. However, their collective behavior is still poorly understood. Progress in understanding the collective behavior of dislocations has primarily come in one of two modes: the simulation of systems of interacting discrete dislocations and the treatment of density measures of varying complexity which are considered as continuum fields. A summary of contemporary models of continuum dislocation dynamics is presented. This includes, in order of complexity, the two-dimensional statistical theory of dislocations, the field dislocation mechanics treating the total Kröner-Nye tensor, vector density approaches which treat geometrically necessary dislocations on each slip system of a crystal, and high-order theories which examine the effect of dislocation curvature and distribution over orientation. Each of theories contain common themes, including statistical closure of the kinetic dislocation transport equations and treatment of dislocation reactions such as junction formation. An emphasis is placed on how these common themes rely on closure relations obtained by analysis of discrete dislocation dynamics experiments. The outlook of these various continuum theories of dislocation motion is then discussed.

1 Introduction

Almost one hundred years have passed since dislocations were first asserted to be the carriers of plastic deformation in crystals [1–3]. And yet metal plasticity remains very much an open problem. Why is this the case? Many interesting phenomena regarding the plastic behavior of crystalline materials have their roots in the collective behavior of dislocations. While the behavior of individual dislocations has long been well understood, as they begin to interact they give rise to complex emergent behaviors.

Just as quantum theorists will never provide exact solutions to the many-body Schrödinger equation, our community will never provide exact solutions to many of the problems associated with the collective motion of dislocations. However, one strategy that is proving useful is the description of the dislocation field in a crystal using measures of increasing generality in the hopes of distilling relations between particular behaviors and the dislocation structure at a particular length scale. The purpose of this paper is to present several such efforts to describe the dislocation system. In doing so, we will encounter problems whose solutions are within the grasp of these various theories as well as some horizons of dislocation dynamics which remain puzzling.

Presented here are four models that describe the evolution of dislocation densities in a crystal, that is four models of continuum dislocation dynamics (CDD). They differ widely in their approaches, but all are instructive towards building a cohesive picture of the collective behavior of dislocations. In this presentation we hope to situate our own work on the vector density approach to dislocation dynamics in the present field of CDD frameworks. Additionally, we will examine the strengths and limits of each model, and try to understand how each can inform the other in advancing our community's understanding of plastic behavior.

However, models describing the evolution of various dislocation density fields by no means have an exclusive claim to supremacy in plasticity theory. Rather continuum approaches enjoy a healthy camaraderie with theories of discrete dislocation dynamics (DDD) [4–8], which treat the evolution of a collection of discrete lines in a crystal. DDD calculations show promise in revealing information about the self-organization of dislocations, where the effect of short-range interactions such as dislocation reactions have been found to be significant [9–11]. As the field has progressed, novel phenomenological rules for these interactions as well as for the mobility of dislocations have been developed which are typically informed from lower scale atomistic calculations [6, 12–14]. Many novel situations benefit from the specificity of considering the positions of individual dislocation lines. These include studies of strain bursts and avalanche dynamics in finite crystals [15–17], interactions of glide dislocations with other material defects such as stacking fault tetrahedra, prismatic loops, voids, and secondary phases [18–20]. However, the downfall of these discrete models is a computational complexity wall produced by the multiplication of dislocations in a system as strain increases. While significant efforts have been made in improving the computational efficiency of DDD using novel computational methods–e.g. multipole method for long range stress calculations [4, 21], subcycling time integration schemes [22, 23], GPU-accelerated schemes [24], and fast Fourier transform-based schemes [25]–computations become prohibitively expensive beyond $\sim$1% strain. Even if this wall were not an issue, the kinematics of discrete lines at such finite deformations begin to break down the assumptions on which the entire method is based [26, 27]. As the field of discrete dislocation dynamics advances and suitable boundary conditions are devised to compare DDD with the mechanical environment of CDD [28], data gathered from DDD experiments helps to inform CDD models. In addition to an overview of CDD methods, we hope to give a glimpse into how discrete simulation data is used to inform these continuum models of dislocation dynamics.

With all this in mind, we outline the paper as follows. We summarize: in section 2, the two-dimensional (2D) models pioneered by Groma, Zaiser, and coworkers; in section 3, the field dislocation mechanics (FDM) of Acharya and coworkers; in section 4, the vector density approach to CDD which we, the present authors, commonly employ; lastly in section 5, the most general kinematics of curved dislocations developed by Hochrainer and associates. We hope to illustrate how all of these inform, extend, or generalize each other, as well as how each is in turn informed by DDD experiments.

2 Two-dimensional theories

The first forays into statistical considerations of dislocations were motivated by interpreting x-ray diffraction line broadening in terms of the dislocation content of a crystal [29–31]. In this line of thinking there arose a statistical model of straight, parallel edge dislocations to deal more precisely with the x-ray line broadening problem [32], based on the Born-Bogoliubov-Green-Yvon-Kirkwood (BBGKY) density hierarchy description of particle systems [33–35]. The analogy to particle systems appears by considering these perfectly straight and parallel dislocations of Burgers vector $\hat{x}$ to be two species of particles located in a plane (which we will refer to as the xy-plane). These two species (positive and negative) arise from the tangent vector of the dislocation lying along $+\hat{z}$ or $-\hat{z}$. The signed dislocation density measure, if chosen as the random variable of consideration, would cause cancellation in some scenarios. As a result, the density field is often considered to be dependent on the orientation space $\mathbb{T}$, which in this case is simply $\mathbb{T} := -1, +1$. The statistical process of defining the continuum fields begins with the discrete dislocation system, having density:

$$\rho_{\pm}^{(D)}(\boldsymbol{r}) = \sum_{i=1}^{N_{\pm}} \delta(\boldsymbol{r} - \boldsymbol{r}_i) \tag{1}$$

where $\boldsymbol{r}_i$ is the location of the ith of $N_{\pm}$ positive or negative dislocations, respectively. Considering the average behavior of these discrete densities over many such possible configurations results in a hierarchy of continuum densities (cf. BBGKY hierarchies):

$$\rho_{\pm}(\boldsymbol{r}) := \left\langle \rho_{\pm}^{(D)}(\boldsymbol{r}) \right\rangle \tag{2}$$

$$\rho_{++}(\boldsymbol{r}, \boldsymbol{r'}) := \left\langle \rho_{+}^{(D)}(\boldsymbol{r}) \rho_{+}^{(D)}(\boldsymbol{r'}) \right\rangle \tag{3}$$

$$\rho_{+-}(\boldsymbol{r}, \boldsymbol{r'}) = \rho_{-+}(\boldsymbol{r'}, \boldsymbol{r}) := \left\langle \rho_{+}^{(D)}(\boldsymbol{r}) \rho_{-}^{(D)}(\boldsymbol{r'}) \right\rangle \tag{4}$$

$$\rho_{--}(\boldsymbol{r}, \boldsymbol{r'}) := \left\langle \rho_{-}^{(D)}(\boldsymbol{r}) \rho_{-}^{(D)}(\boldsymbol{r'}) \right\rangle \tag{5}$$

$$\cdots$$

A straightforward averaging of the equations of motion of the individual dislocations results in the following evolution equations for the single point densities:

$$\partial_t \rho_{+} = -M_0 b\, \partial_x \Big[\rho_{+}(\boldsymbol{r}) \tau_{\text{ext}} + \int \{ \rho_{++}(\boldsymbol{r}, \boldsymbol{r'}) - \rho_{+-}(\boldsymbol{r}, \boldsymbol{r'}) \} \tau_{\text{int}}(\boldsymbol{r} - \boldsymbol{r'})\, d^2\boldsymbol{r'} \Big] \tag{6}$$

$$\partial_t \rho_{-} = +M_0 b\, \partial_x \Big[\rho_{-}(\boldsymbol{r}) \tau_{\text{ext}} - \int \{ \rho_{--}(\boldsymbol{r}, \boldsymbol{r'}) - \rho_{-+}(\boldsymbol{r}, \boldsymbol{r'}) \} \tau_{\text{int}}(\boldsymbol{r} - \boldsymbol{r'})\, d^2\boldsymbol{r'} \Big] \tag{7}$$

where M_0 is a mobility constant, b the length of the Burgers vector, τ_{ext} the externally applied shear stress, and τ_{int} the kernel of the interaction stress between two edge dislocations. These equations are not usable in their present form without a closure relation for the two-point densities. It is common practice in density hierarchy approaches to factor out the dependence on the single-point densities [36], expressing the two-point densities in the following manner

$$\rho_{s_1 s_2}(\boldsymbol{r}, \boldsymbol{r'}) := \rho_{s_1}(\boldsymbol{r})\rho_{s_2}(\boldsymbol{r'})\left(1 + d_{s_1 s_2}(\boldsymbol{r} - \boldsymbol{r'})\right) \tag{8}$$

where s_1, s_2 are the desired species (positive or negative) of dislocation to be represented, and $d_{s_1 s_2}$ are the dislocation correlation functions. By assuming that the correlation functions decay fast compared to the lengths on which $\rho_\pm$ varies, all correlation effects can be expressed in terms of local field variables at $\boldsymbol{r}$ [37–40]. This approximation allows the evolution equations for the total dislocation density $\rho(x, y) := \rho_+ + \rho_-$ and the geometrically-necessary dislocation (GND) density $\kappa(x, y) := \rho_+ - \rho_-$ to be expressed as [41]

$$\partial_t \rho = -M_0 b \partial_x \left[\kappa\left(\tau_{\mathrm{mf}} - \tau_{\mathrm{b}}\right) - \rho\, \tau_{\mathrm{d}}\right] \tag{9}$$

$$\partial_t \kappa = -M_0 b \partial_x \left[\rho\left(\tau_{\mathrm{mf}} - \tau_{\mathrm{b}} - \tau_{\mathrm{f}}\left(1 - \left(\frac{\kappa}{\rho}\right)^2\right)\right) - \kappa\, \tau_{\mathrm{d}}\right] \tag{10}$$

