Statistical mechanics treatment of the evolution of dislocation distributions in single crystals

A. El-Azab*
Pacific Northwest National Laboratory, MSIN: K1-83, 902 Battelle Boulevard, P.O. Box 999, Richland, Washington 99352
(Received 12 July 1999; revised manuscript received 9 December 1999)

A statistical mechanics framework for the evolution of the distribution of dislocations in a single crystal is established. Dislocations on various slip systems are represented by a set of phase-space distributions each of which depends on an angular phase space coordinate that represents the line sense of dislocations. The invariance of the integral of the dislocation density tensor over the crystal volume is proved. From the invariance of this integral, a set of Liouville-type kinetic equations for the phase-space distributions is developed. The classically known continuity equation for the dislocation density tensor is established as a macroscopic transport equation, showing that the geometric and crystallographic notions of dislocations are unified. A detailed account for the short-range reactions and cross slip of dislocations is presented. In addition to the nonlinear coupling arising from the long-range interaction between dislocations, the kinetic equations are quadratically coupled via the short-range reactions and linearly coupled via cross slip. The framework developed here can be used to derive macroscopic transport-reaction models, which is shown for a special case of single-slip configuration. The boundary value problem of dislocation dynamics is summarized, and the prospects of development of physical plasticity models for single crystals are discussed.

I. INTRODUCTION

The plastic straining of a metallic crystal is synonymous with the transport of dislocation lines in the crystal. During their motion, dislocations interact with each other via long-range forces in a manner similar to the long-range interactions among charged particles. Dislocations also undergo short-range reactions leading to immobilization or destruction of the reacting dislocation species. These reactions are strongly dependent on the line direction of dislocations. Furthermore, by the fact that dislocations are continuous curved linear entities, their motion normally leads to significant length change or multiplication. The dislocation line density in a deforming crystal may increase by several orders of magnitude during deformation. In addition, dislocations change their glide planes by cross slipping between crystallographic planes sharing the same slip direction. This complex dynamics is believed to be the origin of the induced dislocation density and plastic strain heterogeneity in deforming crystals.[1,2] Therefore, explicit representation of the reactions and transport of dislocations is vital to successful prediction of dislocation and deformation patterns.

Some models dealing with highly idealized dislocation configurations have been developed.[3–10] Such models have been found too simple to capture the three-dimensional character of transport and reactions of dislocations. Almost three decades ago it was argued that the framework of statistical mechanics can be applied to develop a dislocation-based plasticity theory.[11] This argument was based on the fact that the distribution of dislocations in a crystal is statistical in nature. Two attempts at developing a formal kinetic treatment, exploiting the statistical and dynamical nature of the dislocation population in deforming crystals, have been made.[12,13] However, the complex short-range dislocation interactions and discrete nature of crystallographic slip have not been accounted for. Relatively recently, the method of dislocation dynamics has been significantly developed.[14,15] With explicit representation of the dynamics and interactions of discrete dislocations, the method is believed to be promising in resolving certain questions related to the origin of strain and dislocation density heterogeneity in crystals at the mesoscale. Even though it deals with discrete dislocation systems, the simulation method is naturally classified as a statistical mechanics approach to dislocation transport and reactions in deforming crystals.

The main objective of the present work is to develop a statistical mechanics framework for the spatiotemporal evolution of dislocations and, in turn, single-crystal plasticity for the case of small plastic distortions. As shown later, this framework can be considered a continuum analog of the method of discrete dislocation dynamics simulation since it accounts for the transport and reactions of dislocations in an otherwise linear elastic crystal. The present development preserves the framework of the classical theory of dislocation fields which rigorously describes two important aspects of plasticity: the equilibrium of the lattice stress field and compatibility of the deformation field.

The paper is organized as follows. The mathematical formulation of the present framework is presented in Sec. II. A set of phase-space distributions is introduced to represent the evolving dislocation populations on all slip systems. The requirement that the deforming crystal must remain compact is used to define an invariant global quantity which is given by the integral of the dislocation density tensor over the crystal volume. Tensorial Liouville-type equations for the contributions of slip systems to this global invariant are then determined. Considering no higher-order spatial correlations, a set of kinetic equations governing the evolution of the scalar phase-space distributions is derived, with source terms representing short-range interactions, multiplication, and cross slip. The continuity equation of the macroscopic dislocation density tensor is established from the mixed zeroth-velocity-first-angular moment of the kinetic equations. The angular dependence of the phase-space distributions is brought in to account for the line sense of dislocations. In Sec. III, a single-slip configuration model is recovered as a special case. Section IV includes a summary of the initial-boundary-value problem of dislocation dynamics. A discussion of the prospects of this approach in formulating macroscopic dislocation transport-reaction and crystal plasticity models is given in Sec. V.

