A continuum model for dislocation dynamics in three dimensions using the dislocation density potential functions and its application in understanding the micro-pillar size effect

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Abstract

In this paper, we propose a dislocation-based three-dimensional continuum model to study the plastic behaviors of crystalline materials with physical dimensions ranging from the order of microns to submillimeters. It is shown that the proposed continuum model not only provides a proper summary of the underlying discrete dislocation dynamics, but also is the realization of the classical continuous plasticity theories in the context of dislocation dynamics. In the continuum model here, the dislocation substructures are represented by two families of dislocation density potential functions (DDPFs), denoted by $\phi$ and $\psi$. The slip planes of dislocations are thus characterized by the contour surfaces of $\psi$, while the dislocation curves on each slip plane are identified by the contour curves of $\phi$ on that plane. By adopting such way in representing the dislocation substructures, the geometries and the density distribution of the dislocation ensembles can be simply expressed in terms of the spatial derivatives of the DDPFs. More importantly, one can use the DDPFs to explicitly write down an evolutionary system of equations, which is shown to be an result of the upscaling of the underlying discrete dislocation dynamics. The derived system includes i) a constitutive stress rule, which describes how the internal stress field is determined in the presence of the dislocation networks and applied loads; ii) a plastic flow rule, which describes how the motion of the dislocation ensemble is driven by the existing stress field. The derived continuum model using the DDPFs are validated through comparisons with the discrete dislocation dynamical simulation and experimental results. As an application of the derived model, the “smaller-being-stronger” size effect observed in the uniaxial compression
tests of single-crystalline micropillars is studied and an explicit formula between the flow stress and the pillar size $D$ is derived. The obtained formula shows excellent agreement with the experimental observations and it suggests that the flow stress scales with the pillar size by $\log(D)/D$.

**Keywords:** Dislocations, Crystal plasticity, Continuum model, Size effect, Micro-pillars, Finite elements

1. **Introduction**

Understanding the plastic properties of crystalline materials is one of the key issues in controlling the process of manufacturing metallic components. For crystalline structures of size ranging from the order of millimeters or above, the classical continuum plasticity (CCP) theories have shown their abilities in predicting the elastic-plastic behaviors of the materials when being deformed. However, when studying the widely observed size effect on the strength of crystals at the micro- or nano-scale (e.g. Venkatraman and Bravman, 1992; Uchic et al., 2004, 2009; Jang et al., 2012), the CCP theories which are generally size-independent find their limitations. Although the CCP theories have been modified by including the plastic strain gradient terms so as to incorporate some internal length scales (e.g. Fleck and Hutchinson, 1993; Nix and Gao, 1998; Gurtin, 2002; Aifantis and Ngan, 2007), these phenomenological plasticity theories are still far from satisfactory to meet the demand from the micro- or nano-technology (Chakravarthy and Curtin, 2011). On the other hand, since it has been widely agreed that the dislocations are the major carriers of crystalline plasticity, the discrete dislocation dynamical (DDD) models have also been developed to investigate the underlying mechanism governing the plastic deformation of micro- or nano-crystals. Compared to the CCP theories, the focus of the DDD models is on the behaviors of individual dislocations, which are treated as line singularities embedded into an elastic media, and the internal stress field is generally calculated by the superposition

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method proposed by Van der Giessen and Needleman (1995), that is, the internal stress field is the superposition of the stress field due to all dislocation loops in an infinite media, which can be calculated by using the Peach-Kölher stress formula (Hirth and Lothe, 1982) and the stress field due to the elastic response to an image boundary condition. With the stress field calculated, under the imposed laws for dislocation multiplication, annihilation, gliding, climbing, etc., the microstructural changes within crystals can be investigated by tracking the evolution of these dislocation curves. Under such frameworks, the three-dimensional DDD simulation approaches have been well developed (e.g. Kubin et al., 1992; Moulin et al., 1997; Zbib et al., 1998; Fivel et al., 1998; Faradjian et al., 1999; Ghoniem et al., 2000; Gómez-García et al., 2000; von Blanckenhagen et al., 2001; Weygand et al., 2002; Xiang et al., 2003; Han et al., 2003; Benzerga et al., 2004; Quek et al., 2006; Arsenlis et al., 2007; Rao et al., 2007; El-Awady et al., 2008; Tang et al., 2008; Senger et al., 2008; El-Awady et al., 2009; Zhao et al., 2012; Fitzgerald et al., 2012; Zhou and LeSar, 2012; Ryu et al., 2013; Zhu et al., 2013). The DDD models have been well applied to provide insights in explaining many plastic behaviors observed in micro- or nano-crystalline structures, such as in thin films (e.g. von Blanckenhagen et al., 2001; Weygand et al., 2002; Quek et al., 2006; Zhou and LeSar, 2012) and in micro-pillars (e.g. Rao et al., 2007; El-Awady et al., 2008; Tang et al., 2008; Senger et al., 2008; El-Awady et al., 2009; Ryu et al., 2013). However, the three-dimensional DDD simulations become too computationally intensive to be implemented for crystals having the size exceeding the order of several microns, to the best of the authors’ knowledge.

Therefore, plasticity theories designed to efficiently describe the deformation process for crystals of size from microns to sub-millimeters are still highly expected. Such plasticity theories in demand should possess two characteristics. First, the resolution of the expected plasticity theories should be higher than that of the CCP theories, that is, the information about the dislocation substructures should be properly taken into account in the expected plasticity theories. Second, the expected theories need to be less computationally intensive compared to the three-dimensional DDD simulation for metallic samples of size at the order of several microns or above. Fueled by such demands, the dislocation-based continuum
plasticity theories have recently drawn considerable attentions of many researchers. In the continuum models, the focus is not on individual dislocations, but the collective behaviors of the dislocation ensembles. The length scales associated with such continuum models lie between the length scales associated with the CCP and DDD models. The objects “observed” at the length scale characterized by the continuum model (termed as “the continuum scale” in the rest of this paper), become continuous dislocation density distributions represented by the Nye’s dislocation density tensor (Nye, 1953; Kröner, 1963). One of the main goals in such dislocation density based models is to establish continuum laws which are consistent with the underlying discrete dislocation dynamics and such laws include

i) A constitutive stress rule: the determination of the internal stress field in the presence of a given continuous dislocation density distribution and applied loads.

ii) A plastic flow rule: a description of the collective motion of the dislocations, which result in plastic flows in crystals in response to the existing internal stress field.

The plastic deformation process of crystals, therefore, is described by coupling the above two rules.

As the simplest case of such continuous ways in representing dislocation ensembles, the collective behaviors of systems of straight and parallel dislocations have been studied considerably well (e.g. Groma et al., 2003; Voskoboinikov et al., 2007; Kochmann and Le, 2008; Hall, 2011; Liu et al., 2011; Oztop et al., 2013; Geers et al., 2013; Zhu and Chapman, 2014). In these works, the translationally symmetric dislocations can be treated as point singularities (or poles) in their perpendicularly transversal planes. The distribution of these poles are thus expressed by a (scalar) variable characterizing the dislocation density, and thus the complexity of the system is dramatically reduced.

However, the development in systematically building three-dimensional dislocation-based continuum plasticity theories is still far from satisfactory despite a number of valuable works (e.g. Nye, 1953; Kröner, 1963; Kosevich, 1979; Head et al., 1993; Rickman and Vinals, 1997; El-Azab, 2000; Acharya, 2001; Arsenlis and Parks, 2002; Sedláček et al., 2003; Alankar et al., 2009, 2011; Mayeur et al., 2011; Sandfeld et al., 2011; Engels et al., 2012; Hochrainer
et al., 2014; Li et al., 2014; Mayeur and McDowell, 2014; Cheng et al., 2014). The main difficulty in the establishment of such continuum theories is due to the fact that the complex networks of curved dislocation substructures make it extremely difficult to explicitly summarize for constitutive laws from the underlying discrete dislocation dynamics.

To overcome such difficulties, Xiang (2009) introduced the idea of the coarse-grained disregistry functions (CGDFs) originating from the exact disregistry functions used in the Peierls-Nabarro (PN) models (Peierls, 1940; Nabarro, 1947; Xu and Argon, 2000; Xiang et al., 2008). In PN models, the exact disregistry functions take the profile of a regularized jump with height of a Burgers vector over the dislocation core when going across a dislocation on its slip plane. The CGDF is to approximate the exact disregistry function by a smoothly varying profile without resolving details of the dislocation cores, so that the dislocation curves can be described the contours of the CGDF with an integer value multiplied by the modulus of the Burgers vector. With the smooth CGDF defined in this way, the dislocation substructures can be well represented. For example, quantities describing the dislocation geometries, such as the dislocation line directions and curvatures, and the Nye's dislocation density tensor are both found simple functions of the CGDF and its spatial derivatives.

More importantly, with the help of the CGDF, one may explicitly formulate the two laws mentioned above, which are needed for building a continuum model for the dislocation dynamics on one single slip plane. Here to distinguish from the full three-dimensional model to be presented in this paper, the continuum model for dislocation dynamics on one slip plane is termed as the “two-dimensional case”. It has been rigorously shown by Xiang (2009) that the resolved shear stress due to a family of dislocation loops belonging to a single slip plane can be decomposed into a long-range dislocation-dislocation elastic interaction and a short-range self-induced line tangent force and they are both expressible in terms of the CGDFs. It is worth noting that the line tangent force plays crucial roles in many dislocation-based mechanisms, such as particle strengthening (Orowan, 1948; Friedel, 1956; Argon, 2008). With the resolved shear stress calculated in this way, the plastic flow is formulated by an evolutionary equation of the CGDF (Zhu and Xiang, 2010). The Frank-Read (FR) sources, one of the major mechanisms for dislocation multiplications, are also well
incorporated into the continuum model characterized by the CGDF based on the underlying
discrete dislocation dynamics (Zhu et al., 2014). As one of its applications, the derived two-
dimensional continuum model is used to study the pile-up of dislocation loops within a
rectangular grain and a two-dimensional Hall-Petch law, that is, an explicit formula for the
yield (or flow) stress depending on the grain geometries is derived as a function without any
adjustable parameters not only of the physical dimension of the grains but also the grain
aspect ratio (Zhu et al., 2014).

In this paper, we discuss the generalization of the two-dimensional continuum model
using the CGDF into the three-dimensional space, where there are a number of slip planes
belonging to various slip systems. To achieve such generalization, we refer to the idea used
in representing a single dislocation curve by two level set functions by Xiang et al. (2003) to
define two families of dislocation density potential functions (DDPFs) as follows. To each
activated slip system, a DDPF denoted by $\psi$ is assigned, so that the slip planes are identified
by the contour surfaces of $\psi$ taking integer values. With the slip planes determined by $\psi$,
the dislocation curves on each slip plane can thus be expressed in a similar manner as the
two-dimensional case, that is, another DDPF $\phi$ is defined such that the dislocation curves
on each slip plane are represented by the contours of $\phi$ restricted on the plane. With the
introduction of the DDPFs, we can summarize for a constitutive stress rule and a plastic
flow rule from the underlying dislocation dynamics.

For the constitutive stress rule, it is derived by sequentially expressing the Nye’s dislo-
cation density tensor, the plastic distortion, the elastic strain tensor in terms of the DDPFs
according to the equations established in the classical plasticity theories. It will further be
shown that the resolved shear stress components calculated in the DDD models effectively
equals to the sum of two parts. One part is due to the local self-induced line tangent ef-
fect, which can be explicitly formulated in terms of $\phi$ and $\psi$. The other part is due to
the (long-range) stress field determined by the derived constitutive stress rule and the force
balance equation along with the boundary conditions. To compute this long-range stress
field, a finite element (FE) formulation is proposed. It will be further shown that many
well-developed tools used in the FE methods for purely linearly elastic problems are well
The second constitutive law derived for the continuum model in this paper, is the plastic flow rule for face-centered-cubic (FCC) crystals at room temperature, where the anti-planar motions of dislocations, such as cross-slipping and climbing of dislocations, are not taken into account. Under the continuum framework here, the plastic flow rule is found to be an evolutionary equation of the DDPF $\phi$, which is derived based on the conservation of the amount of the plastic shears, that is, the local change in plastic shears is due to the net dislocation flux and the dislocation generation by the FR sources, both of which are formulated in analogy with the two-dimensional cases (Zhu and Xiang, 2010; Zhu et al., 2014).

These derived equations homogenized from the underlying discrete dislocation dynamics form a closed system evolving with time as listed from Eq. (64) to Eq. (71), so that one can use the continuum model to keep tracking of the deformation process of crystals as follows: a given stress state drives the plastic flow, corresponding to the dislocation generation, transportation and annihilation at a smaller scale and a redistributed (continuous) dislocation network alters the stress state and so on.

With the derived continuum plasticity models using the DDPFs, we further study the size effect on crystalline strength observed in the uniaxial compression tests of monocrystalline micro-pillars. Such size effect can be simply described to be that the pillar strength measured by the flow stress $\sigma_{\text{flow}}$ decreases as the pillar size $D$ increases. Experimentally, it is suggested that $\sigma_{\text{flow}}$ scales inversely with $D$ by a power law that

$$\sigma_{\text{flow}} \sim D^{-m},$$

where $m$ is found to be from 0 to 1, varying from metal to metal (Uchic et al., 2009). Typically there are two classes of models proposed to rationalize this smaller-being-stronger effect. The first type falls into the family of the “dislocation starvation” models (Greer et al., 2005; Greer and Nix, 2006). They argued that a crystal smaller in size does not provide enough space for dislocation multiplication. The consequence is that the solid in “starved states” gets its yield strength increased. The second category of models attribute
the observed size effect to the initial distribution of the dislocation sources. It is suggested
that many bowing-out sources originally of the FR type pinned at both ends may intersect
with the free surface due to the spatial limitation in small volumes, ending up with many
single-arm sources of shorter length. As a result, the effective length of the FR sources in
small crystals is reduced, leading to a rise in the source activation stress (Parthasarathy
et al., 2007). There are attempts by using the DDD simulation with a pre-set initial source
distribution to rationalize such size effect (e.g. El-Awady et al., 2008; Senger et al., 2008; El-
Awady et al., 2009; Shao et al., 2014). Also, there are models using statistical approaches
to reproduce the power law expression in Eq. (1) (e.g. Gu and Ngan, 2013). In the last
part of this paper, by following the trace of the source models, we apply the derived three-
dimensional continuum models to study the plasticity of single-crystalline micro-crystals
being compressed. The simulation results by using the derived continuum model are shown
excellent agreement with the experimental data by Dimiduk et al. (2005). Through ex-
amining the internal micro-structural states with the derived continuum model, an explicit
formula for the flow stress of nickel is derived to be

\[
\sigma_{\text{flow}} = \frac{15\mu b}{4\pi m_s D} \log \left( \frac{D}{6r_c} \right) + \frac{\sigma_{\text{flow}}^{\text{bulk}}}{2},
\]

(2)

where \(\sigma_{\text{flow}}^{\text{bulk}}\) is the bulk flow stress; \(b\) is the modulus of the Burgers vector; \(D\) is the sample
diameter; \(\mu\) is the shear modulus; \(m_s\) is the Schmid factor of the activated slip system; \(r_c\)
is the cut-off dislocation core radius. Eq. (2) suggests that the flow stress scales with the
sample size with

\[
\sigma_{\text{flow}} \sim \log(D)/D.
\]

(3)

This paper is arranged as follows. In Sec. 2, the representation of dislocation networks in
the three-dimensional space by the DDPFs is introduced. This is followed by the derivation of
the constitutive stress rule and the plastic flow rule. In Sec. 3, the numerical implementation
to the derived system of equations is discussed. In Sec. 4, some numerical examples are shown
and the derived continuum model is validated through comparing with the DDD simulation
results. In Sec. 5, the derived continuum model is applied to study the size effect arising in
the uniaxial compression tests of single-crystalline micro-pillars.
To better illustrate the method, the following notations are used throughout the paper unless specified. The Cartesian coordinates are denoted by \( \mathbf{r} = (x, y, z)^T \), where \(^T\) stands for the “transpose of”. We use bold Greek letters, for example \( \mathbf{\sigma} \), to denote the second-order tensors of size \( 3 \times 3 \) and bold English letters, for example \( \mathbf{r} \) and \( \mathbf{l} \), to denote a vector of three dimensions unless specified. The \( i \)-th entry of a vector, for example \( \mathbf{r} \), is denoted by \( (\mathbf{r})_i \) or simply by \( r_i \) if any ambiguity is avoided. The \( ij \)-th entry of a second-order tensor, for example \( \mathbf{\sigma} \), is denoted by \( (\mathbf{\sigma})_{ij} \) or simply \( \sigma_{ij} \). A super- or sub-script (or both) are attached to a variable to better indicate its physical meaning if necessary. Unless specified, the following notation are used in the rest of this paper to denote the operations including the vector gradient \( (\nabla \mathbf{u})_{ij} = \partial u_i / \partial r_j \); the cross product \( (\mathbf{m} \times \mathbf{n})_i = \sum_{j,k=1}^{3} \epsilon_{ijk} m_j n_k \) with \( \epsilon_{ijk} \) the permutation tensor; the inner product of two vectors \( \mathbf{m} \cdot \mathbf{n} = \sum_{i=1}^{3} m_i n_i \); the inner product of two second-order tensors \( \mathbf{\alpha} : \mathbf{\beta} = \sum_{i,j=1}^{3} \alpha_{ij} \beta_{ij} \); the magnitude of a vector \( |\mathbf{u}| = \sqrt{\mathbf{u} \cdot \mathbf{u}} \); the symmetric part of a second-order tensor \( \text{sym}(\mathbf{\alpha}) = (\mathbf{\alpha} + (\mathbf{\alpha})^T) / 2 \); the outer product of two vectors \( (\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j \); the row “curl” of a second-order tensor \( (\nabla \times \mathbf{\alpha})_{ij} = \sum_{k,l=1}^{3} \epsilon_{jkl} \alpha_{il,k} \).