where the dislocations evolve under the influence of the mean-field stress τ_{mf}, as well as emergent effective stresses: the back stress τ_{b}, the flow stress τ_{f}, and the diffusion stress τ_{d}. These quantities are defined as follows:

$$\tau_{\mathrm{mf}} = \tau_{\mathrm{ext}} + \int \kappa(\boldsymbol{r'})\tau_{\mathrm{int}} d^2\boldsymbol{r'} \tag{11}$$

$$\tau_{\mathrm{b}} = \frac{D}{\rho}\partial_x \kappa \tag{12}$$

$$\tau_{\mathrm{f}} = \alpha\sqrt{\rho} \tag{13}$$

$$\tau_{\mathrm{d}} = \frac{A}{\rho}\partial_x \rho \tag{14}$$

where D, A, and α are dimensionless constants. More specifically, they are integral moments of the correlation functions [40]. The effects of these effective stresses are clearly seen in the behavior of equations (9,10) in the limit of $|\kappa| \ll \rho$, that is, a nearly homogeneous system. In such a case, terms quadratic in $|\kappa|/\rho$ are neglected: the diffusion stress τ_{d} leads to diffusion in the evolution of ρ, the back stress τ_{b} partially negates the mean-field stress and is related to pile-ups of dislocations, while the flow stress τ_{f} represents the dynamic breaking and forming of dipoles and results in a Taylor-type flow stress. From the outset, these correlation dependent terms have been calibrated against 2D DDD simulations. These correlation functions began to be calculated as measures of the dislocation microstructure [42, 43], and were then co-opted for their kinetic relevance to these effective stresses [35, 38].

In recent years Groma and coworkers have stressed that the equations of motion have a phase-field-type structure [44]. That is to say, they can be expressed as gradients of chemical potentials which are, in turn, variational derivatives of a potential function with respect to a state variable. That is, these evolution equations can be expressed as follows for weakly polarized systems ($\kappa \ll \rho$) [41]:

$$\partial_t \begin{pmatrix} \rho \\ \kappa \end{pmatrix} = \left[\partial_x \begin{pmatrix} \zeta(\delta P/\delta\rho) & \delta P/\delta\kappa \\ \delta P/\delta\kappa & \zeta(\delta P/\delta\rho) \end{pmatrix} \right] \begin{pmatrix} \rho \\ \kappa \end{pmatrix} \tag{15}$$

where a so-called "plastic potential" P is introduced, having the form:

$$P[\chi, \kappa, \rho] := P_{\mathrm{mf}}[\chi, \kappa] + P_{\mathrm{corr}}[\rho, \kappa] \tag{16}$$

$$P_{\mathrm{mf}}[\chi, \kappa] := \int -\frac{1-\nu}{4\mu}(\nabla^2\chi)^2 + b\chi\,\partial_y\kappa\; d^2\boldsymbol{r} \tag{17}$$

$$P_{\mathrm{corr}}[\rho, \kappa] := Gb^2 \int A\rho \ln\left(\frac{\rho}{\rho_0}\right) + \frac{D}{2}\frac{\kappa^2}{\rho}\; d^2\boldsymbol{r} \tag{18}$$

In the above expressions, χ represents the Airy stress potential; minimization of P_{mf} with respect to χ gives $\tau_{\mathrm{mf}} := \partial_x\partial_y\chi$ in terms of κ.

The only term in the plastic potential which does not naturally appear in the elastic energy functional is a portion of the natural logarithm term which produces the diffusion stress [37]. In the energy functional, this logarithm represents the self-energy of the dislocation line and is free from any correlation dependence. However, in the plastic potential (equation 18), an integral of the correlation (i.e. A) appears.

While this system may seem simplistic on the surface, it has many lessons to teach about the role of statistical considerations in the collective motion of dislocations. In the more than twenty years of comparative studies with DDD experiments, many nuances of the statistical description have been discovered. These comparisons have shown, for example, the aforementioned emergence of correlation dependent effective stresses [35, 38], a discrepancy between the mobility of the discrete dislocations and dislocation density fields [45], and a dependence of the effective stresses on density resolution as well as on the local stress field [46]. Moreover, it has shed valuable light on the role of the collective motion of dislocations in plasticity at inclusion interfaces [47], the behavior of dislocation pile-ups [48], and the emergence of dislocation patterns [40, 41, 49]. A recent stochastic implementation has shown useful in describing problems related to intermittent dislocation flow [41, 49, 50]. This simplified continuum model seems to be a veritable fount of interesting behavior, and as such it will help inform directions of inquiry for 3D continuum methods, to which we now turn our attention.

3 Field Dislocation Mechanics

Since dislocations were identified as the carriers of permanent deformation in a solid, there has been a considerable interest in the internal mechanical fields they produce. In the bulk, the stress field is a combination of the internal stress, which depends on the spatial distribution of dislocations, and the external stress, which arises from the applied boundary conditions. As a result, the evolution of the internal dislocation microstructure should be accounted for in order to accurately predict the mechanical response. The elastic theory of continuously distributed dislocations (ECDD) [51] describes the internal mechanical fields in terms of the Kröner-Nye dislocation density tensor $\boldsymbol{\alpha}$ [52]. This tensor represents the geometrically necessary dislocations of each unique Burgers vector by considering:

$$\boldsymbol{\alpha}(\boldsymbol{r}) := \sum_{\gamma} \rho^{[\gamma]}_{\mathrm{GND}}(\boldsymbol{r}) \left(\boldsymbol{\xi}^{[\gamma]}(\boldsymbol{r}) \otimes \boldsymbol{b}^{[\gamma]} \right) \tag{19}$$

where $\rho^{[\gamma]}_{\mathrm{GND}}(\boldsymbol{r})$ is the total line length of GNDs at $\boldsymbol{r}$ due to slip system γ, $\boldsymbol{\xi}$ the net direction of the GNDs, and $\boldsymbol{b}^{[\gamma]}$ the Burgers vector of that slip system. Due to the summation across slip systems, some information regarding the GND content is lost. Some theories of plasticity have treated this problem by assuming the underlying dislocations to be pure edge and screw type (Arsenlis et al., 2004; Leung et al., 2015). Still, there are several theories which directly treat the evolution of $\boldsymbol{\alpha}$ (see the works of Gurtin [53], Zbib [54–56], and Acharya [57, 58]). We will focus on the current form of field dislocation mechanics (FDM) due to Acharya [57]. The geometrically linear version of FDM consists of the following basic equations [59],

$$\boldsymbol{\nabla} \times \boldsymbol{\beta}^{\mathrm{P}} = -\boldsymbol{\alpha}, \tag{20}$$

$$\boldsymbol{\beta}^{\mathrm{P}}_{\parallel} = \tilde{\boldsymbol{\beta}}^{\mathrm{P}}_{\parallel}, \tag{21}$$

$$\boldsymbol{\varepsilon} := \frac{1}{2}\left(\boldsymbol{\beta} + \boldsymbol{\beta}^{T}\right), \quad \boldsymbol{\varepsilon}^{\mathrm{P}} := \frac{1}{2}\left(\boldsymbol{\beta}^{\mathrm{P}} + (\boldsymbol{\beta}^{\mathrm{P}})^{T}\right), \tag{22}$$

$$\boldsymbol{\sigma} = \mathbb{C}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{P}}), \qquad \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = 0 \tag{23}$$

$$\partial_t \boldsymbol{\alpha} = -\boldsymbol{\nabla} \times (\boldsymbol{\alpha} \times \boldsymbol{V}) + \boldsymbol{s}, \tag{24}$$

$$\partial_t \tilde{\boldsymbol{\beta}}^{\mathrm{P}} = \boldsymbol{\alpha} \times \boldsymbol{V}. \tag{25}$$

In the above, $\boldsymbol{\beta}$ is the displacement gradient, $\tilde{\boldsymbol{\beta}}^{\mathrm{P}}$ and $\boldsymbol{\beta}^{\mathrm{P}}$ are the slip and plastic distortions, respectively. $\tilde{\boldsymbol{\beta}}^{\mathrm{P}}_{\parallel}$ and $\boldsymbol{\beta}^{\mathrm{P}}_{\parallel}$ are their compatible parts, $\boldsymbol{\sigma}$ the stress tensor, and $\mathbb{C}$ the fourth-order elastic modulus tensor. $\boldsymbol{V}$ is the dislocation velocity tensor, and $\boldsymbol{s}$ is a dislocation source term. The plastic distortion is decomposed into an incompatible part and a compatible part, which are determined by equations (20) and (21), respectively. Equations (22) and (23) are the standard stress constitutive equation and equilibrium equation. Equation (24) depicts the evolution of dislocation density tensor, and its derivation is based on localizing an integral balance law for the Burgers vector of dislocations that thread an arbitrary surface. Equation (25) represents the evolution of the slip distortion due to the motion of dislocations.

The novel contribution of FDM is equation (21). It should be pointed out that the decomposition of the plastic distortion into a compatible and incompatible part is an important feature of FDM compared with other continuum dislocation approaches. In ECDD [51], only equations (20), (22) and (23) are considered to predict the internal stress field when the dislocation density field is known in a configuration. Acharya [57] showed that the equations of ECDD are inadequate for the unique determination of the physical displacement field due to the gauge invariance of equation (20). In fact, the compatible part of plastic distortion depends on the history of dislocation evolution, so equations (24) and (25) are required to determine the physical displacement. The evolution of the dislocation density tensor is motivated by the work of Mura [60] and Kosevich [61]. However, FDM adopts a different stance with respect to the specification of the plastic deformation and the dislocation flux in comparison to these earlier works. In the first version of FDM, the unphysical nonuniqueness of the plastic distortion field was solved by using an orthogonal projection associated with an inner-product and an additional field equation involving this projection [57]. It was later replaced by a more physical formulation [62], which includes an additional position vector field. It has also shown in a recent work [63] that the decomposition of plastic distortion as in FDM can also help in reducing the numerical errors compared with direct time integration of equation (25).