2. Continuum plasticity model by the dislocation density potential functions

In this section, the continuum model for dislocation dynamics on one slip plane using a two-dimensional coarse-grained disregistry function (CGDF) is firstly reviewed. Then we consider building a three-dimensional model analogically. This can be achieved by the introduction of the DDPFs, by the help of which a constitutive stress rule and a plastic flow rule are derived, both through summarizing the underlying DDD models. These derived equations form a closed evolutionary system governing the plastic deformation of crystals and they are listed in the end of this section.

2.1. Review of the two-dimensional continuum plasticity model described by a CGDF

Recalling from Xiang (2009), a family of dislocation curves in one slip plane can be represented by a continuous two-dimensional CGDF, whose contours of the integer value multiplied by the magnitude of the Burgers vector are the dislocation curves. For example as shown in Fig. 1(a), if the (two-dimensional) CGDF is denoted by \( \phi_{2d} \), then the \( i \)-th
Figure 1: (a) A family of dislocation loops on one slip plane ($x$-$y$ plane) can be represented by a two-dimensional CGDF $\phi_{2d}(x,y)$: the dislocation curves are represented by the contours of $\phi_{2d}(x,y)$ with integer values multiplied by the modulus of the Burgers vector. For example, $\phi_{2d} = ib$ characterizes the $i$-th dislocation curve on the slip plane. (b) A three-dimensional continuously distributed dislocation network belonging to a same slip system can be expressed by two DDPFs $\phi$ and $\psi$. The slip planes are identified by the integer values of $\psi$ while on each slip plane the contours of $\phi$ taking integer values are dislocation curves. For example, the $i$-th dislocation curve on the $j$-th slip plane denoted by $\gamma_j^i$ is expressed as $\{r|\phi(r) = i \text{ and } \psi(r) = j\}$. It is worth noting that the unit of $\phi_{3d}$ (which is non-dimensionalized) is slightly different from its two-dimensional counterpart $\phi_{2d}$ (of unit $b$) for the purpose of being systematic. The dislocation tangent $t$, the in-plane normal $n$ and the slip normal $m$ form a local orthogonal triad.

dislocation curve in the slip plane, which is the $x$-$y$ plane, is given by $\phi_{2d} = ib$, where $b$ is the modulus of the Burgers vector. With this formulation, the “in-plane” dislocation normal denoted by $n$, which is the (two-dimensional) unit vector normal to the dislocation curve and in the slip plane, is calculated by the normalized “in-plane” gradient of the CGDF $\phi_{2d}$

$$n = \frac{1}{\sqrt{(\partial \phi_{2d}/\partial x)^2 + (\partial \phi_{2d}/\partial y)^2}} \left(\frac{\partial \phi_{2d}}{\partial x}, \frac{\partial \phi_{2d}}{\partial y}\right)^T.$$  \hspace{1cm} (4)$$

With the introduction of $\phi_{2d}$, we can also express the dislocation total length per area by

$$\frac{1}{b} \sqrt{\left(\frac{\partial \phi_{2d}}{\partial x}\right)^2 + \left(\frac{\partial \phi_{2d}}{\partial y}\right)^2}.$$  \hspace{1cm} (5)$$
Moreover, the introduction of $\phi_{2d}$ enables us to express the discrete sum of the resolved shear stress due to all individual dislocations by an integral in $\mathbb{R}^2$

$$
\tau_{2d}^{\text{long}} = \frac{\mu}{4\pi} \int_{\mathbb{R}^2} \frac{(x - \tilde{x}) \frac{\partial \phi_{2d}(\tilde{x}, \tilde{y})}{\partial x} + (y - \tilde{y}) \frac{\partial \phi_{2d}(\tilde{x}, \tilde{y})}{\partial y}}{(x - \tilde{x})^2 + (y - \tilde{y})^{3/2}} \, d\tilde{x} d\tilde{y}
+ \frac{\mu \nu}{4\pi(1 - \nu)b^2} \int_{\mathbb{R}^2} \frac{(b_1 \frac{\partial \phi_{2d}(\tilde{x}, \tilde{y})}{\partial x} + b_2 \frac{\partial \phi_{2d}(\tilde{x}, \tilde{y})}{\partial y})(b_1(x - \tilde{x}) + b_2(y - \tilde{y}))}{(x - \tilde{x})^2 + (y - \tilde{y})^{3/2}} \, d\tilde{x} d\tilde{y},
$$

(6)

where $\mu$ and $\nu$ are the shear modulus and the Poisson’s ratio, respectively. However, it has been shown rigorously by Xiang (2009) that $\tau_{2d}^{\text{long}}$ given by Eq. (6) only takes the long-range resolved shear stress into account while the local self-induced line tangent effect, which proves to be important in many dislocation-based mechanisms, is missing. This self-induced resolved shear stress $\tau_{2d}^{\text{self}}$ is rigorously calculated by Xiang (2009) in terms of the CGDF $\phi_{2d}$ by

$$
\tau_{2d}^{\text{self}} = \frac{\mu b \kappa}{4\pi} \left( \frac{1 + \nu}{1 - \nu} - \frac{3\nu}{1 - \nu} \left( \frac{b_1 \frac{\partial \phi_{2d}}{\partial x} + b_2 \frac{\partial \phi_{2d}}{\partial y}}{\sqrt{\left( \frac{\partial \phi_{2d}}{\partial x} \right)^2 + \left( \frac{\partial \phi_{2d}}{\partial y} \right)^2}} \right)^2 \right) \log \left( \frac{b}{r_c} \sqrt{\left( \frac{\partial \phi_{2d}}{\partial x} \right)^2 + \left( \frac{\partial \phi_{2d}}{\partial y} \right)^2} + 1 \right),
$$

(7)

where $r_c$ is the width of the dislocation core and $\kappa$ is the local signed curvature of the dislocations calculated by

$$
\kappa = \frac{\partial}{\partial x} \left( \frac{\partial \phi_{2d}}{\partial x} \sqrt{\left( \frac{\partial \phi_{2d}}{\partial x} \right)^2 + \left( \frac{\partial \phi_{2d}}{\partial y} \right)^2} \right) + \frac{\partial}{\partial y} \left( \frac{\partial \phi_{2d}}{\partial y} \sqrt{\left( \frac{\partial \phi_{2d}}{\partial x} \right)^2 + \left( \frac{\partial \phi_{2d}}{\partial y} \right)^2} \right).
$$

(8)

Hence the total resolved shear stress field $\tau_{2d}$ is calculated by

$$
\tau_{2d} \approx \tau_{2d}^{\text{long}} + \tau_{2d}^{\text{self}}.
$$

(9)

In the two-dimensional case, the plastic flow is governed by a kinematic equation of the dislocation ensembles, which is

$$
\frac{\partial \phi_{2d}}{\partial t} + v_n \sqrt{\left( \frac{\partial \phi_{2d}}{\partial x} \right)^2 + \left( \frac{\partial \phi_{2d}}{\partial y} \right)^2} = s_{2d},
$$

(10)

where $v_n$ is the dislocation moving speed along in-plane normal direction; $s_{2d}$ formulates the effect due to the dislocation multiplication by Frank-Read sources (Zhu and Xiang, 2010; Zhu et al., 2014).
2.2. Continuous distribution of dislocations represented by three-dimensional DDPFs

Such way in representing the dislocation ensembles can be generalized into the three-dimensional space, where there may be more than one active slip systems, characterized by different slip directions. Here we first discuss the representation of the dislocation ensembles belonging to one slip system with a same Burgers vector \( b \). Then we consider the case of multiple slip systems by combining the effect from each single-slip system together.

In this paper, we consider the case of FCC crystals at room temperature, where all dislocations are restricted in their primary slip planes as shown in Fig. 1(b). Therefore, all slip planes within \( \Omega \), the domain occupied by the solid, are perpendicular to a common unit slip normal vector denoted by \( m \).

To generalize from the existing results in the two-dimensional case, we first need to identify the positions of the slip planes. This can be done by introducing a continuously defined three-dimensional DDPF denoted by \( \psi(r) \) in the following way, where \( r \) is a point in the three-dimensional space. If indices are assigned to all possible slip planes in the sequence along the direction of \( m \) as shown in Fig. 1(b), \( \psi \) is defined such that the \( j \)-th slip plane is the contour plane of \( \psi \) characterized by \( \psi = j \).

For example, when all slip planes are distributed uniformly, that is, the spacings between all neighboring slip planes are of the same size \( d \) as shown in Fig. 1(b), then \( \psi \) is formulated by

\[
\psi = \frac{m \cdot (r - r^0)}{d},
\]

where \( r^0 \) is a point on the 0-th slip plane.

With the slip planes identified by \( \psi \), one can then introduce another smoothly defined three-dimensional DDPF \( \phi_{3d} \), so that on each slip plane the contours of \( \phi_{3d} \) of height \( i \), \( i \in \mathbb{Z} \), where \( \mathbb{Z} \) is the set for all integers, are dislocation curves. It is noted that the three-dimensional DDPF \( \phi_{3d} \) here is defined in a non-dimensional sense, compared to the way in defining its counterpart in the two-dimensional case \( \phi_{2d} \), which is of unit \( b \). The reason behind such slight difference is for the purpose of making the definitions of the DDPF \( \phi_{3d} \) and \( \psi \) (both non-dimensional) systematic. Therefore, when generalizing the results associated
with $\phi_{2d}$ to three dimensions, a factor of $b$ needs to be dropped. Since the focus of this paper is of three dimensions, we simply use $\phi$ to denote the three-dimensional DDPF $\phi_{3d}$ without causing any ambiguities.

Therefore, the $i$-th dislocation curve on the $j$-th slip plane can be mathematically represented by

$$\{ \mathbf{r} | \phi(\mathbf{r}) = i, \psi(\mathbf{r}) = j, i, j \in \mathbb{Z} \}$$

in the continuum model here. It is also worth noting that the DDPFs with smooth profiles here provide a proper representation to the dislocation substructures, especially when the dislocations are condensingly distributed, that is, the physical dimension of a crystalline specimen is much greater than the spacings between the neighboring dislocations in it, and this is in general the situation in materials with size at the order of microns or above.

Another issue worth being pointed out is that the physical meaning of $d$ in Eq. (11) can be thought as the minimum spacing between two possibly activated slip planes. In fact, when only in-plane dislocation motion is considered, one can fix Eq. (11) as the expression for $\psi$. If a plane identified by $\psi(\mathbf{r}) = j$ is not actually activated, one can let $\phi(\mathbf{r})$ vanish on that plane. Then according to Eq. (11), the slip normal $\mathbf{m}$ is actually determined by

$$\mathbf{m} = \frac{\nabla \psi}{|\nabla \psi|} = d \nabla \psi$$

and the slip plane density (of unit per length) is calculated by

$$|\nabla \psi| = \frac{1}{d}$$

throughout this paper. In fact, $d$ introduced in this way provides a parameter to characterize the length scale of spacings between neighboring dislocations.

When there are multiple slip systems activated, one can assign a pair of DDPFs to each individual slip system in the same manner as described above, that is, for the slip system $\alpha$, a pair of $\phi^\alpha$ and $\psi^\alpha$ are defined so that the $i$-th dislocation curve on the $j$-th slip plane in the $\alpha$-th slip system is given by $\{ \mathbf{r} | \phi^\alpha(\mathbf{r}) = i, \psi^\alpha(\mathbf{r}) = j, i, j \in \mathbb{Z} \}$. Throughout this paper, a variable with a superscript "$\alpha$" means that it is defined associated with the $\alpha$-th slip system. The illustration of our method here always starts with the case of single slip systems and
the case of multiple slip systems are investigated by combining the effects due to individual single slip systems. Thus when the context is for single slip system, the superscript “α” is dropped temporarily.

It is worth noting that in body-centered-cubic (BCC) crystals or FCC crystals at high temperature, where the dislocation anti-planar motion is more frequent, the underlying dislocation networks can still be represented under the framework characterized by \( \phi^\alpha \) and \( \psi^\alpha \). In that case, \( \psi^\alpha(r) = j \) becomes a curved surface rather than a plane and this issue will be discussed in details in another paper.

2.3. Dislocation geometries represented by the DDPFs

With the DDPFs introduced above, we are able to explicitly describe the geometric structures of the dislocation networks, such as the dislocation tangent (field) \( l \) as shown in Fig. 1(b). It is recalled that, in the continuum model derived here, the dislocation curves are represented by the contours of \( \phi \) restricted on that plane and this is the same as the set-up used in the two-dimensional case. Hence the in-plane normal \( n \) to a dislocation curve as shown in Fig. 1(b), can be expressed as a generalization of Eq. (4), that is, \( n \) is the normalized “in-plane” gradient of \( \phi \), which equals to the projection vector of the full gradient of \( \phi \) denoted by \( \nabla \phi \) onto planes normal to the slip normal in the three-dimensional space. Mathematically, this in-plane gradient of \( \phi \) is given by \( \nabla_{\text{in-plane}} \phi = \nabla \phi - (m \cdot \nabla \phi)m \) and the dislocation in-plane normal \( n \) is expressed by normalizing \( \nabla_{\text{in-plane}} \phi \). Thus the dislocation tangent \( l \), can also be calculated by \( l = n \times m = \frac{\nabla \phi \times m}{|\nabla \phi \times m|} \), since \( \{l, n, m\} \) form an orthogonal triad. Due to the fact that \( l \) calculated in this way is still a unit vector, we obtain

\[
|\nabla_{\text{in-plane}} \phi| = |\nabla \phi - (m \cdot \nabla \phi)m| = |\nabla \phi \times m|. \tag{15}
\]

With regard to the fact that \( m = \nabla \psi / |\nabla \psi| \), \( l \) can be re-written in terms of the DDPFs by

\[
l = \frac{\nabla \phi \times \nabla \psi}{|\nabla \phi \times \nabla \psi|}. \tag{16}
\]

Then the dislocation in-plane normal \( n \) is also calculated in terms of the DDPFs by

\[
n = m \times l = \frac{\nabla \psi \times (\nabla \phi \times \nabla \psi)}{|\nabla \phi \times \nabla \psi||\nabla \psi|}. \tag{17}
\]
Moreover, with the Frenet-Serret formulas, we have
\[
\kappa \mathbf{n} = (\mathbf{l} \cdot \nabla \mathbf{l}_1, \mathbf{l} \cdot \mathbf{n}_2, \mathbf{l} \cdot \mathbf{n}_3)^\top,
\]
where \(\kappa\) denotes the signed curvature of the dislocation curve with respect to \(\mathbf{l}\). Thus with the expressions for \(\mathbf{l}\) and \(\mathbf{n}\) in Eq. (16) and (17), respectively, \(\kappa\) is also represented by using the DDPFs
\[
\kappa = \mathbf{n} \cdot (\kappa \mathbf{n}) = \sum_{i=1}^{3} n_i \mathbf{l} \cdot \nabla \mathbf{l}_i.
\]

2.4. Representation of the Nye’s dislocation density tensor by DDPFs

As mentioned in Sec. 1, one of the key issues in many existing dislocation-based continuum models is to describe the dislocation substructures as a continuous dislocation density distribution. A systematic way in expressing such continuous density distribution is by using the Nye’s dislocation density tensor \(\alpha\) (Nye, 1953)
\[
\alpha = \sum_{\alpha} \rho_{\text{num}}^\alpha (b^\alpha \otimes l^\alpha),
\]
where \(\rho_{\text{num}}^\alpha\) is the dislocation number density associated with the \(\alpha\)-th slip system and it is defined to be the dislocation total length per volume. Here we still consider the expression of \(\alpha\) in terms of \(\phi\) and \(\psi\) for the case of single slip systems first.

It is worth noting that the definition of the number density \(\rho_{\text{num}}\) is associated with an internal length scale parameterized by \(\epsilon\). To be precise, \(\rho_{\text{num}}\) is determined as follows. At any point \(\mathbf{r}\), a cube \(\Omega^\epsilon\) of size \(\epsilon\) containing \(\mathbf{r}\) is chosen as shown in Fig. 2. If the length of the dislocation curves inside \(\Omega^\epsilon\) is denoted by \(l_{\text{tot}}^\epsilon\), then \(\rho_{\text{num}}\) is calculated by \(l_{\text{tot}}^\epsilon/|\Omega^\epsilon|\), where \(|\Omega^\epsilon|\) is the volume of \(\Omega^\epsilon\). Here \(\epsilon\) is chosen much smaller compared to \(L\), the size of \(\Omega\), so that number density distribution at each point determined in this way is roughly unique. Here the internal length scale parameter \(\epsilon\) associated with the continuum model is required to satisfy
\[
d \ll \epsilon \ll L,
\]
where \(d\) is recalled to be the spacing between the neighboring slip planes and it can be regarded as a length scale parameter associated with the DDD models. Eq. (21) guarantees
Figure 2: The dislocation number density $\rho_{\text{num}}$ at $\mathbf{r}$ is calculated to be the dislocation total length within a cuboid $\Omega'$ of size $\epsilon$ containing $\mathbf{r}$ divided by $|\Omega'|$. The definition of $\rho_{\text{num}}$ is associated with an internal length scale parameter $\epsilon$. In the continuum model here, the length scale parameter $\epsilon$ satisfies Eq. (21). If looking along the slip normal $\mathbf{m}$, we see dislocations residing on one of the representative slip planes as shown in the top left figure. If looking along the dislocation tangent $\mathbf{l}$, the bottom left figure is what we see. In fact by its definition, $\rho_{\text{num}}$ is approximately equal to the product of two quantities. One is the dislocation total length per area in $\Omega' \cap \Gamma_k$, where $\Gamma_k$ is one of the slip planes intersecting with $\Omega'$. The other quantity is the slip plane density (of unit number per length). The slip planes in the continuum model here can be thought as layers of thickness $d$ as suggested in the bottom left figure.

that the dislocation substructures are properly taken into account at a coarser scale compared to that of the DDD models. In fact, the internal length scale parameter $\epsilon$ controls the resolution of the continuum model: when $\epsilon$ is of the same order of $d$, the density distribution becomes a sum of $\delta$-functions characterized by individual dislocation curves and the resulting “continuum” model effectively becomes a DDD model.

Now we consider the expression of the number density $\rho_{\text{num}}$ by using the DDPFs. Actually by its definition, $\rho_{\text{num}}$ approximately equals to the product of two quantities as shown in Fig. 2. One is the dislocation total length per area in $\Omega' \cap \Gamma_k$, where $\Gamma_k$ is one of the slip planes intersecting with $\Omega'$ as shown in the top left figure in Fig. 2. According to the result from the two-dimensional case given by Eq. (5), the total length per area is calculated by the magnitude of the in-plane gradient of $\phi$ given by Eq. (17), which equals to $|\nabla \phi \times \mathbf{m}|$. The other quantity needed to calculate $\rho_{\text{num}}$ is the slip plane density (of unit number per length)
as shown in the bottom left figure in Fig. 2 and by its definition, the slip plane density is $|\nabla \psi|$. Hence the dislocation number density is calculated by

$$\rho_{\text{num}} = |\nabla \phi \times m| \cdot |\nabla \psi| = |\nabla \phi \times \nabla \psi|,$$

(22)

where the second identity is due to the fact that $m = \nabla \psi / |\nabla \psi|$. In fact, the slip planes in the three-dimensional continuum model here can be thought as layers of thickness $d$ as suggested in the bottom left figure of Fig. 2.

For the case with multiple slip systems, one can analogically express the number density $\rho_{\text{num}}^a$ by Eq. (22) for the $a$-th slip system. Therefore, incorporating Eq. (16) and (22) into Eq. (20) gives the expression of the Nye’s dislocation density tensor in our continuum model characterized by the DDPFs

$$\alpha = \sum_a b^a \otimes (\nabla \phi^a \times \nabla \psi^a)$$

$$= \sum_a \begin{pmatrix} b_1^a \left( \frac{\partial \phi^a}{\partial x} \frac{\partial \psi^a}{\partial y} - \frac{\partial \phi^a}{\partial y} \frac{\partial \psi^a}{\partial x} \right) & b_1^a \left( \frac{\partial \phi^a}{\partial x} \frac{\partial \psi^a}{\partial z} - \frac{\partial \phi^a}{\partial z} \frac{\partial \psi^a}{\partial x} \right) & b_1^a \left( \frac{\partial \phi^a}{\partial y} \frac{\partial \psi^a}{\partial z} - \frac{\partial \phi^a}{\partial z} \frac{\partial \psi^a}{\partial y} \right) \\ b_2^a \left( \frac{\partial \phi^a}{\partial x} \frac{\partial \psi^a}{\partial y} - \frac{\partial \phi^a}{\partial y} \frac{\partial \psi^a}{\partial x} \right) & b_2^a \left( \frac{\partial \phi^a}{\partial x} \frac{\partial \psi^a}{\partial z} - \frac{\partial \phi^a}{\partial z} \frac{\partial \psi^a}{\partial x} \right) & b_2^a \left( \frac{\partial \phi^a}{\partial y} \frac{\partial \psi^a}{\partial z} - \frac{\partial \phi^a}{\partial z} \frac{\partial \psi^a}{\partial y} \right) \\ b_3^a \left( \frac{\partial \phi^a}{\partial x} \frac{\partial \psi^a}{\partial y} - \frac{\partial \phi^a}{\partial y} \frac{\partial \psi^a}{\partial x} \right) & b_3^a \left( \frac{\partial \phi^a}{\partial x} \frac{\partial \psi^a}{\partial z} - \frac{\partial \phi^a}{\partial z} \frac{\partial \psi^a}{\partial x} \right) & b_3^a \left( \frac{\partial \phi^a}{\partial y} \frac{\partial \psi^a}{\partial z} - \frac{\partial \phi^a}{\partial z} \frac{\partial \psi^a}{\partial y} \right) \end{pmatrix} \cdot (23)

2.5. Constitutional stress rule in the continuum model

In this subsection, we discuss the derivation of a constitutive stress law consistent with the underlying discrete dislocation dynamics for the continuum model characterized by DDPFs. The derivation takes two steps. First, we re-write the constitutive relations commonly used in classical plasticity models in the context of DDPFs, so as to derive for an expression for the stress field. Then we prove that the stress field obtained in this way along with a local self-induced stress field reproduces the stress field calculated in the underlying DDD models.

2.5.1. The derivation of a constitutive equation for stress field

When a body experiences a small deformation, the following three constitutive equations are satisfied according to the classical theories. Firstly, the total distortion, which is the gradient of the displacement $u$ can be decomposed into an elastic distortion denoted by $\beta^e$
and a plastic distortion denoted by $\beta^p$

$$\nabla u = \beta^e + \beta^p. \quad (24)$$

Secondly the Nye’s dislocation density tensor is the spatial gradient of the plastic distortion (Kröner, 1958)

$$\nabla \times \beta^p = -\alpha = -\sum_\alpha b^\alpha \otimes (\nabla \phi^I \times \nabla \psi^\alpha). \quad (25)$$

Thirdly the stress field $\sigma$ satisfies the Hooke’s law (the isotropic case):

$$\sigma = 2\mu \varepsilon^e + \frac{2\mu}{1-2\nu} tr(\varepsilon^e) I, \quad (26)$$

where “tr” denotes the “trace of”; $I$ is the $3 \times 3$ identity matrix; $\varepsilon^e$ is the elastic strain tensor related to the elastic distortion by $\varepsilon^e = \text{sym}(\beta^e)$.

Now we re-write the above constitutive equations in the context of the DDPFs. From Eq. (25), one can solve for $\beta^p$ by

$$\beta^p = -\sum_\alpha \phi^\alpha (b^\alpha \otimes \nabla \psi^\alpha). \quad (27)$$

It is worth noting that the general form of the solutions to Eq. (25) is Eq. (27) added by $\nabla w$, where $w$ is an arbitrary vector field. Later we will discuss how the arbitrariness of $w$ influences the outcomes of the derived equations.

By using Eq. (24) and (27), we are able to express the elastic strain tensor by

$$\varepsilon^e = \text{sym}(\nabla u) + \sum_\alpha \phi^\alpha \text{sym}(b^\alpha \otimes \nabla \psi^\alpha). \quad (28)$$

Incorporating Eq. (28) with the Hooke’s law in Eq. (26) and using the fact that $b^\alpha \cdot \nabla \psi^\alpha = 0$, we have

$$\sigma = \mathcal{L}(\nabla u) + 2\mu \sum_\alpha \phi^\alpha \text{sym}(b^\alpha \otimes \nabla \psi^\alpha), \quad (29)$$

where the linear operator $\mathcal{L}$ is defined to be

$$\mathcal{L}(\nabla u) = 2\mu \left( \text{sym}(\nabla u) + \frac{\nu}{1-2\nu}(\nabla \cdot u) I \right). \quad (30)$$
Therefore, Eq. (29) is derived as a formula for stress field in the presence of given dislocation substructures described by DDPFs.

It is worth noting that when a solid body is purely elastic (dislocation free), $\phi^\alpha = 0$ and Eq. (29) becomes $\sigma = \mathcal{L}(\nabla u)$, which is exactly the constitutive law for stress used in classical linear elasticity.

Eq. (29) suggests that the stress field in a plastically deformed body is attributed to two effects. The first part $\mathcal{L}(\nabla u)$ calculates the contribution from the gradient of the displacement. The second part $2\mu \sum_\alpha \phi^\alpha \text{sym}(b^\alpha \otimes \nabla \psi^\alpha)$ reflects how the stress field gets affected by the plastic slips carried out by the dislocation ensembles.

To close the system, the force balance equation in the absence of the body force is used

$$\nabla \cdot \sigma = 0. \quad (31)$$

In general, two types of boundary conditions are prescribed with the boundary $\partial \Omega$ decomposed by $\partial \Omega = \partial \Omega_d \cup \partial \Omega_t$. One is the displacement boundary conditions imposed on $\partial \Omega_d$

$$u|_{\partial \Omega_d} = u^b. \quad (32)$$

The other is the traction boundary conditions imposed on $\partial \Omega_t$

$$\sigma|_{\partial \Omega_t} \cdot k = t^b, \quad (33)$$

with $k$ the outer unit normal to the surface $\partial \Omega_t$.

Finally we discuss how the arbitrariness of $w$ introduced by solving Eq. (25) affects the outputs of the above set of equations. Actually, if we add $\nabla w$ to Eq. (27) and incorporate it to the expression for $\epsilon^e$ in Eq. (28), it can be seen that $w$ virtually plays a same role as the displacement $u$. In another word, $w$ can be envisaged as an image displacement field. But this image effect finally gets absorbed by the imposed boundary conditions, thus it does not affect the actual stress field.

2.5.2. Stress field summarized from the underlying DDD models

Now we consider the stress field in a finite body at the view point of the discrete dislocation dynamics. To make our illustration better address the underlying idea, we consider a
simpler situation first: i) crystals with singly activated slip systems are temporarily studied; ii) all dislocations form loops inside \( \Omega \); iii) only the traction boundary condition in Eq. (67) is imposed on \( \partial \Omega \). Actually, when the displacement boundary conditions are also present, the case can be proved with analogy.

Given dislocation substructures in a finite body \( \Omega \) subjected to an applied traction \( t_b \) on \( \partial \Omega \), the conventional approach in calculating the stress field \( \sigma_{dd} \) in the DDD models is by using the superposition method proposed by Van der Giessen and Needleman (1995). Here a subscript “dd” is affiliated with a variable indicating it is defined in the sense of the discrete dislocation dynamics. The superposition method suggests that the internal stress field \( \sigma_{dd} \) satisfies

\[
\sigma_{dd} = \sigma_{\text{inf}}^{dd} + \sigma_{\text{ima}}^{dd},
\]

where \( \sigma_{\text{inf}}^{dd} \) is the stress field due to all isolated loops in the whole three-dimensional space \( \mathbb{R}^3 \) and \( \sigma_{\text{ima}}^{dd} \) is the image stress field solution to a purely linearly elastic problem subjected to the boundary condition that

\[
\sigma_{\text{ima}}^{dd} \big|_{\partial \Omega} \cdot k = t_b - \sigma_{\text{inf}}^{dd} \big|_{\partial \Omega} \cdot k.
\]

For a single dislocation loop \( \gamma_{ij} \), its exerted stress field in \( \mathbb{R}^3 \) at a point \( r \) denoted by \( \sigma_{dd}^{\gamma_{ij}} \) is given by the Peach-Köehler stress formula

\[
\sigma_{dd}^{\gamma_{ij}}(r) = \frac{\mu}{2\pi} \int_{\gamma_{ij}} \text{sym} \left( \frac{b \times (r - \tilde{r})}{|r - \tilde{r}|^3} \right) \cdot l \, ds + \frac{\mu}{4\pi(1 - \nu)} \int_{\gamma_{ij}} (l \cdot (b \times \nabla) \nabla \otimes \nabla - \Gamma \nabla^2)|r - \tilde{r}| \, ds,
\]

where “\( \nabla \)” denotes taking the gradient with respect to \( r \); \( s \) is the arclength of the dislocation loop \( \gamma_{ij} \); \( \tilde{r} \) goes over all points in \( \gamma_{ij} \). Thus the stress field due to all discrete loops in \( \mathbb{R}^3 \) is calculated by

\[
\sigma_{dd}^{\text{inf}}(r) = \sum_{j=1}^{M} \sum_{i=1}^{N_j} \sigma_{dd}^{\gamma_{ij}}(r),
\]

where \( N_j \) is the number of the dislocation loops on the \( j \)-th slip plane and \( M \) is the total number of slip planes. It is worth noting that when using Eq. (37) to evaluate the stress field at a point on dislocations, it becomes singular, and such singularities are removed by introducing the regularized \( \delta \)-functions.
Now we consider approximating $\sigma_{\text{inf}}^{\text{dd}}$ in the context of the continuum model derived here. In analogy with the results in the two-dimensional continuum model by Eq. (6), the leading order approximation to $\sigma_{\text{inf}}^{\text{dd}}$ based on Eq. (37) is found to be an integral in terms of $\phi$ and $\psi$ given by

$$
\sigma_{\text{con}}^{\text{inf}}(r) = \frac{\mu}{2\pi} \int_{\mathbb{R}^3} \text{sym} \left( \frac{b \times (r - \tilde{r})}{|r - \tilde{r}|^3} \otimes (\nabla \phi(\tilde{r}) \times \nabla \psi(\tilde{r})) \right) d\tilde{V} \\
+ \frac{\mu}{4\pi(1 - \nu)} \int_{\mathbb{R}^3} (b \cdot \nabla \phi(\tilde{r}))(\nabla \psi(\tilde{r}) \cdot \nabla)(\nabla \otimes \nabla - I \nabla^2)|r - \tilde{r}| d\tilde{V},
$$

(38)

where $d\tilde{V}$ is an infinitesimal volume associated with position $\tilde{r}$. Here a subscript “con” is affiliated with a variable indicating that it is calculated in the sense of the continuum model derived in this paper. One way in rationalizing the derivations of Eq. (38) is to decompose $\Omega$ into many infinitesimally small regions, each of which is of volume $\Delta V$. Then in each small region, the dislocation segments inside can be envisaged as a super dislocation segment of “Burgers vector” $b|\nabla \phi \times \nabla \psi|\Delta V$, which is the actual Burgers vector multiplied by the total length in that small region. The tangent vector of this super dislocation segment is given by Eq. (16), i.e. $l = (\nabla \phi \times \nabla \psi)/|\nabla \phi \times \nabla \psi|$. Hence the stress field at any point due to this continuous dislocation density distribution is the integrating effect over all small regions in a same sense how the Peach-Köhler stress tensor is built. Actually, if we replace $ld$ in the Peach-Köhler stress tensor in Eq. (36) by $(\nabla \phi \times \nabla \psi)d\tilde{V}$, $\sigma_{\text{con}}^{\text{inf}}$ given by Eq. (38) is obtained.