To close the FDM theory, a theoretical guideline to deriving constitutive closure, driving forces for the dislocation velocity, and dislocation nucleation rates were derived from minimal, but essential, thermodynamical grounds [62, 64]. These studies showed the driving force is in accord with the Peach-Koehler force on a single dislocation from the total local stress. A phenomenological mesoscopic field dislocation mechanics (PMFDM) was also developed [58, 59] which results from an elementary space-time averaging of the equations of FDM. PMFDM is able to study practical problems of mesoscopic and macroscopic plasticity with linkage to the theory of continuously distributed dislocations.

FDM theory has been analytically shown to possess the capability of predicting fundamental features of dislocation plasticity in solids, for example, it predicts the stress field of edge and screw dislocations in an isotropic medium [57]. Numerical schemes of FDM has also been implemented to study more complicated and practical problems, for example, size effects [58], dislocation walls [65], the effect of passivation and grain boundaries [66], as well as dislocation microstructures [67, 68].

The theory of FDM is more often compared to crystal plasticity models than to DDD experiments [66, 67]. However, we include it among the discussion of continuum models of dislocation dynamics because not only of its important link to the classical theories of distributed dislocations, but also its importance to solutions of the mechanical fields in continuum dislocation dynamics. In fact, solutions for the mechanical fields based on the Kröner-Nye tensor $\boldsymbol{\alpha}$ are beginning to be used even in discrete dislocation mechanics [25, 69] due to a lower computational complexity relative to the number of dislocation segments considered. However, the mechanical fields due to $\boldsymbol{\alpha}$ are analogous to the mean-field stress of equation (11), and additional statistical effects would need to be considered [70] in a more complete theory.

Because the total dislocation density tensor $\boldsymbol{\alpha}$ is used in the dislocation evolution equation, the physical meaning of the associated dislocation velocity $\boldsymbol{V}$ is not straightforward [71]. Moreover, it seems to be difficult to consider dislocation junction reactions between different slip systems when the evolution equation is only based on the total dislocation density tensor. The source terms in equation (24) are included to describe dislocation nucleation [64], but junction reactions would require more nuance.

4 Vector-Density Based Theories

The representation that needs the least information to properly resolve the kinematics of curved dislocation lines is one which treats dislocations as vector densities and distinguishes between densities on different slip systems [71]. This vector density approach has also been called the theory of purely geometrically necessary dislocations [72, 73]. Its creation was motivated by a desire to study the onset of dislocation patterning [74] and the emergence of lattice misorientations as sub-grains begin to form [75]. In considering the basis of the vector density approach, it is helpful to consider the problem of discrete dislocation dynamics as the evolution of a collection of line objects $\mathcal{L}^{[\alpha]}$ corresponding to the dislocation objects on each slip system α. These line objects can be recast as discrete densities analogously to the 2D case (equation 1):

$$\boldsymbol{\rho}^{(D)}_{\mathcal{L}^{[\alpha]}}(\boldsymbol{r}) = \int_{\mathcal{L}^{[\alpha]}} \delta(\boldsymbol{r} - \boldsymbol{r}_l) d\boldsymbol{l} \tag{26}$$

where $d\boldsymbol{l}$ includes the tangent direction of the line object at $\boldsymbol{r}_l$. The smooth vector density field is then obtained by means of any suitable ensemble average such that:

$$\boldsymbol{\rho}^{[\alpha]}(\boldsymbol{r}) = \left\langle \boldsymbol{\rho}^{(D)}_{\mathcal{L}^{[\alpha]}}(\boldsymbol{r}) \right\rangle \tag{27}$$

$$\left| \hat{\boldsymbol{a}} \cdot \boldsymbol{\rho}^{[\alpha]}(\boldsymbol{r}) \right| = \left\langle \left| \hat{\boldsymbol{a}} \cdot \boldsymbol{\rho}^{(D)}_{\mathcal{L}^{[\alpha]}}(\boldsymbol{r}) \right| \right\rangle \tag{28}$$

where for any arbitrary constant vector $\hat{\boldsymbol{a}}$. The second requirement (28) is referred to as the line bundle assumption [76] and is a formal definition of how the theory considers only GNDs. This assumption implies that all the underlying discrete dislocations considered by the smooth vector density $\boldsymbol{\rho}^{[\alpha]}$ have tangent vector parallel to the vector density. As a result, the ensemble average operation in equation (27) has no cancellation (which would produce statistically stored dislocations), and the magnitude of the vector density is equal to the total dislocation line density at each point. In such a regime, the streamlines of the density field (Fig. 1) can be considered as the approximate positions of the underlying discrete dislocations. The accuracy of this approximate position is relative to the resolution on which the vector-density is evaluated: at distances shorter than the chosen resolution, interactions must be considered in a statistical manner. The behavior of these short-range interactions has been seen to be strongly dependent on the chosen length scale used to describe the density fields, as the line bundle assumption breaks down above the average dislocation spacing [76].

By means of the line-bundle assumption, the transport equation can be expressed as [73, 77, 78]

$$\partial_t \boldsymbol{\rho}^{[\alpha]} = \boldsymbol{\nabla} \times \left\langle \boldsymbol{v}^{[\alpha]} \times \boldsymbol{\rho}^{[\alpha]} \right\rangle + \dot{\boldsymbol{\rho}}^{[\alpha]}_{\text{source}} - \dot{\boldsymbol{\rho}}^{[\alpha]}_{\text{sink}} \tag{29}$$

where $\boldsymbol{v}^{[\alpha]}$ is the velocity of the line object $\mathcal{L}^{[\alpha]}$ and $\dot{\boldsymbol{\rho}}^{[\alpha]}_{\text{source}}, \dot{\boldsymbol{\rho}}^{[\alpha]}_{\text{sink}}$ can be used to transfer dislocation densities between slip systems, as in the case of dislocation reactions or cross-slip. In the self-consistent field formulation (i.e. neglecting correlation effects) the slip rate vector $\langle \boldsymbol{v}^{[\alpha]} \times \boldsymbol{\rho}^{[\alpha]} \rangle$ is expressed by means of the Peach-Koehler force:

$$\begin{aligned} \left\langle \boldsymbol{v}^{[\alpha]} \times \boldsymbol{\rho}^{[\alpha]} \right\rangle &= \left\langle \boldsymbol{v}^{[\alpha]} \right\rangle \times \boldsymbol{\rho}^{[\alpha]} \\ &= \left(M b \, \tau^{[\alpha]} \, \hat{\boldsymbol{v}}^{[\alpha]} \right) \times \boldsymbol{\rho}^{[\alpha]} \end{aligned} \tag{30}$$

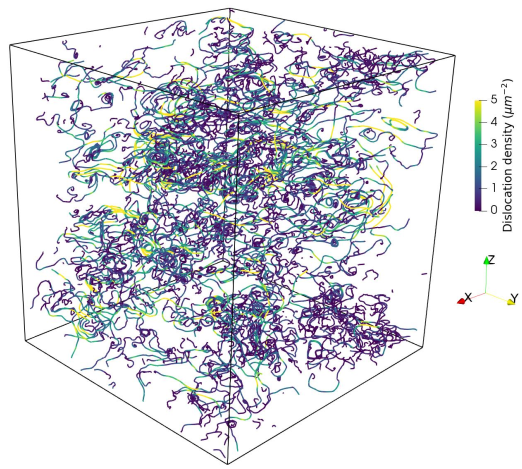

Fig. 1 Streamlines of the density field of dislocations on a single slip system in the line bundle regime. Taken from a typical vector density-based CDD simulation of a (5x5x5.3) μm^3 crystal volume of steel strained to 0.6%. These streamlines represent the approximate position of the underlying discrete dislocation objects.

where M is a mobility constant, b is the length of the Burgers vector, $\tau^{[\alpha]}$ is the resolved shear stress on slip system α, and $\hat{\boldsymbol{v}} := \hat{\boldsymbol{n}}^{[\alpha]} \times (\boldsymbol{\rho}^{[\alpha]}/|\boldsymbol{\rho}^{[\alpha]}|)$ is the direction normal to the slip plane and the dislocation density vector.

The line-bundle assumption not only produces a simplified transport equation (29), but also allows treatment of dislocation reactions by a conventional reaction rate-type theory [79]. In this construction, two reacting slip systems β, γ produce a product density on slip system α:

$$\dot{\boldsymbol{\rho}}^{[\alpha]}_{\text{source}} = \boldsymbol{\rho}^{[\beta]} \cdot \boldsymbol{R}^{[\beta,\gamma]\to[\alpha]} \cdot \boldsymbol{\rho}^{[\gamma]} \tag{31}$$

allowing dislocations to leave the slip-system by means of their respective sink terms. The rate constant $\boldsymbol{R}^{[\beta,\gamma]\to[\alpha]}$ for this process is defined based on the relative velocities of dislocations in the two reagent slip systems and a length scale parameter which characterizes the effective junction length [79]. The reaction rate takes into consideration the effect of orientation of the reacting dislocations based on an energy criterion to decide whether the reaction is feasible or not. This is possible because the orientation of the underlying dislocations is well-defined due to the line-bundle assumption. These rate constants can then be calibrated against junction data from DDD experiments [80, 81].

Moreover, while equation (30) allows for the consideration the transport equation in a self-consistent field context, the dislocation correlation functions of the vector density system has recently been shown [76] to have a simple form, whereby the two-point density may be expressed (cf. equation 8):

$$\left\langle \rho_i^{(D)[\alpha]}(\boldsymbol{r}) \rho_j^{(D)[\beta]}(\boldsymbol{r'}) \right\rangle = \rho_i^{[\alpha]}(\boldsymbol{r}) \rho_j^{[\beta]}(\boldsymbol{r'}) \left(1 + d^{(i,j)[\alpha,\beta]}(\boldsymbol{r} - \boldsymbol{r'})\right) \tag{32}$$

where $\rho_i^{(D)[\alpha]}(\boldsymbol{r})$ represents the ith component of $\boldsymbol{\rho}^{(D)}_{\mathcal{L}^{[\alpha]}}(\boldsymbol{r})$. Due to a corollary of the line bundle assumption, there is no tensor summation in the above equation. The correlation functions for the case of $\alpha = \beta$ were evaluated from DDD experiments [76], and were seen to decay at length scales similar to the spatial gradients of $\boldsymbol{\rho}^{[\alpha]}$. Incorporating these correlation-induced effects would still produce effects analogous to the 2D effective stresses (equations 11-14), but a local density approximation (as in [37]) would not be appropriate.