However, similar as the two-dimensional case as pointed out by Xiang (2009), if one uses $\sigma_{\text{con}}^{\text{inf}}$ as the stress field at a point on dislocation due to all other dislocation loops, the stress field due to the local line tangent effect denoted by $\sigma_{\text{self}}$ is missing. Mathematically, this means the stress field at a point $r$ on a dislocation calculated in DDD models satisfies

$$
\sigma_{\text{dd}}^{\text{inf}}(r) = \sigma_{\text{con}}^{\text{inf}}(r) + \sigma_{\text{self}}(r).
$$

(39)

It is worth noting that the resolved shear component of $\sigma_{\text{self}}$ is only needed to track the plastic flow, so we keep $\sigma_{\text{self}}$ unspecified until the next subsection.

If multiple slip systems are activated, Eq. (39) still holds, while $\sigma_{\text{con}}^{\text{inf}}$ is redefined by
adding the contribution from different slip systems together

\[
\sigma_{\text{con}}(r) = \frac{1}{2\pi} \sum_{\alpha} \int_{\mathbb{R}^3} \text{sym} \left( \frac{b^\alpha \times (r - \tilde{r})}{|r - \tilde{r}|^3} \otimes (\nabla \phi^\alpha(\tilde{r}) \times \nabla \psi^\alpha(\tilde{r})) \right) d\tilde{V} \\
+ \frac{1}{4\pi(1-\nu)} \sum_{\alpha} \int_{\mathbb{R}^3} (b^\alpha \cdot \nabla \phi^\alpha(\tilde{r})) (\nabla \psi^\alpha(\tilde{r}) \cdot \nabla) (\nabla \otimes \nabla - \mathbf{I} \nabla^2) |r - \tilde{r}| d\tilde{V}.
\]  

(40)

It is worth noting that the calculation of \( \sigma_{\text{inf}} \) by Eq. (39) used for the case of multiple slip systems still neglects the short range interactions between dislocations from different slip systems. We will discuss the roles played by such short range interactions in another paper.

To accommodate the traction boundary conditions, we here also define an image stress field denoted by \( \sigma_{\text{ima}} \), which is the solution to a purely elastic problem along with the boundary condition that \( \sigma_{\text{ima}}|_{\partial \Omega} \cdot k = t^b - \sigma_{\text{inf}}|_{\partial \Omega} \cdot k \). Since the line tangent effect only casts effect on dislocations, \( \sigma_{\text{self}} \) does not account for the traction on the actual boundaries. Hence the boundary condition for \( \sigma_{\text{ima}} \) can be re-written by

\[
\sigma_{\text{ima}}|_{\partial \Omega} \cdot k = t^b - \sigma_{\text{inf}}|_{\partial \Omega} \cdot k.
\]

(41)

A comparison between Eq. (35) and (41) suggests that

\[
\sigma_{\text{ima}} = \sigma_{\text{con}}.
\]

(42)

Therefore, combining Eq. (34), (39) and (42), the stress field computed in DDD models can be reproduced in the continuum model here by

\[
\sigma_{\text{dd}} = \sigma_{\text{inf}} + \sigma_{\text{self}} + \sigma_{\text{ima}}.
\]

(43)

Now we relate the right hand side of Eq. (43) to the derived constitutive stress rule given by Eq. (29) in Sec. 2.5.1. It can be shown that \( \sigma_{\text{inf}} \) by Eq. (40) is actually one solution to the constitutive stress law in Eq. (29) and the force balance equation (31). The detailed proof is not included in the paper due to the limitation in space. The underlying idea in the proof follows Kröner (1958)’s way in solving for the stress field due to a dislocation loop in \( \mathbb{R}^3 \). If we replace \( b \) and \( l \) in Kröner (1958)’s calculation by \( b^\alpha |\nabla \phi^\alpha \times \nabla \psi^\alpha| \) and \( (\nabla \phi^\alpha \times \nabla \psi^\alpha)/|\nabla \phi^\alpha \times \nabla \psi^\alpha| \), respectively, we can see that the resulting governing equations
become exactly Eq. (29) and (31) and one solution to them is $\sigma_{\text{con}}^{\text{inf}}$ expressed by Eq. (40). This means that

$$\sigma_{\text{long}} = \sigma_{\text{con}}^{\text{inf}} + \sigma_{\text{con}}^{\text{ima}}$$

(44)

not only solves Eq. (29) and (31), but also satisfies the boundary conditions.

Therefore, by using Eq. (43) and (44), the stress field calculated in DDD models can be reproduced in the continuum model by

$$\sigma_{\text{dd}} = \sigma_{\text{long}} + \sigma_{\text{self}}.$$  

(45)

The long-range stress field $\sigma_{\text{long}}$, including the dislocation-dislocation elastic interaction and the stress response to applied loads, is solved from the constitutive stress rule of Eq. (29) and the force balance equation (31) along with the boundary conditions, while the local self-induced line tangent effect formulated by $\sigma_{\text{self}}$ will be discussed explicitly in the next subsection.

Finally, we consider the situation when not all dislocations in $\Omega$ form closed loops. In that case, one can always (implicitly) extend an open curve, say $\gamma_j^i$ to a closed one $\bar{\gamma}_j^i$. Then one can perform the same analysis as in this subsection and it can be seen that the stress field due to the extended part is fully accommodated by the resulting image stress field. Therefore, the evaluation of $\sigma_{\text{dd}}$ given by Eq. (45) also works for the cases where there are dislocation curves intersecting with the solid surfaces.

2.6. Plastic flow rule in the continuum model by DDPFs

In FCC crystals at room temperature, dislocations in general move on their slip planes due to the presence of a stress field and plastic flows are thus induced by the collective motion of these dislocations. In the three-dimensional model here, the associated plastic flow rule can be described by

$$\frac{\partial \phi^\alpha}{\partial t} + v_n^\alpha |\nabla \phi^\alpha \times \mathbf{m}^\alpha| = s^\alpha$$

(46)

in analogy with Eq. (10), where $v_n^\alpha$ is the moving speed of dislocations belonging to the $\alpha$-th slip plane along the in-plane normal and $s^\alpha$ formulates the dislocation generation by Frank-Read sources to be discussed in details in the next subsection.
Mathematically, Eq. (46) can be regarded as a kinematic equation of level-set functions, the family of which $\phi^\alpha$ also belongs to. Physically, Eq. (46) can be considered as a result of the conservation of the amount of the plastic shears. Here since no anti-planar motion of dislocations is considered here, the amount of the plastic shears is conserved on each slip plane. It is recalled from bottom left figure in Fig. 2 that in the three-dimensional continuum model, each slip plane is characterized by a layer of thickness $d$ or equivalently $1/|\nabla \psi|$ and the conservation of the dislocation length can be built within that layer. In Eq. (46), $\partial \phi^\alpha / \partial t$ describes the rate of change in the plastically sheared state (or equivalently the dislocation density potential) and it is due to two reasons: the generation of dislocation loops by Frank-Read sources and the net dislocation flux formulated by 

$$v_n^\alpha \sum_{\psi} \nabla \phi^\alpha \times \nabla \psi^\alpha / |\nabla \psi^\alpha|,$$

which equals to the product of the (local) total dislocation length and the translating speed. It is worth noting that there is no need to assign extra rules for dislocation annihilation in the continuum model here, since Eq. (46) automatically handles the topological changes in the contours of $\phi^\alpha$ (a numerical example of the two-dimensional case can be found in Zhu et al. (2014)).

The dislocation transportation speed $v_n^\alpha$ in Eq. (46) is related to the resolved shear stress component of the existing stress field by an empirically imposed dislocation mobility law. In the continuum model here, $v_n^\alpha$ is calculated by

$$v_n^\alpha = m_g b^\alpha \left( \tau_{\text{long}}^\alpha + \tau_{\text{self}}^\alpha \right),$$

where $\tau_{\text{long}}^\alpha$ and $\tau_{\text{self}}^\alpha$ are the shear component of $\sigma_{\text{long}}$ and $\sigma_{\text{self}}$ in Eq. (45) resolved in the $\alpha$-th slip system, respectively; $m_g$ is the dislocation gliding coefficient. It is worth noting that when formulating the dislocation line tangent effect, the “self-force” is the most commonly used term. In this paper, we use the self resolved shear stress $\tau_{\text{self}}^\alpha$ for the purpose of being systematic. In fact, $\tau_{\text{self}}^\alpha$ is simply different from the self force by a factor of $b^\alpha$.

The long-range resolved shear component $\tau_{\text{con}}^\alpha$ is calculated by

$$\tau_{\text{long}}^\alpha = \frac{b^\alpha}{b^\alpha} \cdot \left( \sigma_{\text{long}} \frac{\nabla \psi^\alpha}{|\nabla \psi^\alpha|} \right).$$

Since the dislocation curves are confined in their slip planes here, $\tau_{\text{self}}^\alpha$ can be explicitly
written in terms of $\phi^\alpha$ and $\psi^\alpha$ by

$$
\tau_{\text{self}}^\alpha = \frac{\mu b^\alpha}{4\pi} \left( \frac{1 + \nu}{1 - \nu} \cdot \frac{3\nu}{|b^\alpha|^2 |\nabla \psi^\alpha|} \cdot \frac{|\nabla \psi^\alpha|^2 (b^\alpha \cdot \nabla \phi^\alpha)^2}{|b^\alpha|^2 |\nabla \psi^\alpha \times \nabla \phi^\alpha|^2} \right) \kappa^\alpha \cdot \log \left( \frac{|\nabla \psi^\alpha|}{2\pi \tau_c |\nabla \psi^\alpha \times \nabla \phi^\alpha|} + 1 \right),
$$

(49)
as generalized from the two-dimensional result given by Eq. (7), where the in-plane signed curvature $\kappa^\alpha$ is calculated by Eq. (19).

It is worth noting that if we take the temporal derivative of Eq. (27), we obtain

$$
\dot{\beta}^p = - \sum_{\alpha} \dot{\phi}^\alpha |\nabla \psi^\alpha| b^\alpha \otimes m^\alpha,
$$

(50)

where $\dot{\cdot}$ stands for $\partial/\partial t$. If we check the kinematic equation for the plastic distortion by Rice (1971), which is widely used in the classical continuum plasticity model, it can be seen that Eq. (27) is exactly of the same form as Rice (1971)'s equation. A comparison between them suggests that $\dot{\phi}^\alpha |\nabla \psi^\alpha|$ is the fulfillment of the (signed) slip system shearing rate $\dot{\gamma}^\alpha$, one of the key internal variables used in the classical continuum plasticity models, in the context of dislocation dynamics.

In general, boundary conditions are also needed for the evolutionary equation (46). One extreme case is that the dislocations can exit the solid from its surfaces freely. In this case, no boundary conditions are required since the profiles of $\phi^\alpha$ on the surfaces are fully determined by the (dislocation and stress) states inside the solid. The extreme case on the other end is where the dislocations are impenetrable to a surface. In that case, $\phi^\alpha$ on the surface is fixed to be zero, since no plastic slip takes place on that boundary.

The total plastic strain rate is conventionally defined to be the rate of area swept by all dislocations multiplied by the respective modulus of the Burgers vector per volume. In the three-dimensional continuum model, the plastic strain rate denoted by $\dot{\epsilon}_p^{\text{tot}}$ is given by

$$
\dot{\epsilon}_p^{\text{tot}} = \frac{1}{|\Omega|} \sum_{\alpha} \int_{\Omega} b^\alpha \frac{\partial \phi^\alpha}{\partial t} |\nabla \psi^\alpha| dV,
$$

(51)

where $dV$ is an infinitesimal volume, as generalized from the results given by Zhu and Xiang (2010) in the two-dimensional continuum model.
2.7. Incorporation of the Frank-Read sources into the continuum model

In this subsection, we search for an expression of the source term \( s^a \) for Eq. (46) by incorporating the Frank-Read sources into the continuum model. To achieve this goal, we first review the method used for the incorporation of an FR source into the two-dimensional continuum model by Zhu et al. (2014). Then the method is generalized in the context of the three-dimensional continuum model and it is found that the collective effect due to a large number of FR sources is equivalent to a continuously distributed source at the length scale characterized by the derived continuum model. Again for simplicity, we start with the case of single slip systems and the superscript “a” can be dropped temporarily.

2.7.1. Incorporation of a Frank-Read source into the two-dimensional continuum model

A Frank-Read source is a dislocation segment pinned at its two ends. When the resolved shear stress \( \tau \) acting on it exceeds a critical value, known as the activation stress denoted by \( \tau_c \) here, the bowing-out segment may evolve to an unstable kidney-like shape and eventually becomes a dislocation loop and a dislocation segment similar as the initial segment in shape, so that this dislocation multiplication process can be repeated (Hirth and Lothe, 1982). The time it takes an FR source to perform an operating cycle is known as the nucleation time denoted by \( t_{\text{nuc}} \) here.

If observed at the continuum level, the operation of an FR source takes a profile not of cyclically loop releasing, but of dislocation flux originating from a small source region. In the context of the two-dimensional continuum model reviewed in Sec. 2.1, the operation of an FR source is described by a continuously rising-up process in the value of the CGDF \( \phi_{2d} \) within the source region and three parameters from the dislocation substructures are needed to control such rising-up process at the continuum scale. They are the source activation stress \( \tau_c \), the source operating rate, which equals to \( 1/t_{\text{nuc}} \) and the source region denoted by \( \Gamma_s^{2d} \), which is defined to be the (two-dimensional) region enclosed by a newly released dislocation loop.

The nucleation stress \( \tau_c \) here is evaluated by adopting the critical stress formula given
by Foreman (1967)

\[ \tau_c = \frac{C_s \mu b}{2\pi l} \log \left( \frac{l}{r_c} \right), \]  

(52)

where \( C_s \) depends on the source character and the Poisson ratio \( \nu \) (with \( \nu = 1/3 \), \( C_s = 1 \) for an edge-oriented source and \( C_s = 1.5 \) for an screw-oriented source); \( l \) is the length of the FR source; \( r_c \) represents the dislocation core radius as used in the evaluation for the self-induced resolved shear stress given by Eq. (49).

To determine the other two parameters \( t_{nuc} \) and \( \Gamma_{2d}^s \), Zhu et al. (2014) use two symmetrically evolving spirals, which both grow in length and rotate about their vortices, to model the dynamical profile of an FR source within one operating cycle. By this method, the nucleation time \( t_{nuc} \) is calculated by

\[ t_{nuc} = \frac{Q_{ch}}{m_g b^2 (|\tau| - \tau_c)}, \]  

(53)

where \( m_g \) is the gliding coefficient the same as defined in the law of motion (47); \( Q_{ch} \) depends only on the source orientation fitted from the DDD simulation (\( Q_{ch} = 6.1278 \) for edge-oriented source, \( Q_{ch} = 3.0413 \) for screw-oriented source). For an FR source of length \( l \) and centered at \((x_s, y_s)\) in the two-dimensional space (the slip plane in this case is the \( x \)-\( y \) plane), the corresponding source region \( \Gamma_{2d}^s \) is found to be a region enclosed approximately by an ellipse

\[ \Gamma_{2d}^s = \left\{ (x, y) \left| \frac{(x - x_s)^2}{(a_1 l)^2} + \frac{(y - y_s)^2}{(a_2 l)^2} \leq 1 \right. \right\}, \]  

(54)

where \( a_1 \) and \( a_2 \) are calculated to be 2.4610 and 2.2488, respectively (Zhu et al., 2014).

With \( \tau_c \), \( t_{nuc} \) and \( \Gamma_{2d}^s \) determined by Eq. (52), (53) and (54), respectively, the FR source is incorporated into the two-dimensional continuum model using the (two-dimensional) CGDF \( \phi_{2d} \) in the following sense. Given \( \tau > \tau_c \), an FR source continuously changes the value of \( \phi_{2d} \) at a speed of \( 1/t_{nuc} \) by pumping dislocation loops enclosing \( \Gamma_{2d}^s \) into the system. Mathematically, the source term \( s_{2d} \) in the two-dimensional model in Eq. (10) is given by

\[ s_{2d} = -\frac{m_g b^2 (\tau - \text{sign}(\tau)\tau_c)}{Q_{ch} l} H(|\tau| - \tau_c) \cdot \chi_{\Gamma_{2d}^s}, \]  

(55)

where \( \chi_{\Gamma_{2d}^s} \) is the characteristic function in \( \Gamma_{2d}^s \), i.e. \( \chi_{\Gamma_{2d}^s} \) is 1 in \( \Gamma_{2d}^s \) and vanishes elsewhere and \( H(\cdot) \) is the Heaviside function satisfying \( H(s) = 1 \) for \( s \geq 0 \) and 0 for \( s < 0 \).
2.7.2. Incorporation of Frank-Read sources into the three-dimensional continuum model

The incorporation of a Frank-Read source into the three-dimensional model follows similar steps as in the two-dimensional case. Still three parameters, the activation stress $\tau_c$, the source operating rate $1/t_{\text{nuc}}$ and the source region are needed to formulate the source operating process at the continuum level. In fact, $\tau_c$ and $t_{\text{nuc}}$ are found to be calculated by exactly the same formula in Eq. (52) and (53), respectively.