Because of the line bundle assumption which allows for such close analogy with the underlying discrete dislocation lines, many of the closure relations in the vector density formulation (e.g. correlation functions, reaction rate terms, etc.) are easily formulated in terms of statistics that can be gathered from DDD experiments [76, 79–81]. However, this invites a possible accusation that the vector density dislocation dynamics are simply a numeric approximation to DDD by which nothing is gained. In practice, this is not the case. Before moving on we would like to highlight several recent achievements of the vector density approach which go beyond the capabilities of DDD.

Even in this line bundle regime, the dislocation density vector still describes the collective motion of dislocations. As a result, the mechanical fields that result can show the effect of their collective behavior. For instance, lattice misorientation provides information about the abrupt lattice direction change in a single crystal, which demarcates subgrain structures in deformed metals. At these regions of concentrated misorientation, there arise so-called geometrically necessary boundaries and incidental dislocation boundaries which are observed in transmission electron microscopy experiments [82–84]. These structures, as well as other heterogeneities in the GND field, play a vital role in the context of recrystallization [85]. Preliminary vector density dislocation dynamics studies have suggested that the emergence of dislocation patterns and subgrains is tied to the introduction of cross-slip and dislocation reactions [80, 86]. Upon introduction of reaction terms, subgrain structures began to emerge (cf. Fig. 2) [86]. These capabilities of predicting the onset of subgrain formation will allow fruitful comparison with recent *in-situ* methods for measuring the lattice rotations of subgrains [87]. It is comparisons such as these that will advance our understanding of the effect of dislocation structures on the plastic behavior of metals.

Additionally, it is worth noting that continuum dislocation dynamics models are capable of accounting for the kinematics of finite deformation [67, 73, 88, 89]. We omit for present consideration the numerous phenomenological crystal theories to focus on theories which explicitly consider the kinematics of dislocation densities. In this setting, the multiplicative decomposition of the deformation gradient is used to introduce elastic and plastic effects on the body (cf. the decomposition of the distortion field in equation 20-21). These models all leverage the use of the Kröner-Nye dislocation density tensor, which Cermelli [90] showed to transform using Piola type transformations by analyzing Burgers circuits in both reference and deformed configurations. In FDM, the dislocation density tensor in the deformed configuration represents the dislocation system and closure relations are formed with this in mind. In the vector density approach, the dislocation density tensor is decomposed into slip system parts and either a scalar or vector density representation of dislocations are formed. Hochrainer and Weger [73] derive the transport equations for the vector density in the intermediate configuration by decomposing the dislocation density tensor in the microstructure configuration into slip system components.

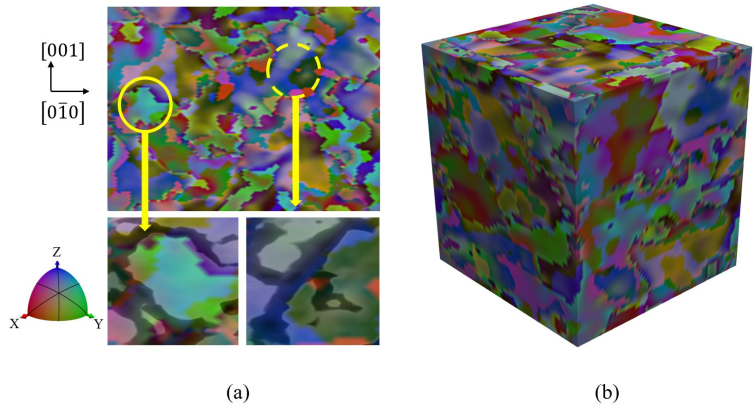

Fig. 2 Lattice rotations in a (5x5x5.3) μm^3 crystal volume of copper at 0.6% strain shown as an RGB plot where red, green and blue corresponds to the components of the normalized lattice rotation vector along [100], [010], and [001], respectively. Visualization of (a) slice along (100) plane, (b) the bulk. Two regions in (a) have beeny enlarged to show the GND density distribution superimposed (black) on the lattice rotation fields.

Starkey et al. [88] derive not only the transport relations but driving forces as well in both the deformed and reference configuration by using the two-point dislocation density tensors. Consistency between these two vector density models can be seen by taking the time derivative of the transformation relations between the referential and microstructure vector densities and plugging in the transport relations for the referential densities. In all these works, the driving forces are obtained by examining the free energy dissipation inequality for each of the corresponding configurations. This allows the corresponding Mandel stress to drive the dislocation motion in each configuration and in some cases, an additional contribution to the driving force emerges from gradients of the free energy. Because the computational complexity of the vector density system does not scale with the total dislocation density and because the kinematics are preserved in the case of finite deformation, the vector density approach is not constrained to the small strain regime as is the case for DDD. Barring a breakdown of the line-bundle assumption at high strains, there does not seem to be an upper strain limit on the efficacy of vector density approaches. It is our opinion that in pushing dislocation dynamics to ever higher strains, vector density dislocation dynamics will emerge as a useful tool in describing microscopic plasticity.

5 Higher Order Theories

As with the 2D models of dislocation motion, to be truly length-scale agnostic the dislocation density measures must retain some information regarding the underlying dislocations' distribution over an orientation space [91]. First pioneered by Hochrainer and associates [78, 92, 93], considerable work has been done on the kinematics of curved line systems when this orientation distribution is taken into account. This presentation of the kinematics will follow most closely [94]. The formulation of these high-order kinematics of curved lines was motivated by the fact that without the line bundle constraint mentioned previously, the transport equation for the density field (29) cannot be expressed in terms of the density vector because the the average slip rate vector is no longer proportional to the cross product of the average density and velocity fields, i.e.:

$$\left\langle \boldsymbol{v}^{[\alpha]} \times \boldsymbol{\rho}^{[\alpha]} \right\rangle \not\propto \left\langle \boldsymbol{v}^{[\alpha]} \right\rangle \times \left\langle \boldsymbol{\rho}^{[\alpha]} \right\rangle \tag{33}$$

To amend this issue, the dislocation density must be treated similarly to the 2D case: as a distribution not only over real space $\mathcal{M}$, but also over an orientation space $\mathbb{T}$, the unit circle parametrized by $\varphi = [0, 2\pi)$. This orientation space defines the line tangent $\hat{\boldsymbol{l}}(\varphi) := \cos(\varphi)\hat{\boldsymbol{b}} + \sin(\varphi)\hat{\boldsymbol{a}}$, where by $\hat{a}$ we represent the positive edge dislocation direction $\hat{\boldsymbol{a}} := \hat{\boldsymbol{n}} \times \hat{\boldsymbol{b}}$. Rather than the ensemble average of space curves, the high-order density represents an ensemble average of 'lifted curves' which are represented at every point by the tuple of not only their line direction $\boldsymbol{l}$ but also their curvature k, forming a 4-vector $\boldsymbol{L}$ which moves according to the 4-vector $\boldsymbol{V}$:

$$\boldsymbol{L}(\boldsymbol{r}, \varphi) := \left(\hat{\boldsymbol{l}}(\varphi), k(\boldsymbol{r}, \varphi)\right) \tag{34}$$

$$\boldsymbol{V}(\boldsymbol{r}, \varphi) := \left(v(\boldsymbol{r}, \varphi)\hat{\boldsymbol{l}}_{\perp}(\varphi), \vartheta(\boldsymbol{r}, \varphi)\right) \tag{35}$$

where $\hat{\boldsymbol{l}}_{\perp}(\varphi) := (\hat{\boldsymbol{l}}(\varphi) \times \hat{\boldsymbol{n}})$ and $\vartheta(\boldsymbol{r}, \varphi)$ is an orientation velocity which captures the rotation of the lines. As opposed to the vector-density measure, which represents a spatial distribution times a line direction in real space, the high-order density also retains a component in the orientation space:

$$\boldsymbol{\rho}_{\mathrm{HO}}(\boldsymbol{r}, \varphi) := \rho(\boldsymbol{r}, \varphi)(\hat{\boldsymbol{l}}(\varphi), k(\boldsymbol{r}, \varphi)) \tag{36}$$

After the averaging process, note that the $k(\boldsymbol{r}, \varphi)$ represents the average curvature of all dislocation lines passing through $\boldsymbol{r}$ which have tangent direction $\hat{\boldsymbol{l}}(\varphi)$, and so the component of $\boldsymbol{\rho}_{\mathrm{HO}}^{[\alpha]}$ in the orientation 'direction' is referred to as the curvature density $q(\boldsymbol{r}) := \rho(\boldsymbol{r}, \varphi)k(\boldsymbol{r}, \varphi)$. The key operation of this kinematic formulation is that the orientation velocity, ϑ, is expressible as the directional derivative of the real-space velocity, v, in 4-space along $\boldsymbol{L}$:

$$\begin{aligned} \vartheta(\boldsymbol{r}, \varphi) &= \hat{\boldsymbol{\nabla}}_{\boldsymbol{L}} v(\boldsymbol{r}, \varphi) \\ &= \left[\left(\hat{\boldsymbol{l}}(\varphi) \cdot \boldsymbol{\nabla}\right) + k(\boldsymbol{r}, \varphi)\partial_{\varphi}\right] v(\boldsymbol{r}, \varphi) \end{aligned} \tag{37}$$

where $\hat{\boldsymbol{\nabla}}$ represents the 4-space gradient operator, and $\boldsymbol{\nabla}$ represents the conventional gradient operator in the spatial dimensions.