The source region in the three-dimensional model becomes a cylinder denoted by $\Omega_s$. The base of the cylinder is given by the domain enclosed by the ellipse formulated by Eq. (54) and its height equals to $d$, the spacing between neighboring slip planes, since the dislocations in the three-dimensional continuum model are considered of “thickness” $d$ as shown in Fig. 2. Therefore, the source region $\Omega_s$ in the three-dimensional space $\Omega_s$ is given by

$$\Omega_s = \{ r | r = r_s + \lambda_1 \cos \theta e_1 + \lambda_2 \sin \theta e_2 + \lambda_3 m \},$$

where $\theta \in [0, 2\pi)$; $\lambda_1 \in [0, a_1l]$; $\lambda_2 \in [0, a_2l]$; $\lambda_3 \in [-d/2, d/2]$; $r_s$ is the position of the source center. By this way, the source term due to an individual FR source denoted by $s_{\text{ind}}$ can be formulated by

$$s_{\text{ind}} = -\frac{m_s b (\tau - \text{sign}(\tau) \tau_c)}{Q_{\text{ch}} l} H(|\tau| - \tau_c) \cdot \chi_{\Omega_s}^{3d},$$

in analogy with Eq. (55). It is worth noting that the unit of $s_{\text{ind}}$ is different from $s^{2d}$ in Eq. (55) by a factor of $b$. This is because of the difference in the unit of $\phi$ of three dimensions and $\phi^{2d}$ of two dimensions.

It is worth noting that the derived continuum model with FR sources incorporated here is valid in the regime governed by

$$b \ll l \sim d \ll L,$$

where $L$ is the size of $\Omega$. The condition (58), which is in general the practical case, indicates that the source region $\Omega_s$ almost degenerates to a point viewed at the continuum scale and actually it can be shown that

$$\chi_{\Omega_s} \approx |\Omega_s| \delta(r_s) = \pi a_1 a_2 l^2 d \delta(r_s),$$

in Eq. (59).
where $\delta(\cdot)$ is the Dirac-$\delta$ function; $|\Omega_s|$ is the volume of $\Omega_s$; $a_1$ and $a_2$ are of the same value as in Eq. 54. At the continuum level, the singular feature in the source term due to the existence of the $\delta$-function is removed by employing the regularized Dirac function denoted by $\delta_{\text{reg}}(\cdot)$.

When there are $S$ operating FR sources assigned with indices $k = 1, \cdots, S$, the source term $s$ in Eq. (46) can be obtained as the sum of the contribution by each single point source formulated by combining Eq. (57) and (59)

$$s = -m_g \pi a_1 a_2 db \sum_{k=1}^{S} \frac{l_k(\tau - \text{sign}(\tau)\tau^k)}{Q_{\text{ch}}^k} H(|\tau| - \tau^k)_{\text{reg}}(r - r^k_s),$$  

(60)

where the index $k$ is affiliated to a variable to indicate it is defined with regards to the $k$-th source. For example, $l_k$ is the length of the $k$-th source and $\tau^k_c$ is its activation stress given by $\tau^k_c = C_s^k \mu b / (2\pi l_k) \log (l_k/r_c)$; $Q_{\text{ch}}^k$ is the $k$-th orientation parameter and $r^k_s$ is the $k$-th source center, etc.

### 2.7.3. Initialization of the source term

From the computational point of view, the source term $s$ given by Eq. (60) is of little use, because one has to determine in turn whether a source is activated by checking $H(\tau - \tau^k_c)$ each time step and this is extremely time consuming when the total source number is very large. To overcome such computational difficulties, we derive from Eq. (60) for an expression of the source term given by

$$s = (\tau - \tau_0(r)) g(r) H(|\tau| - \tau_0),$$  

(61)

where

$$g(r) = -\pi m_g a_1 a_2 b \sum_{k} \frac{l_k}{Q_{\text{ch}}^k} \delta_{\text{reg}}(r - r^k_s)$$  

(62)

and

$$\tau_0(r) = \frac{\mu b}{2\pi d} \frac{1}{g(r)} \sum_{k} \left( \frac{C_s^k \delta_{\text{reg}}(r - r^k_s)}{Q_{\text{ch}}^k} \log \left( \frac{l_k}{r_c} \right) \right).$$  

(63)

The expression for $s$ given by Eq. (61) suggests that the collective behaviors of FR sources can be described as the operation of a continuously distributed dislocation source field. $g(r)$
reflects how the rate of plastic shears due to the (continuous) source at \( r \) depends on the resolved shear stress and \( \tau_0(r) \) can be considered as the on-site source activation stress at \( r \).

To derive for Eq. (61) from Eq. (60), we simply introduce

\[
q = -\pi m_a a_1 a_2 d_b \sum_{k=1}^{S} \left( \frac{l_k (\tau - \text{sign}(\tau) \tau_0)}{Q_k} \delta_{\text{reg}}(r - r_k^s) \right),
\]

which is obtained by dropping the Heaviside functions from \( s \) in Eq. (60). Rearranging the expression for \( q \), we find that \( q = g(r)(\tau - \tau_0(r)) \), where \( g(r) \) and \( \tau_0(r) \) are the same as defined by Eq. (62) and (63), respectively. Considered from a continuous point of view, the source activation at each point is controlled by whether the resolved shear stress overcomes the on-site activation stress \( \tau_0 \) and this gives rise to the introduction of the Heaviside function in Eq. (61).

In Fig. 3, two examples are presented to intuitively show how to continuously formulate the operation of a number of individual FR sources in a non-dimensionalized sense. If starting with individual FR sources generated following a uniform distribution in space as displayed in Fig. 3(a), the profiles of its corresponding \( g(r) \) on several selected slip planes are drawn in Fig. 3(b). It can be observed that \( g(r) \) attains a relatively high value on the bottom slip plane in Fig. 3(b) because the number of individual sources are high in the same place in Fig. 3(a). Similar correspondence can also be spotted in Fig. 3(c) and (d), where the discrete sources are generated following a normal distribution in space.

Here it is worth noting that in crystals of micro size, some FR sources may evolve to single-arm spiral sources after reacting with the free surfaces (Parthasarathy et al., 2007) and they are also effectively captured in the source term here. This is because the parameters controlling the FR sources in the continuum model are derived by approximating the source operating cycles by two symmetrically evolving spirals.

When multiple slip systems are considered, the source term \( s^\alpha \) for the \( \alpha \)-th slip system can be expressed by adding a superscript “\( \alpha \)” to all associated variables in Eq. (61).
Figure 3: Continuous formulation of a number of operating FR sources in a non-dimensionalized sense: (a) the sources are generated following the uniform distribution in space and the source length is also produced by the uniform distribution; (b) the continuous distribution of \( g(\mathbf{r}) \) obtained by using Eq. (62) with regards to the configuration in (a) on several slip planes; (c) the positions of the source are generated by a normal distribution in space with their lengths obtained by a uniform distribution; (d) the continuous distribution of \( g(\mathbf{r}) \) obtained by using Eq. (62) with regards to the configuration in (c) on several slip planes. By comparison, it is observed that, where the discrete sources are condensed, the value of \( g(\mathbf{r}) \) is correspondingly larger in terms of a lighter color in (b) and (d).

2.8. Summary of the system of the derived equations

Therefore, based on the underlying discrete dislocation dynamics, a set of equations to describe the plastic deformation of crystals of finite size are derived under the continuum framework characterized by the DDPFs. The derived equations are summarized as follows.

1. The stress rule: given the dislocation substructures described by \( \phi^{\alpha} \) and \( \psi^{\alpha} \), the long-range stress field \( \sigma_{\text{long}} \) is determined by

\[
\sigma_{\text{long}} = 2\mu \left( \text{sym}(\nabla \mathbf{u}) + \frac{\nu \text{tr}(\nabla \mathbf{u})}{1-2\nu} \mathbf{I} + \sum_{\alpha} \phi^{\alpha} \text{sym}(\mathbf{b}^{\alpha} \otimes \nabla \psi^{\alpha}) \right) \tag{64}
\]

and the force balance equation

\[
\nabla \cdot \sigma_{\text{long}} = 0 \tag{65}
\]

with the displacement boundary conditions

\[
\mathbf{u} |_{\partial \Omega_d} = \mathbf{u}^b \tag{66}
\]
and the traction boundary conditions
\[ \sigma |_{\partial\Omega_1} \cdot k = t^b. \] (67)

2. The plastic flow rule: the collective motion of the dislocations belonging to the slip system \( \alpha \) is described by an evolutionary equation of \( \phi^\alpha \)
\[ \frac{\partial \phi^\alpha}{\partial t} + v^\alpha_n \frac{[\nabla \phi^\alpha \times \nabla \psi^\alpha]}{[\nabla \psi^\alpha]} = g^\alpha(r) \left( \tau^\alpha - \tau^\alpha_0(r) \right) H(\tau - \tau^0(r)), \] (68)
where the transportation speed of the dislocation ensembles is determined by the law of motion that
\[ v^\alpha_n = m g^\alpha \left( \tau^\alpha_{\text{long}} + \tau^\alpha_{\text{self}} \right); \] (69)
\( g^\alpha(r) \) and \( \tau^\alpha_0(r) \) are two field variables given by Eq. (62) and (63), respectively. The shear stress component resolved in the \( \alpha \)-th slip system \( \tau^\alpha_{\text{long}} \) and \( \tau^\alpha_{\text{self}} \) are calculated by
\[ \tau^\alpha_{\text{long}} = \frac{b^\alpha}{b^\alpha} \cdot \left( \sigma_{\text{long}} \frac{\nabla \psi^\alpha}{[\nabla \psi^\alpha]} \right) \] (70)
and
\[ \tau^\alpha_{\text{self}} = \frac{\mu b^\alpha}{4\pi} \left( \frac{1 + \nu}{1 - \nu} - \frac{3\nu}{1 + \nu} \right) \left( \frac{[\nabla \psi^\alpha]^2 (b^\alpha \cdot \nabla \phi^\alpha)^2}{[b^\alpha]^2 [\nabla \psi^\alpha \times \nabla \phi^\alpha]^2} \right) \kappa^\alpha \cdot \log \left( \frac{[\nabla \psi^\alpha]}{2\pi r_c [\nabla \psi^\alpha \times \nabla \phi^\alpha]} + 1 \right), \] (71)
respectively, where the signed curvature \( \kappa^\alpha \) is given by Eq. (19).

3. Numerical implementation of the derived continuum model

In this section, we discuss the numerical solutions to the derived system of equations listed from Eq. (64) to (71). The focus will be put on i) the computation of the stress field satisfying Eq. (64) and (65) with boundary conditions (66) and (67); 2) the evolution of \( \phi^\alpha \) governed by Eq. (68).

For a better explanation of the numerical approaches to the continuum model here, we choose the computational domain to be a cuboid of size \( D \times D \times L \) and the \( x, y \) and \( z \) axis are set to be parallel to the edges of the cuboid. Hence the computational domain is
represented by \( \Omega = [-D/2, D/2] \times [-D/2, D/2] \times [-L/2, L/2] \) and the aspect ratio of the cuboid height to its bottom edge is then given by \( L/D \).

The boundary conditions for the stress field here are set to be consistent with the experimental set-ups used in the uniaxial compression tests of micro-pillars. On the bottom surface, no displacement is allowed along \( z \) direction, which is the loading direction, giving rise to \( u_3|_{z=-L/2} = 0 \), and on the top surface the displacement boundary condition \( u_3|_{z=L/2} = u_0^b \) is imposed on \( u_3 \) due to indentation. On these two surfaces, the shear force is set to be free. On the other four side surfaces, the traction free boundary conditions are imposed.

In this paper, \( \Omega \) is meshed by the C3D8 bricks, one of the most commonly used elements for the FE discretization of a three-dimensional body. In this case, the vertices of each brick are exactly the grid points for \( \phi^\alpha \) when using the finite difference scheme to track its evolution according to Eq. (68).

3.1. Finite element formulation to determine the long-range stress field

For a solid in force balance satisfying Eq. (31), its internal stress field subject to the boundary conditions (32) and (33) has a weak form that \( \int_{\Omega} \sigma : (\nabla v) dV = \int_{\partial \Omega} t^b \cdot v dS \) for any test vector functions \( v \in \{ v | v = 0, \text{ on } \partial \Omega_d \} \). Replacing the stress field in the above weak form by the constitutive stress rule given by Eq. (29), we obtain the weak form associated with the derived continuum model to be

\[
\int_{\Omega} (\nabla v) : \mathcal{L}(\nabla u) dV = \int_{\partial \Omega_t} t \cdot v dS - 2\mu \sum_{\alpha} \int_{\Omega} \phi^\alpha \text{sym}(b^\alpha \otimes \nabla \psi^\alpha) : (\nabla v) dV. \tag{72}
\]

To carry out the FE computation, we define a vector \( u_{FE} \) of length \( 3N \), where \( N \) is the number of nodes, to containing all nodal values of \( u \). Similarly, a vector \( v_{FE} \) of length \( 3N \) contain all nodal values of the test function field \( v \), is defined with the same arrangement as \( u_{FE} \). In the FE formulation, both \( u \) and \( v \) are approximated by formulas interpolated by the corresponding nodal values within each element. It is worth noting that the nodal values of \( \phi^\alpha \) have been updated by the finite difference scheme from the last time step. Hence the last integral of Eq. (72) can be effectively considered as a term due to a “body force”.

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For simplicity, $\phi^\alpha$ in the FE formulation here is treated as piecewise constants, which are evaluated as the average of the eight nodal values in each element.

By this way, the integrals in Eq. (72) can be explicitly evaluated, giving rise to a vector-matrix form that $\mathbf{v}_{FE} \cdot (K_{FE} \mathbf{u}_{FE}) = \mathbf{v}_{FE} \cdot \mathbf{f}_{FE}$, where $K_{FE}$ is the stiffness matrix of size $3N \times 3N$. The process in generating $K_{FE}$ is known as the assembling of the elements. Since the above vector-matrix form holds for all possible $\mathbf{v}_{FE}$, we finally reach a linear system for the nodal values $\mathbf{u}_{FE}$

$$K_{FE} \mathbf{u}_{FE} = \mathbf{f}_{FE}. \tag{73}$$

To incorporate the displacement boundary conditions into the linear system, we employ the conventionally used approximating method, that is, if the $n$-th nodal value of $\mathbf{u}_{FE}$ is predetermined by $(\mathbf{u}_{FE})_n = u_b$, then the $n$-th equation in Eq. (73) is added by $A(\mathbf{u}_{FE})_n = Au_b$, where $A$ is a large number taken to be $10^{12}$ for the simulation results presented in this paper.

It has been shown that the integral term on the left side of Eq. (72), from which $K_{FE}$ is obtained, is exactly of the same form as used in the FE formulation in classical linear elasticity. Therefore, many well-developed tools for purely elastic problems, such as meshing, assembling for $K_{FE}$ and solving the linear system in Eq. (73), can be inherited by the FE formulation proposed here. The assembling for $\mathbf{f}_{FE}$ is also typical, since it is from the traction boundary conditions and a “body” force in terms of $\phi$ and $\psi$, the discretizations of which are also well studied in classical linear elasticity. The detailed procedures in assembling for Eq. (73) can be found in many text books on FE method (e.g. Li et al., 2006).

When $\mathbf{u}_{FE}$ is obtained from Eq. (73), the nodal values for the long-range stress field $\sigma_{long}$ can be computed according to the constitutive stress rule with Eq. (29), where the first-order spatial derivatives of $\mathbf{u}$ are needed. To compute the derivatives of $\mathbf{u}$, if the evaluation point is not on the boundary, the central difference is used. Otherwise, the single-sided difference is used for the estimation of the spatial derivative of $\mathbf{u}$. Then the resolved long-range shear stress component $\tau_{long}^\alpha$ can be computed according to Eq. (70).
3.2. Finite difference scheme for the evolution of $\phi^\alpha$

The finite difference method is implemented to update $\phi^\alpha$ according to Eq. (68), which by combing Eq. (69) is re-written by

$$\frac{\partial \phi^\alpha}{\partial t} + m^\alpha b^\alpha (\tau_{\text{long}}^\alpha + \tau_{\text{self}}^\alpha) |m^\alpha \times \nabla \phi^\alpha| = s^\alpha. \quad (74)$$

The temporal derivative of $\phi^\alpha$ in Eq. (74) is approximated by using the Euler scheme. For spatial derivatives, the approximating schemes are chosen depending on the actual physics. For example, the second term of Eq. (74) can be considered as a convection term due to two sources: one by a self-induced “force” $\tau_{\text{self}}^\alpha$ and the other by an externally-driven “force” $\tau_{\text{long}}^\alpha$. To guarantee the stability of the evolution for $\phi^\alpha$, we here follow the idea by Burchard et al. (2001), where two similar types of convection effects are also included in their evolutionary equations of the level-set functions. For “convection” driven by $\tau_{\text{self}}^\alpha$, the central difference is used to evaluate all spatial derivatives of $\phi^\alpha$ needed for $|m^\alpha \times \nabla \phi^\alpha|$ and for the determination of $\tau_{\text{self}}^\alpha$ by Eq. (49). For “convection” caused by $\tau_{\text{long}}^\alpha$, we use the first-order upwind scheme. Specifically in this paper, we use Eq. (16) and (18) to rewrite $\tau_{\text{long}}^\alpha |m^\alpha \times \nabla \phi^\alpha|$ by

$$\tau_{\text{long}}^\alpha |m^\alpha \times \nabla \phi^\alpha| = \tau_{\text{long}}^\alpha \frac{\partial \phi^\alpha}{\partial n^\alpha} = \tau_{\text{long}}^\alpha n_1^\alpha \frac{\partial \phi^\alpha}{\partial x} + \tau_{\text{long}}^\alpha n_2^\alpha \frac{\partial \phi^\alpha}{\partial y} + \tau_{\text{long}}^\alpha n_3^\alpha \frac{\partial \phi^\alpha}{\partial z}. \quad (75)$$

From Eq. (75), it can be seen that the “wind direction” is indicated by the sign of the products of $\tau_{\text{long}}^\alpha$ and the component of $n^\alpha$, the in-plane normal, which is evaluated from Eq. (17) by using the central differences to approximate all spatial derivatives of $\phi^\alpha$. Therefore, we here approximate $\partial \phi^\alpha / \partial x$ at a point $(x_j, y_i, z_k)$ with the upwind scheme by

$$(\frac{\partial \phi^\alpha}{\partial x})_{j,i,k}^{\text{up}} = \begin{cases} \frac{\phi^\alpha(x_j, y_i, z_k; t) - \phi^\alpha(x_{j-1}, y_i, z_k; t)}{\Delta x} & \text{if } \tau_{\text{long}} n_1^\alpha > 0; \\ \frac{\phi^\alpha(x_{j+1}, y_i, z_k; t) - \phi^\alpha(x_j, y_i, z_k; t)}{\Delta x} & \text{if } \tau_{\text{long}} n_1^\alpha < 0, \end{cases} \quad (76)$$

and so on with $(\frac{\partial \phi^\alpha}{\partial y})_{j,i,k}^{\text{up}}$ and $(\frac{\partial \phi^\alpha}{\partial z})_{j,i,k}^{\text{up}}$.

Moreover, the regularized $\delta$-function needed for the source term $s^\alpha$ is given by

$$\delta_{\text{reg}}(r) = \frac{1}{\Delta s_1^{\frac{1}{2}}} \cdot \frac{\pi}{\pi^2 - 4} \left( \cos \frac{\pi |\nabla \psi^\alpha \times r|}{|\nabla \psi^\alpha| \Delta s_1} + 1 \right) \cdot \frac{1}{2\Delta s_2} \left( \cos \frac{\pi (\nabla \psi^\alpha \cdot r)}{|\nabla \psi^\alpha| \Delta s_2} + 1 \right), \quad (77)$$

where $\Delta s_1$ and $\Delta s_2$ are two smoothing parameters.
4. Numerical examples

In this section, the derived continuum plasticity model characterized by the DDPFs is validated through comparison with DDD simulation results.

All simulation results presented in this paper are obtained using $10 \times 10 \times 20$ C3D8 brick elements, and the simulation is performed with Matlab R2010a.

4.1. A single Frank-Read source under constantly applied strains

This example is aimed to provide a first impression about the numerical implementation of the continuum plasticity model. An FR source of length $l = 400b$ and with its activation stress to be $7.8 \times 10^{-4}\mu$, is put at the center of the cuboid $\Omega$ and a $0.3\%$ constant strain is applied to the cuboid by means of indentation on the top surface. The internal structural changes are then simulated starting with a dislocation-free state. It is recalled that the dislocations on each slip plane are represented by the contours of $\phi$, we are thus able to roughly track the evolution of the dislocations at any time slot as shown in Fig. 4. It can be observed that in response to the applied strain, the source keeps releasing dislocation loops.

![Figure 4: Snap shots for the rough distribution of dislocation curves under a constantly applied strain: starting with a dislocation-free state, the solid is applied a constant strain by indentation on top surface. In response to the applied strain, the FR source in the center of $\Omega$ releases dislocation loops.

\[ \text{(a)} \quad t = \frac{5ld}{\mu m_g b^2} \quad \text{(b)} \quad t = \frac{50ld}{\mu m_g b^2} \quad \text{(c)} \quad t = \frac{200ld}{\mu m_g b^2} \quad \text{(d)} \quad t = \frac{2000ld}{\mu m_g b^2} \]
which exit $\Omega$ from the free surfaces. Consequently as shown in Fig. 5, the resolved shear

![Graph showing stress and time relationship](image)

Figure 5: As the FR source keeps releasing dislocation loops to the solid, both the resolved shear stress at the source center and the pressure on the top surface are found dropping. At $t$ roughly being $700L/\left(\mu m^2 g\right)$, the resolved shear stress finally falls below the source activation stress at the source center (indicated by the dashed-dotted line), and the source is thus deactivated.

stress at the source center is found dropping during this loop-releasing process and so does the surface pressure, which is measured as the averaging value of all nodal values for $\sigma_{33}$. These findings agree with the common impression about the role an FR source plays under a constant applied strain: it releases dislocation loops so as to reduce the internal stress state. At $t$ roughly being $700L/\left(\mu m^2 g\right)$, the resolved shear stress finally drops below the source activation stress at the source center (indicated by the dashed-dotted line in Fig. 5), the source is thus deactivated.

The contour surfaces of all components of the displacement field $\mathbf{u}$ on $\partial \Omega$ are drawn in Fig. 6. It suggests that the orientation of the displacement gradient on $\partial \Omega$ is altered to be consistent with the underlying active slip system as a result of the deposition of dislocation loops on the free surfaces. Such deposition mechanism gives rise to (continuous) steps on the free surfaces.
Figure 6: From the contour surfaces of $u_3$ on $\partial \Omega$, the dislocation loops having left the solid produce steps on the free surfaces in accordance with the underlying active slip system. The displacement field is measured in unit of $L$, the pillar height.

4.2. Comparison with the results by DDD simulation

To further validate the derived continuum model by the DDPFs, we have also compared the numerical results with the DDD simulation results obtained by El-Awady et al. (2008), where the compression tests of nickel rods with aspect ratio 3 are simulated.

The parameters used in the simulation here are chosen in accordance with El-Awady et al. (2008) as follows. The loading axis is $<001>$ and a single slip system is activated with the slip direction $[0 \bar{1} 1]$ and slip normal $(111)$. The Schmid’s factor $m_s$ is thus calculated to be 0.4050. The shear modulus is 76GPa; the Poisson’s ratio is 0.347; the strain rate is $200s^{-1}$; the modulus of the Burgers vector $|\mathbf{b}| = 0.25$nm. The dislocation gliding coefficient $m_g$ appearing in the mobility law by Eq. (47) is unspecified by El-Awady et al. (2008), we here follow Senger et al. (2008) to let $m_g = 10^4/(\text{Pa-s})$. The pillar shapes in this paper are cuboids for the ease of implementing the FE formulation with C3D8 elements, compared to cylinders used by El-Awady et al. (2008). The sample sizes here are characterized by the length $D$ of the cuboid base and the cases where $D = 0.5\mu m$ and $1\mu m$ are tested with four samples each here.

In our simulation, the lengths of the FR sources are obtained randomly following the
uniform distribution within \([20\text{nm}, D]\) inside \(\Omega\). The initial dislocation density \(\rho_{\text{initial}}\) is also randomly generated within the range \(1.6 \sim 4 \times 10^{12} \text{m}^{-2}\) and these pre-existing dislocation segments are assumed uniformly assigned to the twelve slip systems, i.e. the initial dislocation density is \(\rho_{\text{initial}}/12\) for each slip system. The statistics about the initial source distribution for various samples are listed in Table 1 and 2. With these isolated FR sources generated, the source term \(s\) needed in the evolutionary equation (68) for \(\phi\) is computed following the algorithm given in Sec. 2.7.3. It is worth noting that the source character parameter, i.e. \(C_s\) in Eq. (52) for every single source is needed for the generation of the source term \(s\). According to El-Awady et al. (2008), to activate a source (probably of edge type) with length \(l = 20\text{nm}\), the resolved shear stress must exceed 1GPa. Incorporating these data into Eq. (52) with the effective core radius to be 0.6\(b\), we find that \(C_s\) in our simulation

| Sample | Mean source length (\(\mu\text{m}\)) | Standard deviation (\(\mu\text{m}\)) | Max source length (\(\mu\text{m}\)) | \(\tau_{\text{min}}^0\) (MPa) | Flow stress (MPa) |
|--------|----------------------------------|-----------------------------------|----------------------------------|----------------|-----------------|
| 1      | 0.1835                           | 0.1104                            | 0.4832                           | 170.7          | 420.0           |
| 2      | 0.2403                           | 0.0935                            | 0.4423                           | 132.8          | 331.5           |
| 3      | 0.2039                           | 0.0992                            | 0.3340                           | 145.5          | 357.9           |
| 4      | 0.1928                           | 0.1083                            | 0.3711                           | 158.9          | 388.8           |

Table 1: Parameters about the individual sources with their lengths obtained following a uniform distribution within \([20\text{nm}, D]\) for samples of size \(D = 0.5\mu\text{m}\). \(\tau_{\text{min}}^0 = \min_{\Omega} \tau_0\), where \(\tau_0\) is given by Eq. (63).

| Sample | Mean source length (\(\mu\text{m}\)) | Standard deviation (\(\mu\text{m}\)) | Max source length (\(\mu\text{m}\)) | \(\tau_{\text{min}}^0\) (MPa) | Flow stress (MPa) |
|--------|----------------------------------|-----------------------------------|----------------------------------|----------------|-----------------|
| 1      | 0.4066                           | 0.2252                            | 0.9196                           | 83.8           | 196.4           |
| 2      | 0.4047                           | 0.2412                            | 0.9995                           | 91.0           | 230.2           |
| 3      | 0.4596                           | 0.2333                            | 0.9605                           | 80.7           | 204.0           |
| 4      | 0.4709                           | 0.2275                            | 0.9349                           | 80.3           | 201.2           |

Table 2: Parameters about the individual sources with their lengths obtained following a uniform distribution within \([20\text{nm}, D]\) for samples of size \(D = 1\mu\text{m}\).
needs to be 1.35 and 2.02 for a single edge source and a screw source, respectively. It is worth noting that $\tau^0_{\text{min}}$ in Table 1 and 2 are defined to be the minimum value of the on-site activation stress $\tau_0$ associated with the continuum source distribution discussed in Sec. 2.7.3, i.e. $\tau^0_{\text{min}} = \min_\Omega \tau_0$, where $\tau_0$ is given by Eq. (63).

The stress-strain curves obtained by the continuum model are shown in Fig. 7(a) for samples of size $D = 0.5\mu m$ and Fig. 7(b) of size $D = 1\mu m$. Our obtained stress-strain curves are shown great agreement with the results by El-Awady et al. (2008) based on the following common features. First, both simulation results indicate an initially elastic regime and an almost perfectly plastic regime, where work-hardening effect is barely observed in the stress-strain curves. Both simulation results also suggest that the applied stress stays roughly unchanged or oscillate around some value in the perfectly plastic regime and this stress is measured as the flow stress of the micro-pillars. The “smaller-being-stronger” size effect on crystalline strength, which is indicated by the flow stress, are both observed in our simulations and in El-Awady et al. (2008). Moreover, it is suggested by both simulation results that there are statistical effects in the flow stress. Such statistical effects are also

Figure 7: The stress-strain curves by the simulation based on the continuum model derived in this paper for samples of size (a) $0.5\mu m$ and (b) $1\mu m$. The vertical intervals denote the ranges for the flow stress abstracted from the simulation results by El-Awady et al. (2008) and the black dots are the averaged value of computed flow stress by El-Awady et al. (2008).
examined in many other literature (e.g. El-Awady et al., 2009; Li et al., 2014).

To make a quantitative comparison between the results by our model and by El-Awady et al. (2008), a vertical interval is drawn to denote the range of the flow stress recorded by El-Awady et al. (2008) and a black dot is used to indicate the average value for each case by El-Awady et al. (2008) in Fig. 7. It can be seen that the flow stresses calculated by our continuum model all fall into the respective ranges characterized by the sample size obtained from the DDD simulation.

The comparison results suggest that the three-dimensional continuum model derived in this paper computationally provide an excellent summary of the underlying discrete dislocation dynamics. In the next section, we will use it to study the mechanism giving rise to the size effect on crystalline strength found in the uniaxial compression tests of micro-pillars.

5. Size effect on strength observed in the uniaxial compression tests of single-crystalline micro-pillars

The “smaller-being-stronger” size effect on strength has been observed in a wide range of pure and composite single crystals at the micrometer scale in the uniaxial compression tests of micro-pillars (Uchic et al., 2009). However, the understanding of the mechanism giving rise to such size effect seems still far from satisfactory. In this section, we follow the traces of the statistically distributed source models introduced in Sec. 1 and use the derived continuum model to study the cause of the size effect on strength of micro-crystals.

5.1. Comparison of the continuum model with the experimental results

In order to apply the continuum model for practical studies, the initial distribution of dislocation sources has to be presumed. However, to the best of the authors’ knowledge, there seems no strong experimental evidence in literature revealing the initial distribution of the FR sources in micro-crystals. Hence we have to first assume an initial source distribution by assembling pieces of information from relevant experimental findings and then get our assumption validated through comparison with experimental data. The total length of the FR sources are associated with the initial distribution of the pre-existing dislocations, whose
number density is suggested to be $3 \times 10^{-12} \text{m}$ by Dimiduk et al. (2005). Similar as in the set up in Sec. 4.2, these pre-existing dislocation segments are assumed to be uniformly distributed in twelve possibly activated slip systems. It has been widely agreed that the initial distribution of the mobile dislocations in each slip system is random in source length, but there seems no wide agreement on the explicit form describing the source distribution. Here we follow the suggestions by Shishvan and Van der Giessen (2010) that, in analogy to the distribution of grain sizes in polycrystals which have been experimentally measured, the FR source size $l$ is set to follow a log-normal distribution with the probability density function to be

$$
\frac{1}{\sqrt{2\pi}\sigma_{sd}} e^{-\frac{(\log(l) - \log(\lambda_m))^2}{2\sigma_{sd}^2}}
$$

(78)

with two parameters $\lambda_m$ and $\sigma_{sd}$ to be determined.

It is worth noting that the log-normal distribution employed here is aimed to resemble the agglomerated effects (such as by FR sources, single-armed sources, etc.) on source lengths due to a finite pillar size. Therefore, the parameter $\lambda_m$, which is envisaged as the effective mean source length affected by the physical dimensions of the samples, is assumed to be a fraction of the pillar size $D$. Here we choose $\lambda_m$ to be $D/15$ and this value will prove to be representative of the practical situation through comparison with experiments. To determine $\sigma_{sd}$ in Eq. (78), we assume that the probability of a source greater than $D$ in size is no more than 0.00001% and $\sigma_{sd}$ is calculated to be about 0.4.

To justify the above set-up of the initial source distribution, the numerical results by the derived continuum model are compared with the experiments by Dimiduk et al. (2005), where single-crystalline nickel is again used as the testing materials. Thus in the simulation presented here, most parameters are chosen the same as used in Sec. 4.2 with the following exceptions: the loading axis is set along [269] and the singly active slip system is of the slip direction along [101] and slip normal ($\overline{111}$) with the Schmid factor $m_s = 0.48$; the aspect ratio is chosen randomly between 2 and 3; the shear modulus here is 78GPa slightly different from Sec. 4.2 in accordance with Dimiduk et al. (2005).

The computed stress-strain curves are shown in Fig. 8 for five groups of samples varying
in size. The size effect on crystalline strength is clearly observed from the simulation results. In each figure, a vertical interval identifies the range of the measured shear stress taken from Dimiduk et al. (2005) at the applied shear strain being roughly 0.1. It can be observed that most computed resolved shear components of the flow stresses just fall into the corresponding intervals characterized by the sample sizes with few exceptions in the case of 5µm.