The main result of this high-order dislocation density measure is that the evolution equation is expressible in terms of a single velocity field, even after ensemble averaging. This is expressed rather simply in terms of the 4-space curl operator as:

$$\partial_t \boldsymbol{\rho}_{\mathrm{HO}} = -\mathrm{Curl}(\boldsymbol{V} \times \boldsymbol{\rho}_{\mathrm{HO}}) \tag{38}$$

Because of unintuitive nature of the high-dimensional differential operators, it is more simply expressed as two coupled evolution equations for the scalar dislocation density and the curvature density:

$$\partial_t \rho = -\left(\hat{\boldsymbol{l}}_\perp \cdot \boldsymbol{\nabla}\right)(\rho v) - \partial_\varphi(\rho\vartheta) + qv \tag{39}$$

$$\partial_t q = \left(\hat{\boldsymbol{l}} \cdot \boldsymbol{\nabla}\right)(\rho\vartheta) - \left(\hat{\boldsymbol{l}}_\perp \cdot \boldsymbol{\nabla}\right)(qv) \tag{40}$$

These high-dimensional transport equations have been applied in the past to some simplified scenarios, notably a simplified micro-bending geometry [95, 96], where they have been seen to generate hardening behavior in the tension and shear deformation of thin-films [97]. However, there has been much interest in simplifying these evolution equations, as solutions of the high-dimensional transport equations require discretizing the orientation space at every point in the crystal. As a result, there have been efforts to create a reduced representation of the angular space. Early attempts at this simplification [98, 99] began to integrate the dislocation density and curvature density over configuration space, but this process was formalized in [100]. This formulation recasts the evolution equations (39, 40) as an infinite hierarchy of coupled equations by taking successive integral moments of the dislocation density tensor. These alignment tensors are expressed as:

$$\rho^{(0)}(\boldsymbol{r}) = \int d\varphi\, \rho(\boldsymbol{r},\varphi) \tag{41}$$

$$\boldsymbol{\rho}^{(1)}(\boldsymbol{r}) = \int d\varphi\, \rho(\boldsymbol{r},\varphi)\, \hat{\boldsymbol{l}}(\varphi) \tag{42}$$

$$\boldsymbol{\rho}^{(2)}(\boldsymbol{r}) = \int d\varphi\, \rho(\boldsymbol{r},\varphi)\, \hat{\boldsymbol{l}}(\varphi) \otimes \hat{\boldsymbol{l}}(\varphi) \tag{43}$$

$$\boldsymbol{\rho}^{(n)}(\boldsymbol{r}) = \int d\varphi\, \rho(\boldsymbol{r},\varphi)\, \hat{\boldsymbol{l}}(\varphi)^{\otimes n} \tag{44}$$

The zeroth and first alignment tensors represent the total and geometrically necessary dislocation content, respectively, at a point in the crystal. Their evolution equations are expressed as follows:

$$\partial_t \rho^{(0)} = \boldsymbol{\nabla} \cdot \left(v\, \hat{\boldsymbol{n}} \times \boldsymbol{\rho}^{(1)}\right) + v\, \boldsymbol{Q}^{(0)} \tag{45}$$

$$\partial_t \boldsymbol{\rho}^{(n)} = \Big[\boldsymbol{\nabla} \times \left(v\, \hat{\boldsymbol{n}} \otimes \boldsymbol{\rho}^{(n-1)}\right) + (n-1)v\, \boldsymbol{Q}^{(n)} - (n-1)\left(\hat{\boldsymbol{n}} \times \boldsymbol{\rho}^{(n+1)}\right) \cdot \boldsymbol{\nabla} v\Big]_{\mathrm{sym}} \tag{46}$$

$$\partial_t q^{(0)} = \nabla \cdot \left(v\, \boldsymbol{Q}^{(1)} - \boldsymbol{\rho}^{(2)} \cdot \boldsymbol{\nabla} v\right) \tag{47}$$

where $\boldsymbol{Q}^{(n)}$ are auxiliary curvature tensors of the form:

$$\boldsymbol{Q}^{(n)} = \int d\varphi\, q(\boldsymbol{r},\varphi)\, \hat{\boldsymbol{l}}_\perp(\varphi) \otimes \hat{\boldsymbol{l}}_\perp(\varphi) \otimes \hat{\boldsymbol{l}}(\varphi)^{\otimes n-2} \tag{48}$$

These equations can be closed at order n if a sufficient form for $\boldsymbol{\rho}^{(n+1)}$ and $\boldsymbol{Q}^{(n)}$ in terms of lower order terms [94, 101]. Comparisons to simplified DDD results showed closure at $n = 1$ (i.e. kinematics of the total and GND densities) to be insufficient to predict microstructure evolution [101, 102] in some cases. Nonetheless, closure of the transport equations at first order seems to be the predominant usage [102–108].

There has been significant work to compare these high-order kinematics of dislocations with DDD experiments [94, 102, 106, 107, 109]. These equations show excellent agreement in many problems regarding collections of expanding dislocation loops [94, 102]. Moreover,many of the closure relations regarding the multipole expansion seem obtainable from DDD as tools emerge to collect curvature and orientation data from segment-based DDD experiments, especially when complemented by the advent of machine learning techniques [102, 106, 107].

Nonetheless, all of the above considerations have regarded only the kinematics of the system, with no regard to the kinetics. That is, they consider how the dislocation density measures move under a prescribed velocity field, they do not give a means of prescribing such a velocity field. The ubiquitous, zeroth-order kinetic strategy is to use some analogy of field dislocation mechanics to solve the long-range stress field resulting from the dislocation eigenstrain field [103, 110] (cf. the mean-field stress in equation 11 or the self-consistent field formulation of equation 30). However, more nuanced kinetics have been proposed. Hochrainer has adapted the free-energy strategy of the 2D plastic potential to this 3D system, introducing back-stress-type driving forces as well as curvature dependent driving forces, albeit in an in an *ad-hoc* manner [111, 112]. A rigorous coarse-graining of the elastic energy functional [37] shows no dependence on the curvature density, but does support the introduction of back-stress terms, which have begun to be used in numerical implementations of high-order CDD [104]. With the exception of the long-range stress field, many of the kinetic effects depend on the dislocation correlation functions. In the high-dimensional CDD equations, the correlation functions are fully dependent on the angular coordinate. In the reduced representation, correlations between many combinations of the alignment tensors and their respective components must be considered [37]. As a result, correlation effects [37] have not been assessed quantitatively at present.

Moreover, while the kinematics are notable for being length scale agnostic, this is somewhat of a hindrance for implementing dislocation reactions. Two theories have been developed to implement reactions, one due to Monavari [113] and another due to Sudmanns [108]. Both involve enumerating possible reaction scenarios (e.g. glissile junctions, frank-read sources, double cross-slip) and implementing them individually. However, the heuristics by which source terms are derived differ significantly. In the implementation by Sudamanns and coworkers [108, 109], reactions create sources of scalar density and curvature. Considering for example glissile junctions of slip systems β, γ resulting in dislocations of type α:

$$\dot{\rho}_{\mathrm{gj}}^{[\alpha]} \propto \rho^{[\beta]} v^{[\beta]} \sqrt{\rho^{[\gamma]}} + \rho^{[\gamma]} v^{[\gamma]} \sqrt{\rho^{[\beta]}} \tag{49}$$

$$\dot{q}_{\mathrm{gj}}^{[\alpha]} \propto \mathrm{sgn}(v^{[\gamma]}) \dot{\rho}_{\mathrm{gj}}^{[\alpha]} \sqrt{\rho_t}, \tag{50}$$

the difficulties of implementation become apparent. The orientation of the reagent slip systems have been seen to strongly affect glissile junction behavior [9], but this information is unavailable in the high-order equations, and homogenization arguments are needed to arrive at relevant reaction volumes dependent on the velocity fields and average dislocation spacings $1/\sqrt{\rho^{[\alpha]}}$. Models such as these show promise in introducing hardening behavior, but they require considerable statistical calibration from more finely resolved models [109].

In short, the higher order kinematics required to maintain a length-scale-agnostic theory of continuum dislocation dynamics capture interesting and unforeseen consequences of the evolution of the average curvature of a dislocation system [97]. It represents a strong theory of the macroscopic effects of dislocation glide on plastic behavior. As the kinematic formulation has reached a simplified and tractable form, larger simulations have become feasible. Recent studies of the deformation of tricrystals [104], microwires [105], and early signs of pattern formation [103], demonstrate the utility of this descriptive framework. However, difficulties regarding incorporation of short-range interactions [111, 112] as well as reaction processes [72, 97, 108, 113, 114] suggest that this will never be a suitable first-principles theory of dislocation motion at high strains.

6 Concluding Remarks

In this contribution, we have summarized several of the current models of continuum dislocation dynamics. We have seen the simplified 2D theory of dislocation motion, which, even if the physical system it considers is relevant only in specific bending geometries, is noteworthy in the fact that it points to the importance of statistical considerations in dislocation dynamics. Research into the 2D system is ongoing as increasingly nuanced statistical considerations reveal new interesting behavior. We examined field dislocation mechanics, which most closely follows the classical theory of distributed dislocations and is notable for its powerful description of internal mechanical fields and deformation kinematics. We considered the vector density approach to dislocation dynamics, which is commonly used by the present authors, with special emphasis on the implications of the line bundle assumption by which it treats only geometrically necessary dislocations. While this approach preserves more of the discrete line information than other continuum models due to its low-level treatment of the dislocation dynamics, several applications which go beyond the capabilities of DDD were discussed. Lastly, we discussed the high-order theory of dislocation dynamics which is capable of describing dislocation glide across all scales. Difficulties pertaining to the closure not only of the kinematics but also the kinetics of the high-order dynamics were discussed; while it shows promise for being a physically based plasticity theory at large scales, it will always be reliant on lower-level theories of dislocation motion.

Throughout, an emphasis has been placed on the role of DDD experiments in informing these continuum models. This is most often in the form of statistical information, which produces virtual effective stresses which enter in the kinetic closure of continuum theories. The 2D theories have the most straightforward relationship with DDD. Nonetheless, with a bit of statistical nuance, the vector density approach obtains these effective stresses, as well as closure relations for dislocation reactions. The high-order theory, as it requires homogenization arguments that have yet to be definitively determined, may require statistical considerations which rely on machine learning techniques to extract salient quantities from DDD.

The outlook for the methods of continuum dislocation dynamics is compelling, to say the least. It seems poised to give us a physical basis for plasticity, not only at micron-scales, but also at the crystal level. As finite deformation methods for continuum dislocation dynamics have now emerged, an entirely new regime of strains now lie open to us. What new strengthening mechanisms might now be within our view? Which outstanding plasticity problems might now be put to rest? In the opinion of the present authors, continuum dislocation dynamics methods could represent a new frontier in plasticity research.

Competing interests

The authors declare that they have no competing interests.

Author's contributions

PL contributed to the discussion of field dislocation mechanics, KS to the discussion of 2D theories and finite deformation considerations in vector density approaches. VV contributed results from vector density approaches as well as discussion of the implementation of reactions in both vector density and high-order theories. YP contributed the introductory discussion of discrete models. AE assisted in determining the scope of the review as well as in the editing process. JPA compiled the manuscript, contributing to the discussion of the high-order theory of dislocation kinematics as well as to the discussion the statistical considerations throughout.

Acknowledgements

This work was supported by the US Department of Energy, Office of Science, Division of Materials Sciences and Engineering, through award number DE-SC0017718 and by the National Science Foundation, Division of Civil, Mechanical, and Manufacturing Innovation (CMMI), through award number 1663311 at Purdue University

References

1. Orowan, E.: Zur kristallplastizität. i. Zeitschrift für Physik **89**(9-10), 605–613 (1934)
2. Polanyi, M.: Über eine art gitterstörung, die einen kristall plastisch machen könnte. Zeitschrift für Physik **89**(9-10), 660–664 (1934)
3. Taylor, G.I.: The mechanism of plastic deformation of crystals. part i.—theoretical. Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character **145**(855), 362–387 (1934)
4. Arsenlis, A., Cai, W., Tang, M., Rhee, M., Oppelstrup, T., Hommes, G., Pierce, T.G., Bulatov, V.V.: Enabling strain hardening simulations with dislocation dynamics. Modelling and Simulation in Materials Science and Engineering **15**(6), 553–595 (2007). doi:10.1088/0965-0393/15/6/001
5. Capolungo, L., Taupin, V.: GD3: generalized discrete defect dynamics. Materials Theory **3**(1), 1–21 (2019). doi:10.1186/s41313-018-0013-9
6. Devincre, B., Madec, R., Monnet, G., Queyreau, S., Gatti, R., Kubin, L.: Modeling Crystal Plasticity with Dislocation Dynamics Simulations: The 'microMegas' Code. In: Mechanics of Nano-Objects, pp. 81–99 (2011). https://www.researchgate.net/publication/258242158
7. Ghoniem, N., Tong, S., Sun, L.: Parametric dislocation dynamics: A thermodynamics-based approach to investigations of mesoscopic plastic deformation. Physical Review B - Condensed Matter and Materials Physics **61**(2), 913–927 (2000). doi:10.1103/PhysRevB.61.913
8. Schwarz, K.W.: Simulation of dislocations on the mesoscopic scale. I. Methods and examples. Journal of Applied Physics **85**(1), 108–119 (1999). doi:10.1063/1.369429
9. Madec, R., Devincre, B., Kubin, L.P.: On the nature of attractive dislocation crossed states. Computational Materials Science **23**(1), 219–224 (2002). doi:10.1016/S0927-0256(01)00215-4
10. Devincre, B., Kubin, L.P., Lemarchand, C., Madec, R.: Mesoscopic simulations of plastic deformation. Materials Science and Engineering A **309-310**, 211–219 (2001). doi:10.1016/S0921-5093(00)01725-1
11. Hussein, A.M., Rao, S.I., Uchic, M.D., Dimiduk, D.M., El-Awady, J.A.: Microstructurally based cross-slip mechanisms and their effects on dislocation microstructure evolution in fcc crystals. Acta Materialia **85**, 180–190 (2015). doi:10.1016/j.actamat.2014.10.067
12. Po, G., Cui, Y., Rivera, D., Cereceda, D., Swinburne, T.D., Marian, J., Ghoniem, N.: A phenomenological dislocation mobility law for bcc metals. Acta Materialia **119**, 123–135 (2016). doi:10.1016/j.actamat.2016.08.016. 1608.01392
13. Malka-Markovitz, A., Devincre, B., Mordehai, D.: A molecular dynamics-informed probabilistic cross-slip model in discrete dislocation dynamics. Scripta Materialia **190**, 7–11 (2021). doi:10.1016/j.scriptamat.2020.08.008
14. Rhee, M., Zbib, H.M., Hirth, J.P., Huang, H., De La Rubia, T.: Models for long-/short-range interactions and cross slip in 3D dislocation simulation of BCC single crystals. Modelling and Simulation in Materials Science and Engineering **6**(4), 467–492 (1998). doi:10.1088/0965-0393/6/4/012
15. Cui, Y., Po, G., Ghoniem, N.: Controlling Strain Bursts and Avalanches at the Nano- to Micrometer Scale. Physical Review Letters **117**(15), 155502 (2016). doi:10.1103/PhysRevLett.117.155502. 1609.07553
16. Cui, Y., Po, G., Ghoniem, N.: Influence of loading control on strain bursts and dislocation avalanches at the nanometer and micrometer scale. Physical Review B **95**(6), 064103 (2017). doi:10.1103/PhysRevB.95.064103
17. Sparks, G., Cui, Y., Po, G., Rizzardi, Q., Marian, J., Maaß, R.: Avalanche statistics and the intermittent-to-smooth transition in microplasticity. Physical Review Materials **3**(8), 080601 (2019). doi:10.1103/PhysRevMaterials.3.080601
18. Crone, J.C., Munday, L.B., Knap, J.: Capturing the effects of free surfaces on void strengthening with dislocation dynamics. Acta Materialia **101**, 40–47 (2015). doi:10.1016/j.actamat.2015.08.067

19. Khraishi, T.A., Zbib, H.M., Diaz De La Rubia, T., Victoria, M.: Modelling of irradiation-induced hardening in metals using dislocation dynamics. Philosophical Magazine Letters **81**(9), 583–593 (2001). doi:10.1080/09500830110069297
20. Cui, Y., Po, G., Ghoniem, N.: Does irradiation enhance or inhibit strain bursts at the submicron scale? Acta Materialia **132**, 285–297 (2017). doi:10.1016/j.actamat.2017.04.055
21. Zbib, H.M., Rhee, M., Hirth, J.P.: On plastic deformation and the dynamics of 3D dislocations. International Journal of Mechanical Sciences **40**(2-3), 113–127 (1998). doi:10.1016/s0020-7403(97)00043-x
22. Sills, R.B., Cai, W.: Efficient time integration in dislocation dynamics. Modelling and Simulation in Materials Science and Engineering **22**(2), 26 (2014). doi:10.1088/0965-0393/22/2/025003
23. Sills, R.B., Aghaei, A., Cai, W.: Advanced time integration algorithms for dislocation dynamics simulations of work hardening. Modelling and Simulation in Materials Science and Engineering (2016). doi:10.1088/0965-0393/24/4/045019
24. Bertin, N., Aubry, S., Arsenlis, A., Cai, W.: GPU-accelerated dislocation dynamics using subcycling time-integration. Modelling and Simulation in Materials Science and Engineering **27**(7), 075014 (2019). doi:10.1088/1361-651X/ab3a03
25. Bertin, N., Upadhyay, M.V., Pradalier, C., Capolungo, L.: 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**(6), 065009 (2015). doi:10.1088/0965-0393/23/6/065009
26. Deshpande, V.S., Needleman, A., Van der Giessen, E.: Finite strain discrete dislocation plasticity. In: Journal of the Mechanics and Physics of Solids, vol. 51, pp. 2057–2083. Pergamon, ??? (2003). doi:10.1016/j.jmps.2003.09.012
27. Irani, N., Remmers, J.J.C., Deshpande, V.S.: Finite strain discrete dislocation plasticity in a total Lagrangian setting. Journal of the Mechanics and Physics of Solids **83**, 160–178 (2015). doi:10.1016/j.jmps.2015.06.013
28. El-Azab, A.: Boundary value problem of dislocation dynamics. Modelling and Simulation in Materials Science and Engineering **8**(1), 37–54 (2000). doi:10.1088/0965-0393/8/1/304
29. Wilkens, M.: The determination of density and distribution of dislocations in deformed single crystals from broadened X-ray diffraction profiles. Physica Status Solidi (a) **2**(2), 359–370 (1970). doi:10.1002/pssa.19700020224
30. Wilkens, M.: Fundamental Aspects of Dislocation Theory. In: National Bureau of Standards, vol. 2, p. 715 (1970)
31. Ungar, T., Mughrabi, H., Rönnpagel, D., Wilkens, M.: X-ray line-broadening study of the dislocation cell structure in deformed [001]-orientated copper single crystals. Acta Metallurgica **32**(3), 333–342 (1984). doi:10.1016/0001-6160(84)90106-8
32. Groma, I.: X-ray line broadening due to an inhomogeneous dislocation distribution. Physical Review B **57**(13), 7535–7542 (1998). doi:10.1103/PhysRevB.57.7535
33. Groma, I.: Link between the microscopic and mesoscopic length-scale description of the collective behavior of dislocations. Physical Review B **56**(10), 5807–5813 (1997). doi:10.1103/PhysRevB.56.5807
34. Groma, I., Balogh, P.: Investigation of dislocation pattern formation in a two-dimensional self-consistent field approximation. Acta Materialia **47**(13), 3647–3654 (1999). doi:10.1016/S1359-6454(99)00215-3
35. Zaiser, M., Miguel, M.C., Groma, I.: Statistical dynamics of dislocation systems: The influence of dislocation-dislocation correlations. Physical Review B **64**(22), 2241021–2241029 (2001). doi:10.1103/PhysRevB.64.224102
36. McQuarrie, D.: Statistical Mechanics, pp. 222–356. University Science Books, Sausalito (2000)
37. Zaiser, M.: Local density approximation for the energy functional of three-dimensional dislocation systems. Physical Review B **92**(17), 174120 (2015). doi:10.1103/PhysRevB.92.174120. arXiv:1508.03652v2
38. Groma, I., Csikor, F.F., Zaiser, M.: Spatial correlations and higher-order gradient terms in a continuum description of dislocation dynamics. Acta Materialia **51**(5), 1271–1281 (2003). doi:10.1016/S1359-6454(02)00517-7
39. Groma, I., Györgyi, G., Kocsis, B.: Dynamics of coarse grained dislocation densities from an effective free energy. In: Philosophical Magazine, vol. 87, pp. 1185–1199. Taylor & Francis Group, ??? (2007). doi:10.1080/14786430600835813. http://www.tandfonline.com/doi/abs/10.1080/14786430600835813 https://www.tandfonline.com/action/journalInformation?journalCode=tphm20
40. Groma, I., Zaiser, M., Dusán Ispánovity, P.: Dislocation patterning in a two-dimensional continuum theory of dislocations. PHYSICAL REVIEW B **93**, 214110 (2016). doi:10.1103/PhysRevB.93.214110
41. Ispánovity, P.D., Papanikolaou, S., Groma, I.: Emergence and role of dipolar dislocation patterns in discrete and continuum formulations of plasticity. Physical Review B **101**(2) (2020). doi:10.1103/PhysRevB.101.024105. 1708.03710v1
42. Gulluoglu, A.N., Srolovitz, D.J., Lesar, R., Lomdahl, P.S.: Dislocation Distributions in Two Dimensions. Scripta Metallurgica **23**, 1347–1352 (1988)
43. Wang, H.Y., Lesar, R., Rickman, J.M.: Analysis of dislocation microstructures: Impact of force truncation and slip systems. Philosophical Magazine A **78**(6), 1195–1213 (1997). doi:10.1080/01418619808239983
44. Groma, I., Györgyi, G., Ispánovity, P.D.: Variational approach in dislocation theory. Philosophical Magazine **90**(27-28), 3679–3695 (2010). doi:10.1080/14786430903401073
45. Kooiman, M., Hütter, M., Geers, M.: Effective mobility of dislocations from systematic coarse-graining. Journal of Statistical Mechanics: Theory and Experiment **2015**(6), 06005 (2015). doi:10.1088/1742-5468/2015/06/P06005
46. Valdenaire, P.-L., Le Bouar, Y., Appolaire, B., Finel, A.: Density-based crystal plasticity: From the discrete to the continuum. PHYSICAL REVIEW B **93**, 214111 (2016). doi:10.1103/PhysRevB.93.214111
47. Yefimov, S., Groma, I., van der Giessen, E.: A comparison of a statistical-mechanics based plasticity model with discrete dislocation plasticity calculations. Journal of the Mechanics and Physics of Solids **52**(2), 279–300 (2004). doi:10.1016/S0022-5096(03)00094-2
48. Schulz, K., Dickel, D., Schmitt, S., Sandfeld, S., Weygand, D., Gumbsch, P.: Analysis of dislocation pile-ups