Therefore, the derived continuum model along with an initially log-normal FR source distribution is shown to be capable in quantitatively reproducing the experimentally observed size-effect on the strength of micro-pillars and, we can use it to study the mechanism that causes such size effect.

5.2. Size effect on the strength of micro-pillars

Based on the above numerical results, we can derive for an explicit formula between the flow stress $\sigma_{\text{flow}}$ and the sample size $D$ to describe the size effect on the strength of micro-pillars by

$$\sigma_{\text{flow}} = \frac{15\mu b}{4\pi m_s} \frac{1}{D} \log \left( \frac{D}{3.6b} \right) + \frac{\sigma_{\text{bulk}}}{2},$$

(79)

where $m_s$ is the Schmid’s factor and a scaling law for $\sigma_{\text{flow}}$ with $D$, according to Eq. (79), can be described by

$$\sigma_{\text{flow}} \sim \frac{1}{D} \log(D),$$

(80)

which displays very similar trend between $\sigma_{\text{flow}}$ and $D$ as the widely used power law, i.e. $\sigma_{\text{flow}} \sim D^{-m}$ with $0 < m < 1$.

The derivation of Eq. (79) is based on several numerical findings by the continuum model derived in this paper. Actually, one can portrait the rough dislocation substructures with the contour curves of $\phi$ on each slip plane, since by definition they characterize the dislocation curves, as shown in Fig. 9, where samples of size $D = 2.4\mu$m, 5µm and 10µm are randomly chosen. The spacing between neighboring slip planes $d$ in generating Fig. 9 is chosen to be 1µm to agree with the set-up of initial density at the order of 1µm$^{-2}$. It is worth noting that since the dislocation number density in each sample is found to be of the same order in magnitude, the dislocation substructures appear more condensing in larger crystals. Moreover, one may keep tracks of the state variables closely related to the plastic
Figure 8: The stress-strain curves obtained by the numerical simulation to the derived continuum model with initial dislocation source length following a log-normal distribution given by Eq. (78). The vertical intervals portrait the ranges of the experimentally measured flow stress at 0.1 strain for samples of different sizes by Dimiduk et al. (2005).
Figure 9: Rough dislocation substructures drawn from randomly picked samples of size (a) $D = 2.4\mu m$, (b) $D = 5\mu m$ and (c) $D = 10\mu m$. It is worth noting that since the dislocation number density in each sample is found to be of the same order in magnitude, the dislocation substructures appear more condensing in larger crystals.

deformation process with our derived continuum model. These state variables include the plastic strain rate, which according to Eq. (51) is given by

$$
\dot{\varepsilon}_p^{\text{tot}} = \frac{b}{|\Omega|} \int_{\Omega} \frac{\partial \phi}{\partial t} |\nabla \psi| dV
$$

and the total dislocation density, which according to Eq. (22) is given by

$$
\rho_{\text{tot}} = \rho_{\text{initial}} + \frac{1}{|\Omega|} \int_{\Omega} |\nabla \phi \times \nabla \psi| dV,
$$

where $\rho_{\text{initial}}$ is the initial number density of the pre-existing dislocations. In Fig. 10, we can see two steady regimes for $\rho_{\text{tot}}$, where their corresponding values appear unchanged and the two steady regimes are connected by a fast transiting region. As for $\dot{\varepsilon}_p^{\text{tot}}$, it can be seen from Fig. 10(b) that the values of $\dot{\varepsilon}_p^{\text{tot}}$ converge to a same value for samples of various size and this value is actually determined by the applied strain rate $200s^{-1}$. The reason is as follows. In the perfectly plastic regime, the internal stress components stay unchanged, that
Figure 10: Evolution of (a) the total number density of dislocations determined by Eq. (82) and (b) the plastic strain (flow) rate determined by Eq. (81) in micro-pillars for randomly picked-up samples of various sizes. We can see two steady regimes for $\rho_{\text{tot}}$, where the corresponding values appear unchanged. The values of $\dot{\epsilon}^p_{\text{tot}}$ are found to converge to a same value for samples of various sizes.

is, $d\sigma/dt = 0_{3\times3}$. If we replace $\sigma$ by using the constitutive stress equation (29) and integrate over $\Omega$ the resulting identity divided by $|\Omega|$, we have an equation from the $\sigma_{33}$ component

$$
\frac{1 - \nu}{1 - 2\nu} \frac{1}{|\Omega|} \int \frac{d}{dt} \left( \frac{\partial u_3}{z} \right) dV = \frac{b_3 m_3}{b} \int \frac{1}{|\Omega|} \frac{d\phi}{dt} |\nabla\psi| dV = \frac{b_3 m_3}{b} \dot{\epsilon}^p_{\text{tot}}, \tag{83}
$$

where the contribution from $\partial u_1/\partial x$ and $\partial u_2/\partial y$ is neglected; the second identity is by using Eq. (81); $m_3$ is the third entry of the slip normal $\mathbf{m}$. In fact, the term $(b_3 m_3)/b$ equals to the Schmid factor $m_s$. If we further assume $u_3$ is linear from 0 to $u_b$, the displacement on the indentation surface, then Eq. (83) becomes

$$
\dot{\epsilon}^p_{\text{tot}} = \frac{1 - \nu}{2(1 - 2\nu)m_s} \frac{d}{dt} \left( \frac{u_b}{L} \right), \tag{84}
$$

where $d(u_b/L)/dt$ is just the applied strain rate. If we let this applied strain rate equal to 200s$^{-1}$ as used in our simulation, it can be calculated from Eq. (84) that the plastic strain rate to accommodate the applied load should be in theory roughly 365s$^{-1}$. It can be seen from Fig. 10(b) that the results from our simulation roughly agree with this theoretical value.
These numerical findings may suggest the following microstructural evolution in samples under a constant applied strain rate induced by compression. When the elastic limit of the samples are reached, the dislocation sources start to release dislocation loops, resulting in the initiation of the plastic flow and a rise in $\rho_{\text{tot}}$. After a short period, the system reaches a steady state, when the applied strain rate is fully accommodated by the plastic flow driven by the dislocation motion. Correspondingly this is the perfectly plastic regime in the stress strain curves in Fig. 8 and the measured engineering stress then is the flow stress $\sigma_{\text{flow}}$. Since the transiting period between the two regimes is rather short, it is reasonable to conclude that $\sigma_{\text{flow}}$ may be highly related to the elastic limits of the samples, which are associated with the strength of the weakest dislocation source.

With the concept of a continuously distributed dislocation source in the continuum model here, the strength of the weakest source denoted by $\tau^0_{\text{min}}$ corresponds to the minimum on-site (continuous) activation stress $\tau_0$ given by Eq. (63). Mathematically, this is $\tau^0_{\text{min}} = \min_{\Omega} \tau_0$. In fact, if we collect the flow stress $\sigma_{\text{flow}}$ and their associated $\tau^0_{\text{min}}$ obtained from all simulation tests and draw them in Fig. 11(a), a strongly linear dependence between $\sigma_{\text{flow}}$ and $\tau^0_{\text{min}}$

$$
\sigma_{\text{flow}} = k_1 \tau^0_{\text{min}} + k_2
$$

formulated by $\sigma_{\text{flow}} = k_1 \tau^0_{\text{min}} + k_2$ is observed. The parameter $k_1$ can be considered as the
ratio of an applied load over its resolved shear component, and it is the reciprocal of \( m_s \), the Schmid factor. The parameter \( k_2 \) is set to be a fraction of \( \sigma_{\text{flow}}^{\text{bulk}} \), the flow stress for bulk materials. This assumption is drawn due to the observation by Dimiduk et al. (2005) the flow stress of the pillars is almost \( \sigma_{\text{flow}}^{\text{bulk}} \) as the pillar size exceeds 40\( \mu \)m. By curve fitting, we find that \( k_2 \) is roughly \( \sigma_{\text{flow}}^{\text{bulk}}/2 \). Therefore, the flow stress is related to the minimum on-site activation stress \( \tau_{\min}^0 \) by

\[
\sigma_{\text{flow}} = \frac{\tau_{\min}^0}{m_s} + \frac{\sigma_{\text{flow}}^{\text{bulk}}}{2}.
\]  

In Fig. 11(a), a comparison between the dashed line drawn by Eq. (85) and the simulation results by the continuum model suggests that, Eq. (79) provides a nice quantitative description for \( \sigma_{\text{flow}} \) as a function of \( \tau_{\min}^0 \). The next step is to relate \( \tau_{\min}^0 \) to the sample size \( D \). The definition of \( \tau_{\min}^0 \) suggests that it is highly related to the activation stress of the weakest single FR source. Actually, one may envisage that \( \tau_{\min}^0 \) depends on an effective length denoted by \( l_{\text{eff}} \) in the same sense in determining the strength of an isolated FR source by Eq. (52), i.e. we can assume \( \tau_{\min}^0 \) satisfies

\[
\tau_{\min}^0 = \frac{C_s \mu b}{2\pi l_{\text{eff}}} \log \left( \frac{l_{\text{eff}}}{r_c} \right),
\]  

where \( C_s \) is dependent on the source character in nickel. It is recalled that the mean length of the randomly distributed FR sources is a fraction of sample size \( D \). Analogically, one can assume \( l_{\text{eff}} \) is also a fraction of \( D \). \( C_s \) here is chosen to be 1.25, the middle value between an edge-oriented source \( (C_s = 1) \) and a screw-oriented source \( (C_s = 1.5) \). Then based on the computed values of \( \tau_{\min}^0 \) under various \( D \), one may fit from Eq. (86) for \( l_{\text{eff}}/D \), which is found to be roughly 1/6. Compared to the mean source length \( D/15 \) used for simulation, \( D/6 \) provides a reasonable estimation to the effective source length of the weakest source.

Therefore, a formula of \( \tau_{\min}^0 \) with sample size \( D \) is obtained by incorporating the values of \( l_{\text{eff}}/D \) and \( C_s \) into Eq. (86)

\[
\tau_{\min}^0 = \frac{9\mu b}{2\pi D} \log \left( \frac{D}{6r_c} \right). 
\]  

Combining Eq. (85) and (87), we obtain the formula for \( \sigma_{\text{flow}} \) depending on \( D \) given by Eq. (79) shown in the beginning of this subsection.
In Fig. 12, the flow stress against the sample size is drawn by using Eq. (79) with $r_c$ taken to be 0.6$b$. It can be seen that the explicit formula describing the size effect on the strength of micro-crystals given by Eq (79) agree well with the experimental and numerical results.

5.3. Discussion

Many other plastic behaviors of a micro-pillar being compressed can also be studied by using the continuum model derived in this paper.

From the rough dislocation substructures given by Fig. 9, one may read the plastic flow pattern induced by the collective motion of the dislocation curves. To do this, we pick up randomly several slip planes in samples of size $5\mu$m and $10\mu$m and draw the contours of $\phi$ as shown in Fig. 13(a) and (b), respectively. It appears from the figures that the plastic flow is caused in general by the motion of dislocations initiated by the sources near one side of the free surfaces and moving towards the opposite side. It is worth noting that the flow pattern shown in Fig. 13(a) and (b) do not mean that the sources inside the micro-pillars
Figure 13: Contours of $\phi$ drawn in a sample (a) of size 5\(\mu\)m and (b) of size 10\(\mu\)m on several picked-up slip planes. (c) The families of the dashed curves and the solid curves should roughly give rise to a same contour profile for the continuum model. This is because the internal length scale associated with the continuum model is too coarse to precisely describe the behaviors of individual dislocation curves. The comparison between the two families of dislocation curves in (c) provides an explanation to the observation in (a) and (b), that the sources near the free surfaces appear more active than the internal ones. It is because the loops generated by the internal sources are more likely to interact with other loops so as to give rise to a coarse-grained plastic flow pattern described by the dashed curves in (c).

are completely deactivated. This is because the internal length scale associated with the continuum model is too coarse to precisely describe the behaviors of individual dislocation curves. As a result, many types of dislocation networks at a finer scale may correspond to similar contour profiles at the coarse-grained level. For example in Fig. 13(c), the families of the dashed curves and the solid curves should roughly give rise to a same contour profile at the continuum scale. Actually, the comparison between the two family of dislocation curves shown in Fig. 13(c) provides an explanation to the phenomena observed in Fig. 13(a) and (b), that the sources near the free surfaces appear more active than the internal ones. It is because the loops generated by the internal sources are more likely to interact with
other loops resulting in a coarse-grained plastic flow pattern, which appears initialing from one free surface and flowing to the opposite surfaces as described by the dashed curves in Fig. 13(c).

With the derived continuum model, one is also able to visualize the deformation process in the shapes of the micro-pillars. This is because a point \( \mathbf{r} \) defined in an undeformed pillar can be tracked at \( \mathbf{r} + \mathbf{u} \) in the compressed pillar at any time in the derived continuum model. By this way, the profile of a deformed pillar of size 5\( \mu \)m during compressions is shown in Fig. 14. It can be seen that the pillar gets sheared as being compressed. The orientation of the plastic shear is found consistent with the underlying activated slip system. Experimentally, such shearing effect induced by plastic slips takes the form of a number of (discrete) steps on the free surfaces (Dimiduk et al., 2005). It is worth noting that the shapes of a compressed micro-pillar computed by using the continuum model provide a coarse-grained description about the shapes of the experimentally observed pillars.

Finally, the role of the boundary values of \( \phi \) is discussed. In fact, it can be seen from the derived constitutive stress rule of Eq. (29) \( \sigma = \mathcal{L}(\nabla \mathbf{u}) + 2\mu \phi \text{sym}(\mathbf{b} \otimes \nabla \psi) \) that the

\[ \sigma = \mathcal{L}(\nabla \mathbf{u}) + 2\mu \phi \text{sym}(\mathbf{b} \otimes \nabla \psi) \]

Figure 14: By the derived continuum model, a point \( \mathbf{r} \) defined in the undeformed pillar can be tracked at \( \mathbf{r} + \mathbf{u} \) in the compressed pillar at any time. In this way, the profiles of the compressed pillars can be sketched. The cuboids formed by the dashed-lines describe the shapes of undeformed pillars.
internal stress field is determined by the total displacement gradient subtracted by the plastic distortion, whose magnitude by Eq. (27) is found governed by the modulus of $\phi$. Thus we may conclude that when the total displacement gradient is fixed, a $\phi$ lower in magnitude plays a less effective role in reducing the internal stress state. This means that the hardening of micro-crystals is highly related to the values of $\phi$ according to the continuum model. An extreme case is when $\phi = 0$, indicating that the dislocations can not penetrate through the boundaries. This corresponds to the hardening effect induced by the dislocation pile-up and from above analysis such hardening effect seems to be a natural outcome of the derived continuum model. The extreme cases on the other end are found on the free surfaces, where no frictional effect takes place in restricting the growth of $\phi$ in magnitude. As a result, the stress state is eased to the best. This may be the reason why no hardening effect is observed in the stress-strain curves in Fig. 8, because the applied strains are fully accommodated by the collective motion of the dislocations, which are able to exit $\Omega$ freely. A further discussion regarding how the hardening of crystals is affected by the values of $\phi$ indicated by the continuum model will be the topic of another paper.

6. Conclusion

In this paper, we derive a dislocation-based continuum model for crystals of size ranging from the order of several microns to sub-millimeters, where neither the discrete dislocation dynamical models nor the strain-gradient continuum plasticity theories work perfectly. In the derived continuum model, the crystalline microstructures are represented by a family of DDPFs $\psi^\alpha$, whose integer values specify slip planes and another family of DDPFs $\phi^\alpha$, whose contours on slip planes characterize dislocation curves. By means of the DDPFs, a closed set of equations are derived to formulate the plastic deformation process. We have shown that the derived equations, which are listed in Sec. 2.8, provide an appropriate summary over the underlying discrete dislocation dynamics. Numerically, an FE formulation is proposed to compute the internal stress field.

The derived continuum model is validated by comparing with the DDD simulation and experiments. As an application of the derived continuum model by the DDPFs, the size
effect on strength of micro-crystals is studied and a formula for the flow stress depending on the sample size is derived as given by Eq. (79).

The presented work can be extended along two directions. Firstly, more mechanisms taking place at the scales of the discrete dislocation dynamical models, need to be taken into account in the continuum model characterized by the DDPFs. For example, the anti-planar dislocation motion, such as the cross-slipping and climbing of dislocations, frequently taking place in BCC or FCC crystals at high temperature, can be incorporated into the continuum model by allowing the contours of $\psi$ to be curved. Besides, there are also potentials and needs to include the dislocation junction formation, dislocation interactions with point defects and grain boundaries, the short-range mutual interactions between dislocations belonging to various slip systems in the continuum model (e.g. Xiang and Srolovitz, 2006; Chen et al., 2010; Zhu and Xiang, 2014). On the other hand, there are also needs for applying the derived continuum model to study the behaviors of crystals at the micrometer scale, such as how the hardening of crystals is governed by the behaviors of the dislocation ensembles indicated by the continuum model characterized by the DDPFs.

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References

A. Acharya. A model of crystal plasticity based on the theory of continuously distributed dislocations. *J. Mech. Phys. Solids*, 49:761–784, 2001.

K.E. Aifantis and A.H.W. Ngan. Modeling dislocation-grain boundary interactions through gradient plasticity and nanoindentation. *Mater. Sci. Eng. A*, 459:251–261, 2007.

A. Alankar, I. N. Mastorakos, and D. P. Field. A dislocation-density-based 3d crystal plasticity model for pure aluminum. *Acta Mater.*, 57(19):5936–5946, 2009.

Alankar Alankar, Philip Eisenlohr, and Dierk Raabe. A dislocation density-based crystal plasticity constitutive model for prismatic slip in-titanium. *Acta Mater.*, 59(18):7003–7009, 2011.

A. S. Argon. *Strengthening mechanisms in crystal plasticity*. Oxford University Press, 2008.
A. Arsenlis and D. M. Parks. Modeling the evolution of crystallographic dislocation density in crystal plasticity. *J. Mech. Phys. Solids*, 50:1979–2009, 2002.

A. Arsenlis, W. Cai, M. Tang, M. Rhee, T. Oppelstrup, T. G. Hommes, T. G. Pierce, and V. V. Bulatov. Enabling strain hardening simulations with dislocation dynamics. *Modelling Simul. Mater. Sci. Eng.*, 15:553–595, 2007.

A. A. Benzerga, Y. Bréchet, A. Neeldeman, and E. Van der Giessen. Incorporating three-dimensional mechanisms into two-dimensional dislocation dynamics. *Modelling Simul. Mater. Sci. Eng.*, 12:159–196, 2004.

P. Burchard, L. T. Cheng, B. Merriman, and S. Osher. Motion of curves in three spatial dimensions using a level set approach. *J. Comput. Phys.*, 170(2):720–741, 2001.

Srinath S. Chakravarthy and W. A. Curtin. Stress-gradient plasticity. *Proc. Nat. Acad. Sci. USA*, 108(38):15716–15720, 2011.

Z. Chen, K. T. Chu, D. J. Srolovitz, J. M. Rickman, and M. P. Haataja. Dislocation climb strengthening in systems with immobile obstacles: Three-dimensional level-set simulation study. *Phys. Rev. B*, 81(5):054104, 2010.

B. Cheng, H. S. Leung, and A. H. W. Ngan. Strength of metals under vibrations - dislocation-density-function dynamics simulations. *Philos. Mag.*, pages 1–21, 2014.

D. M. Dimiduk, M. D. Uchic, and T. A. Parthasarathy. Size-affected single-slip behavior of pure nickel microcrystals. *Acta Mater.*, 53(15):4065–4077, 2005.

J. A. El-Awady, S. B. Biner, and N. M. Ghoniem. A self-consistent boundary element, parametric dislocation dynamics formulation of plastic flow in finite volumes. *J. Mech. Phys. Solids*, 56(5):2019–2035, 2008.

J. A. El-Awady, M. Wen, and N. M. Ghoniem. The role of the weakest link mechanism in controlling the plasticity of micropillars. *J. Mech. Phys. Solids*, 57(1):32–50, 2009.

A. El-Azab. Statistical mechanics treatment of the evolution of dislocation distributions in single crystals. *Phys. Rev. B*, 61:11956–11966, 2000.

P. Engels, A. X. Ma, and A. Hartmaier. Continuum simulation of the evolution of dislocation densities during nanoindentation. *Int. J. Plast.*, 38:159–169, 2012.

A. K. Faradjian, L. H. Friedman, and D. C. Chrzan. Frank-read sources within a continuum simulation. *Modelling Simul. Mater. Sci. Eng.*, 7:479–494, 1999.

S. P. Fitzgerald, S. Aubry, S. L. Dudarev, and W. Cai. Dislocation dynamics simulation of frank-read sources in anisotropic \(\alpha\)-iron. *Modelling Simul. Mater. Sci. Eng.*, 20:1–8, 2012.

M. Fivel, L. Tabourout, E. Rauch, and G. Canova. Identification through mesoscopic simulations of macroscopic parameters of physically based constitutive equations for the plastic behaviour of fcc single crystals. *J. Phys. IV France*, 8:151–158, 1998.
N. A. Fleck and J. W. Hutchinson. A phenomenological theory for strain gradient effects in plasticity. *J. Mech. Phys. Solids*, 41:1825–1857, 1993.

A. J. E. Foreman. The bowing of a dislocation segment. *Philos. Mag.*, 15:1011–1021, 1967.

J. Friedel. *Les dislocations*. Cauthier-Villars, Paris, 1956.

M. G. D. Geers, R. H. H. Peerlings, M. A. Peletier, and L. Scardia. Asymptotic behaviour of a pile-up of infinite walls of edge dislocations. *Arch. Ration. Mech. Anal.*, 209:495–539, 2013.

N. M. Ghoniem, S. H. Tong, and L. Z. Sun. Parametric dislocation dynamics: a thermodynamics-based approach to investigations of mesoscopic plastic deformation. *Phys. Rev. B*, 61:913–927, 2000.

D. Gómez-García, B. Devincre, and L. P. Kubin. Forest hardening and boundary conditions in 2-d simulations of dislocations dynamics. *Mat. Res. Soc. Symp. Proc.*, 578:131–136, 2000.

J. R. Greer and W. D. Nix. Nanoscale gold pillars strengthened through dislocation starvation. *Phys. Rev. B*, 73(24), 2006.

J. R. Greer, W. C. Oliver, and W. D. Nix. Size dependence of mechanical properties of gold at the micron scale in the absence of strain gradients. *Acta Mater.*, 53(6):1821–1830, 2005.

I. Groma, F. F. Csikor, and M. Zaiser. Spatial correlations and higher-order gradient terms in a continuum description of dislocation dynamics. *Acta Mater.*, 51:1271–1281, 2003.

R. Gu and A. H. W. Ngan. Dislocation arrangement in small crystal volumes determines power-law size dependence of yield strength. *J. Mech. Phys. Solids*, 61(6):1531–1542, 2013.

M. E. Gurtin. A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations. *J. Mech. Phys. Solids*, 50:5–32, 2002.

C. L. Hall. Asymptotic analysis of a pile-up of regular edge dislocation walls. *Mater. Sci. Eng. A - Struct.*, 530:144–148, 2011.

X. Han, N. M. Ghoniem, and Z. Wang. Parametric dislocation dynamics of anisotropic crystals. *Philos. Mag.*, 83:3705–3721, 2003.

A. K. Head, S. D. Howison, J. R. Ockendon, and S. P. Tighe. An equilibrium-theory of dislocation continua. *SIAM Rev.*, 35(4):580–609, 1993.

J. P. Hirth and J. Lothe. *Theory of dislocations*. Wiley, New York, 2nd edition, 1982.

T. Hochrainer, S. Sandfeld, M. Zaiser, and P. Gumbsch. Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. *J. Mech. Phys. Solids*, 63:167–178, 2014.

D. C. Jang, X. Y. Li, H. J. Gao, and J. R. Greer. Deformation mechanisms in nanotwinned metal nanopillars. *Nature Nanotechnology*, 7(9):594–601, 2012.

D. M. Kochmann and K. C. Le. Dislocation pile-ups in bicrystals within continuum dislocation theory. *Int. J. Plast.*, 24:2125–2147, 2008.

A. Kosevich. Crystal dislocations and the theory of elasticity. In *Dislocations in Solids*, Vol. 1, pages 33–141.
North-Holland, Amsterdam, 1979.

E. Kröner. *Kontinuumstheorie der Bersetzungen und Eigenspannungen*. Springer-Verlag, Berlin, 1958.

E. Kröner. Dislocation: a new concept in the continuum theory of plasticity. *J. Math. Phys.*, 42:27–37, 1963.

L. P. Kubin, G. Canova, M. Condat, B. Devincre, V. Pontikis, and Y. Bréchet. Dislocation microstructures and plastic flow: a 3d simulation. *Solid State Phenom.*, 23/24:455–472, 1992.

D.S. Li, H. M. Zbib, X. Sun, and M. Khaleel. Predicting plastic flow and irradiation hardening of iron single crystal with mechanism-based continuum dislocation dynamics. *Int. J. Plast.*, 52:3–17, 2014.

K. T. Li, A. X. Huang, and H. Q. Huang. *The finite element method and its application (in Chinese)*. Scientific publisher, Beijing, 2006.

Z. L. Liu, Z. Zhuang, X. M. Liu, X. C. Zhao, and Z. H. Zhang. A dislocation dynamics based higher-order crystal plasticity model and applications on confined thin-film plasticity. *Int. J. Plast.*, 27:201–216, 2011.

J. R. Mayeur and D. L. McDowell. A comparison of gurtin type and micropolar theories of generalized single crystal plasticity. *Int. J. Plast.*, 57(0):29–51, 2014.

J. R. Mayeur, D. L. McDowell, and D. J. Bammann. Dislocation-based micropolar single crystal plasticity: Comparison of multi- and single criterion theories. *J. Mech. Phys. Solids*, 59(2):398–422, 2011.

A. Moulin, M. Condat, and L. P. Kubin. Simulation of frank-read sources in silicon. *Acta Mater.*, 45: 2339–2348, 1997.

F. R. N. Nabarro. Dislocations in a simple cubic lattice. *Proc. Phys. Soc.*, 59:256–272, 1947.

W. D. Nix and H. Gao. Indentation size effects in crystalline materials: a law for strain gradient plasticity. *J. Mech. Phys. Solids*, 46:411–425, 1998.

J. F. Nye. Some geometrical relations in dislocated crystals. *Acta Metall.*, 1:153–162, 1953.

E. Orowan. Discussion. In *Symposium on internal stress in metals and alloys*, page 451. The Institute of Metals, London, 1948.

M. S. Oztop, C. F. Niordson, and J. W. Kysar. Length-scale effect due to periodic variation of geometrically necessary dislocation densities. *Int. J. Plast.*, 41:189–201, 2013.

T. A. Parthasarathy, S. I. Rao, D. M. Dimiduk, M. D. Uchic, and D. R. Trinkle. Contribution to size effect of yield strength from the stochastics of dislocation source lengths in finite samples. *Scripta Mater.*, 56(4):313–316, 2007.

R. Peierls. The size of a dislocation. *Proc. Phys. Soc.*, 52:34–37, 1940.

S. S. Quek, Y. Xiang, Y. W. Zhang, D. J. Srolovitz, and C. Lu. Level set simulation of dislocation dynamics in thin films. *Acta Mater.*, 54(9):2371–2381, 2006.

S. I. Rao, D. M. Dimiduk, M. Tang, T. A. Parthasarathy, M. D. Uchic, and C. Woodward. Estimating the strength of single-ended dislocation sources in micron-sized single crystals. *Philos. Mag.*, 87(30): 56
J. R. Rice. Inelastic constitutive relations for solids: An internal-variable theory and its application to metal plasticity. *J. Mech. Phys. Solids*, 19(6):433–455, 1971.

J. M. Rickman and J. Vinals. Modelling of dislocation structures in materials. *Philos. Mag. A*, 75(5):1251–1262, 1997.

I. Ryu, W. D. Nix, and W. Cai. Plasticity of bcc micropillars controlled by competition between dislocation multiplication and depletion. *Acta Mater.*, 61(9):3233–3241, 2013.

S. Sandfeld, T. Hochrainer, M. Zaiser, and P. Gumbsch. Continuum modeling of dislocation plasticity: Theory, numerical implementation, and validation by discrete dislocation simulations. *J. Mater. Res.*, 26:623–632, 2011.

R. Sedláček, J. Kratochvíl, and E. Werner. The importance of being curved: bowing dislocations in a continuum description. *Philos. Mag.*, 83:3735–3752, 2003.

J. Senger, D. Weygand, P. Gumbsch, and O. Kraft. Discrete dislocation simulations of the plasticity of micro-pillars under uniaxial loading. *Scripta Mater.*, 58(7):587–590, 2008.

S. Shao, N. Abdolrahim, D. F. Bahr, G. Lin, and H. M. Zbib. Stochastic effects in plasticity in small volumes. *Int. J. Plast.*, 52:117–132, 2014.

S. S. Shishvan and E. Van der Giessen. Distribution of dislocation source length and the size dependent yield strength in freestanding thin films. *J. Mech. Phys. Solids*, 58(5):678–695, 2010.

H. Tang, K. W. Schwarz, and H. D. Espinosa. Dislocation-source shutdown and the plastic behavior of single-crystal micropillars. *Phys. Rev. Lett.*, 100(18), 2008.

M. D. Uchic, D. M. Dimiduk, J. N. Florando, and W. D. Nix. Sample dimensions influence strength and crystal plasticity. *Science*, 305(5686):986–989, 2004.

M. D. Uchic, P. A. Shade, and D. M. Dimiduk. Plasticity of micrometer-scale single crystals in compression. *Annu. Rev. Mater. Res.*, 39:361 – 386, 2009.

E. Van der Giessen and A. Needleman. Discrete dislocation plasticity - a simple planar model. *Modelling Simul. Mater. Sci. Eng.*, 3(5):689–735, 1995.

R. Venkatraman and J. C. Bravman. Separation of film thickness and grain-boundary strengthening effects in al thin-films on si. *J. Mater. Res.*, 7(8):2040–2048, 1992.

B. von Blanckenhagen, P. Gumbsch, and E. Arzt. Dislocation sources in discrete dislocation simulations of thin-film plasticity and the hall-petch relation. *Modelling Simul. Mater. Sci. Eng.*, 9:157–169, 2001.

R. E. Voskoboinikov, S. J. Chapman, J. R. Ockendon, and D. J. Allwright. Continuum and discrete models of dislocation pile-ups. i. pile-up at a lock. *J. Mech. Phys. Solids*, 55:2007–2025, 2007.

D. Weygand, L. H. Friedman, E. Van der Giessen, and A. Needleman. Aspects of boundary-value problem solutions with three-dimensional dislocation dynamics. *Modelling Simul. Mater. Sci. Eng.*, 10:437–468,
Y. Xiang. Continuum approximation of the Peach-Koehler force on dislocations in a slip plane. *J. Mech. Phys. Solids*, 57:728–743, 2009.

Y. Xiang and D. J. Srolovitz. Dislocation climb effects on particle bypass mechanisms. *Philos. Mag.*, 86:3937–3957, 2006.

Y. Xiang, L. T. Cheng, D. J. Srolovitz, and W. N. E. A level set method for dislocation dynamics. *Acta Mater.*, 51:5499–5518, 2003.

Y. Xiang, H. Wei, P. B. Ming, and W. E. A generalized Peierls-Nabarro model for curved dislocations and core structures of dislocation loops in Al and Cu. *Acta Mater.*, 56:1447–1460, 2008.

G. Xu and A. S. Argon. Homogeneous nucleation of dislocation loops under stress in perfect crystals. *Philos. Mag. Lett.*, 80:605–611, 2000.

H. M. Zbib, M. Rhee, and J. P. Hirth. On plastic deformation and the dynamics of 3D dislocations. *Int. J. Mech. Sci.*, 40:113–127, 1998.

D. G. Zhao, H. Q. Wang, and Y. Xiang. Asymptotic behaviors of the stress fields in the vicinity of dislocations and dislocation segments. *Philos. Mag.*, 92:2351–2374, 2012.

C. Z. Zhou and R. LeSar. Dislocation dynamics simulations of plasticity in polycrystalline thin films. *Int. J. Plast.*, 30-31:185–201, 2012.

X. H. Zhu and Y. Xiang. Continuum model for dislocation dynamics in a slip plane. *Philos. Mag.*, 90:4409–4428, 2010.

X. H. Zhu and Y. Xiang. Continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries. *J. Mech. Phys. Solids*, 69(0):175–194, 2014.

Y. C. Zhu and S. J. Chapman. A natural transition between equilibrium patterns of dislocation dipoles. *J. Elast.*, 117(1):51–61, 2014.

Y. C. Zhu, S. J. Chapman, and A. Acharya. Dislocation motion and instability. *J. Mech. Phys. Solids*, 61:1835–1853, 2013.

Y. C. Zhu, H. Q. Wang, X. H. Zhu, and Y. Xiang. A continuum model for dislocation dynamics incorporating Frank-Read sources and Hall-Petch relation in two dimensions. *Int. J. Plast.*, 60:19–39, 2014.