using a dislocation-based continuum theory. Modelling and Simulation in Materials Science and Engineering **22**(2), 025008 (2014). doi:10.1088/0965-0393/22/2/025008
49. Wu, R., Tüzes, D., Ispánovity, P.D., Groma, I., Hochrainer, T., Zaiser, M.: Instability of dislocation fluxes in a single slip: Deterministic and stochastic models of dislocation patterning. Physical Review B **98**(5), 54110 (2018). doi:10.1103/PhysRevB.98.054110
50. Ispánovity, P.D., Tüzes, D., Szabó, P., Zaiser, M., Groma, I.: Role of weakest links and system-size scaling in multiscale modeling of stochastic plasticity. Physical Review B **95**(5), 054108 (2017). doi:10.1103/PhysRevB.95.054108. 1604.01645
51. Willis, J.R.: Second-order effects of dislocations in anisotropic crystals. International Journal of Engineering Science **5**(2), 171–190 (1967). doi:10.1016/0020-7225(67)90003-1
52. Nye, J.F.: Some geometrical relations in dislocated crystals. Acta Metallurgica **1**(2), 153–162 (1953). doi:10.1016/0001-6160(53)90054-6
53. Gurtin, M.E.: On the plasticity of single crystals: Free energy, microforces, plastic-strain gradients. Journal of the Mechanics and Physics of Solids **48**(5), 989–1036 (2000). doi:10.1016/S0022-5096(99)00059-9
54. Shizawa, K., Zbib, H.M.: A Thermodynamical theory of plastic spin and internal stress with dislocation density tensor. Journal of Engineering Materials and Technology, Transactions of the ASME **121**(2), 247–253 (1999). doi:10.1115/1.2812372
55. Shizawa, K., Zbib, H.M.: A thermodynamical theory of gradient elastoplasticity with dislocation density tensor. I: Fundamentals. International Journal of Plasticity **15**(9), 899–938 (1999). doi:10.1016/S0749-6419(99)00018-2
56. Shizawa, K., Kikuchi, K., Zbib, H.M.: A strain-gradient thermodynamic theory of plasticity based on dislocation density and incompatibility tensors. Materials Science and Engineering A **309**-**310**, 416–419 (2001). doi:10.1016/S0921-5093(00)01630-0
57. Acharya, A.: A model of crystal plasticity based on the theory of continuously distributed dislocations. Journal of the Mechanics and Physics of Solids **49**(4), 761–784 (2001). doi:10.1016/S0022-5096(00)00060-0
58. Roy, A., Acharya, A.: Size effects and idealized dislocation microstructure at small scales: Predictions of a Phenomenological model of Mesoscopic Field Dislocation Mechanics: Part II. Journal of the Mechanics and Physics of Solids **54**(8), 1711–1743 (2006). doi:10.1016/j.jmps.2006.01.012
59. Acharya, A., Roy, A.: 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**(8), 1687–1710 (2006). doi:10.1016/j.jmps.2006.01.009
60. Mura, T.: Continuous distribution of moving dislocations. Philosophical Magazine **8**(89), 843–857 (1963). doi:10.1080/14786436308213841
61. Kosevich, A.M.: DYNAMICAL THEORY OF DISLOCATIONS. Soviet Physics Uspekhi **7**(6), 837–854 (1965). doi:10.1070/pu1965v007n06abeh003688
62. Acharya, A.: Constitutive analysis of finite deformation field dislocation mechanics. Journal of the Mechanics and Physics of Solids **52**(2), 301–316 (2004). doi:10.1016/S0022-5096(03)00093-0
63. Lin, P., Vivekanandan, V., Starkey, K., Anglin, B., Geller, C., El-Azab, A.: On the computational solution of vector-density based continuum dislocation dynamics models: A comparison of two plastic distortion and stress update algorithms. International Journal of Plasticity **138**, 102943 (2021). doi:10.1016/j.ijplas.2021.102943
64. Acharya, A.: Driving forces and boundary conditions in continuum dislocation mechanics. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences **459**(2034), 1343–1363 (2003). doi:10.1098/rspa.2002.1095
65. Brenner, R., Beaudoin, A.J., Suquet, P., Acharya, A.: Numerical implementation of static Field Dislocation Mechanics theory for periodic media. Philosophical Magazine **94**(16), 1764–1787 (2014). doi:10.1080/14786435.2014.896081
66. Puri, S., Das, A., Acharya, A.: Mechanical response of multicrystalline thin films in mesoscale field dislocation mechanics. Journal of the Mechanics and Physics of Solids **59**(11), 2400–2417 (2011). doi:10.1016/j.jmps.2011.06.009
67. Arora, R., Acharya, A.: Dislocation pattern formation in finite deformation crystal plasticity. International Journal of Solids and Structures **184**, 114–135 (2020). doi:10.1016/j.ijsolstr.2019.02.013. 1812.00255
68. Morin, L., Brenner, R., Suquet, P.: Numerical simulation of model problems in plasticity based on field dislocation mechanics. Modelling and Simulation in Materials Science and Engineering **27**(8), 085012 (2019). doi:10.1088/1361-651X/ab49a0
69. Bertin, N., Capolungo, L.: A FFT-based formulation for discrete dislocation dynamics in heterogeneous media. Journal of Computational Physics **355**, 366–384 (2018). doi:10.1016/j.jcp.2017.11.020
70. Kröner, E.: Benefits and shortcomings of the continuous theory of dislocations. International Journal of Solids and Structures **38**(6-7), 1115–1134 (2001). doi:10.1016/S0020-7683(00)00077-9
71. El-Azab, A., Po, G.: Continuum Dislocation Dynamics: Classical Theory and Contemporary Models. In: Handbook of Materials Modeling, pp. 1–25. Springer, Cham (2018). doi:10.1007/978-3-319-42913-7_18-1. http://link.springer.com/10.1007/978-3-319-42913-7_18-1
72. Weger, B., Hochrainer, T.: Leaving the Slip System - Cross Slip in Continuum Dislocation Dynamics. PAMM **19**(1), 201900441 (2019). doi:10.1002/pamm.201900441
73. Hochrainer, T., Weger, B.: Is crystal plasticity non-conservative? Lessons from large deformation continuum dislocation theory. Journal of the Mechanics and Physics of Solids **141**, 103957 (2020). doi:10.1016/j.jmps.2020.103957
74. Xia, S.X., El-Azab, A.: A preliminary investigation of dislocation cell structure formation in metals using continuum dislocation dynamics. In: IOP Conference Series: Materials Science and Engineering, vol. 89 (2015). doi:10.1088/1757-899X/89/1/012053
75. Xia, S.X., El-Azab, A.: Computational modelling of mesoscale dislocation patterning and plastic deformation of single crystals. Modelling and Simulation in Materials Science and Engineering **23** (2015). doi:10.1088/0965-0393/23/5/055009

76. Anderson, J.P., El-Azab, A.: On the three-dimensional spatial correlations of curved dislocation systems. Materials Theory (in press)
77. Xia, S.X.: Continuum Dislocation Dynamics Modelling of the Deformation of FCC Single Crystals. Phd, Purdue University (2016)
78. Hochrainer, T., Zaiser, M., Gumbsch, P.: A three-dimensional continuum theory of dislocation systems: Kinematics and mean-field formulation. Philosophical Magazine **87**(8-9), 1261–1282 (2007). doi:10.1080/14786430600930218
79. Lin, P., El-Azab, A.: Implementation of annihilation and junction reactions in vector density-based continuum dislocation dynamics. Modelling and Simulation in Materials Science and Engineering **28**(4) (2020). doi:10.1088/1361-651X/ab7d90. 1910.12766
80. Xia, S., Belak, J., El-Azab, A.: The discrete-continuum connection in dislocation dynamics: I. Time coarse graining of cross slip. Modelling and Simulation in Materials Science and Engineering **24**(7), 075007 (2016). doi:10.1088/0965-0393/24/7/075007
81. Deng, J., El-Azab, A.: Temporal statistics and coarse graining of dislocation ensembles. In: Philosophical Magazine, vol. 90, pp. 3651–3678 (2010). doi:10.1080/14786435.2010.497472. https://www.tandfonline.com/action/journalInformation?journalCode=tphm20
82. Godfrey, A., Hughes, D.A.: Scaling of the spacing of deformation induced dislocation boundaries. Acta Materialia **48**(8), 1897–1905 (2000). doi:10.1016/S1359-6454(99)00474-7
83. Hughes, D.A., Liu, Q., Chrzan, D.C., Hansen, N.: Scaling of microstructural parameters: Misorientations of deformation induced boundaries. Acta Materialia **45**(1), 105–112 (1997). doi:10.1016/S1359-6454(96)00153-X
84. Hughes, D.A., Hansen, N., Bammann, D.J.: Geometrically necessary boundaries, incidental dislocation boundaries and geometrically necessary dislocations. Scripta Materialia **48**(2), 147–153 (2003). doi:10.1016/S1359-6462(02)00358-5
85. Humphreys, F.J., Hatherly, M.: Recrystallization and Related Annealing Phenomena. Elsevier, ??? (2012)
86. Vivekanandan, V., Lin, P., Winther, G., El-Azab, A.: On the implementation of dislocation reactions in continuum dislocation dynamics modeling of mesoscale plasticity. Journal of the Mechanics and Physics of Solids **149**, 104327 (2021). doi:10.1016/j.jmps.2021.104327
87. Juul, N.Y., Oddershede, J., Winther, G.: Analysis of Grain-Resolved Data from Three-Dimensional X-Ray Diffraction Microscopy in the Elastic and Plastic Regimes. JOM **72**(1), 83–90 (2020). doi:10.1007/s11837-019-03829-6
88. Starkey, K., Winther, G., El-Azab, A.: Theoretical development of continuum dislocation dynamics for finite-deformation crystal plasticity at the mesoscale. Journal of the Mechanics and Physics of Solids **139**, 103926 (2020). doi:10.1016/j.jmps.2020.103926
89. Po, G., Huang, Y., Ghoniem, N.: A continuum dislocation-based model of wedge microindentation of single crystals. International Journal of Plasticity **114**, 72–86 (2019). doi:10.1016/j.ijplas.2018.10.008
90. Cermelli, P., Gurtin, M.E.: On the characterization of geometrically necessary dislocations in finite plasticity. Journal of the Mechanics and Physics of Solids **49**(7), 1539–1568 (2001). doi:10.1016/S0022-5096(00)00084-3
91. El-Azab, A.: Statistical mechanics treatment of the evolution of dislocation distributions in single crystals. Physical Review B **61**(18), 11956–11966 (2000). doi:10.1103/PhysRevB.61.11956
92. Hochrainer, T.: Evolving systems of curved dislocations: mathematical foundations of a statistical theory. PhD thesis, Karlsruhe Institute of Technology (2007). doi:10.13140/RG.2.1.1630.6407
93. Hochrainer, T., Sandfeld, S., Zaiser, M., Gumbsch, P.: Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. Journal of the Mechanics and Physics of Solids **63**, 167–178 (2014). doi:10.1016/J.JMPS.2013.09.012
94. Monavari, M., Zaiser, M., Sandfeld, S.: Comparison of closure approximations for continuous dislocation dynamics. Materials Research Society Symposium Proceedings **1651**, 13–16510302 (2014). doi:10.1557/opl.2014.62
95. Sandfeld, S., Hochrainer, T., Gumbsch, P., Zaiser, M.: Numerical implementation of a 3D continuum theory of dislocation dynamics and application to micro-bending. Philosophical Magazine **90**(27-28), 3697–3728 (2010). doi:10.1080/14786430903236073
96. Sandfeld, S.: The Evolution of Dislocation Density in a Higher-order Continuum Theory of Dislocation Plasticity. PhD thesis, University of Edinburgh (2010)
97. Sandfeld, S., Thawinan, E., Wieners, C.: A link between microstructure evolution and macroscopic response in elasto-plasticity: Formulation and numerical approximation of the higher-dimensional continuum dislocation dynamics theory. International Journal of Plasticity **72**, 1–20 (2015). doi:10.1016/J.IJPLAS.2015.05.001
98. Sandfeld, S., Hochrainer, T., Zaiser, M., Gumbsch, P.: Continuum modeling of dislocation plasticity: Theory, numerical implementation, and validation by discrete dislocation simulations. Journal of Materials Research **26**(5), 623–632 (2011). doi:10.1557/jmr.2010.92
99. Hochrainer, T., Zaiser, M., Gumbsch, P.: Dislocation transport and line length increase in averaged descriptions of dislocations. AIP Conference Proceedings **1168**, 1133–1136 (2010). 1010.2884
100. Hochrainer, T.: Multipole expansion of continuum dislocations dynamics in terms of alignment tensors. Philosophical Magazine **95**(12), 1321–1367 (2015). doi:10.1080/14786435.2015.1026297
101. Monavari, M., Sandfeld, S., Zaiser, M.: Continuum representation of systems of dislocation lines: A general method for deriving closed-form evolution equations. Journal of the Mechanics and Physics of Solids **95**, 575–601 (2016). doi:10.1016/J.JMPS.2016.05.009
102. Sandfeld, S., Po, G.: Microstructural comparison of the kinematics of discrete and continuum dislocations models. Modelling and Simulation in Materials Science and Engineering **23**(8) (2015). doi:10.1088/0965-0393/23/8/085003
103. Sandfeld, S., Zaiser, M.: Pattern formation in a minimal model of continuum dislocation plasticity. Modelling and Simulation in Materials Science and Engineering **23**(6), 065005 (2015).

doi:10.1088/0965-0393/23/6/065005. 1501.03527

104. Schulz, K., Wagner, L., Wieners, C.: A mesoscale continuum approach of dislocation dynamics and the approximation by a Runge-Kutta discontinuous Galerkin method. International Journal of Plasticity **120**, 248–261 (2019). doi:10.1016/j.ijplas.2019.05.003
105. Zoller, K., Schulz, K.: Analysis of single crystalline microwires under torsion using a dislocation-based continuum formulation. Acta Materialia **191**, 198–210 (2020). doi:10.1016/j.actamat.2020.03.057
106. Song, H., Gunkelmann, N., Po, G., Sandfeld, S.: Data-mining of dislocation microstructures: concepts for coarse-graining of internal energies. Modelling and Simulation in Materials Science and Engineering (2021). doi:10.1088/1361-651x/abdc6b. 2012.14815
107. Steinberger, D., Gatti, R., Sandfeld, S.: A Universal Approach Towards Computational Characterization of Dislocation Microstructure. JOM **68**(8), 2065–2072 (2016). doi:10.1007/s11837-016-1967-1. 1603.04635
108. Sudmanns, M., Stricker, M., Weygand, D., Hochrainer, T., Schulz, K.: Dislocation multiplication by cross-slip and glissile reaction in a dislocation based continuum formulation of crystal plasticity. Journal of the Mechanics and Physics of Solids **132**, 103695 (2019). doi:10.1016/j.jmps.2019.103695
109. Sudmanns, M., Bach, J., Weygand, D., Schulz, K.: Data-driven exploration and continuum modeling of dislocation networks. Modelling and Simulation in Materials Science and Engineering **28**(6) (2020). doi:10.1088/1361-651X/ab97ef
110. Sandfeld, S., Monavari, M., Zaiser, M.: From systems of discrete dislocations to a continuous field description: Stresses and averaging aspects. Modelling and Simulation in Materials Science and Engineering **21**(8) (2013). doi:10.1088/0965-0393/21/8/085006
111. Hochrainer, T.: Thermodynamically consistent continuum dislocation dynamics. Journal of the Mechanics and Physics of Solids **88**, 12–22 (2016). doi:10.1016/J.JMPS.2015.12.015
112. Groma, I., Ispánovity, P.D., Hochrainer, T.: On the dynamics of curved dislocation ensembles. Preprint (2020). 2012.12560
113. Monavari, M., Zaiser, M.: Annihilation and sources in continuum dislocation dynamics. Materials Theory **2**(1), 3 (2018). doi:10.1186/s41313-018-0010-z. 1709.03694
114. Stricker, M., Sudmanns, M., Schulz, K., Hochrainer, T., Weygand, D.: Dislocation multiplication in stage II deformation of fcc multi-slip single crystals. Journal of the Mechanics and Physics of Solids **119**, 319–333 (2018). doi:10.1016/j.jmps.2018.07.003