II. THE STATISTICAL MECHANICS FRAMEWORK

A. The dislocation field

The formulation presented here is based on the notion that, in a deforming crystal, the evolving dislocation field can be described by the method of statistical mechanics. This is motivated by the following facts. First, the spatiotemporal evolution of dislocations is governed by quasi-Newtonian dynamics where the motion of dislocation elements is described by an equation of motion. Second, the corresponding discrete system has a very large number of degrees of freedom. Third, the evolving dislocation field exhibits velocity distributions. These facts are well established. For example, as evident from the computer simulations of discrete dislocation systems, the dislocation population is distributed in the velocity space and exhibits angular dependence.[16]

In a deforming crystal, dislocations are naturally categorized by the slip direction (or Burgers vector) and the slip plane normal. Consider a crystal with N slip systems. For $i=1,N$, denote by $\mathbf{n}^{(i)}$ and $\mathbf{b}^{(i)}$ the unit normal to the slip plane and the Burgers vector, respectively. In the case of finite deformation, both $\mathbf{n}^{(i)}$ and $\mathbf{b}^{(i)}$ must be considered functions of space and time. Only infinitesimal deformation is considered here, hence $\mathbf{n}^{(i)}$ and $\mathbf{b}^{(i)}$ are assumed constant for all slip systems. On a particular slip system, a dislocation element may have a sense vector $\mathbf{t}$ along any direction lying in its slip plane. The motion by *climb* is not considered here since a climbing dislocation has a line direction that may not lie in its slip plane. The dislocation content of a slip system can be conveniently characterized by introducing the distribution $\phi^{(i)}(\mathbf{x},\mathbf{v},\mathbf{t},t)$. Since all directions in a plane can be defined by a single scalar parameter—that is $\mathbf{t}=\mathbf{t}(\theta)$; θ is an angle in the range $[0,2\pi])$—then, $\mathbf{t}$ can be replaced by θ. Hence, $\phi^{(i)}$ can be given the definition: $\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)d\mathbf{x}d\mathbf{v}d\theta$ is dislocation line length contained in the phase-space volume $d\mathbf{x}d\mathbf{v}d\theta$ at time t on the ith slip system. It is to be noted that the $\mathbf{v}$ is orthogonal to $\mathbf{t}$; that is $\mathbf{v}=\mathbf{v}(\mathbf{t}(\theta))$. Hence, $\phi^{(i)}$ depends on θ both implicitly and explicitly.

The conventional field variables are now derived from the distributions $\phi^{(i)}$. The scalar dislocation line density in the crystal is defined as follows:

$$\varrho(\mathbf{x},t)=\sum_{i=1}^{N}\varrho^{(i)}(\mathbf{x},t),\quad \text{where}\quad \varrho^{(i)}(\mathbf{x},t)=\int_{\mathbf{v}}\int_{\theta}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}d\theta. \tag{1}$$

The contribution by dislocations on the ith slip system to the dislocation density tensor $\boldsymbol{\alpha}$ is given by

$$\boldsymbol{\alpha}^{(i)}(\mathbf{x},t)=\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}d\theta \tag{2}$$

and its time rate of change is

$$\dot{\boldsymbol{\alpha}}^{(i)}(\mathbf{x},t)=\frac{\partial\boldsymbol{\alpha}^{(i)}}{\partial t}=\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\dot{\phi}^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}d\theta;$$

$$\dot{\phi}^{(i)}=\frac{\partial\phi^{(i)}}{\partial t}. \tag{3}$$

The reader is refered to Refs. 37, 38, 42, and 43 for a summary of the tensor fields related to dislocations in a distorted crystal. The dislocation density tensor and its time rate of change are obtained as superposition of the partial density tensors and their time rates of change, respectively, that is

$$\boldsymbol{\alpha}(\mathbf{x},t)=\sum_{i=1}^{N}\boldsymbol{\alpha}^{(i)}(\mathbf{x},t),\quad\text{and}\quad\dot{\boldsymbol{\alpha}}(\mathbf{x},t)=\sum_{i=1}^{N}\dot{\boldsymbol{\alpha}}^{(i)}(\mathbf{x},t). \tag{4}$$

To perform the summations in Eq. (4) in three dimensions, the components of all partial density tensors must be referred to the same coordinate system.

The contribution to the dislocation flux tensor $\mathbf{J}$ by dislocations on a slip system is given by

$$\mathbf{J}^{(i)}(\mathbf{x},t)=\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\times\mathbf{v}\otimes\mathbf{b}^{(i)}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}d\theta$$
$$=\mathbf{n}^{(i)}\otimes\mathbf{b}^{(i)}\int_{\mathbf{v}}\int_{\theta}v\,\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}d\theta, \tag{5}$$

where v is the magnitude of $\mathbf{v}$, and $\mathbf{t}\times\mathbf{v}=v\,\mathbf{n}^{(i)}$. The flux tensor $\mathbf{J}^{(i)}$ is itself the rate of plastic distortion, $\dot{\boldsymbol{\beta}}^{P(i)}$, contributed by the ith slip system. The dislocation flux tensor, hence the rate of plastic distortion, is given by

$$\mathbf{J}(\mathbf{x},t)=\dot{\boldsymbol{\beta}}^{P}(\mathbf{x},t)=\sum_{i=1}^{N}\mathbf{J}^{(i)}(\mathbf{x},t). \tag{6}$$

For a given slip system, it is shown that the dislocation density tensor is given by the zeroth-velocity-first-angular moment of the distribution $\phi^{(i)}$, while the dislocation flux tensor is given by the first mixed moment, see Eqs. (3) and (5), respectively.

B. A system invariant

In dynamical simulations of discrete dislocation systems,[14] the evolution of the discrete dislocation system is determined by the changes in the position, number, velocity, direction, and length of the dislocation elements, or the generalized degress of freedom of the dislocation system and their time rate of change.[15] In a phase space, the system evolution is studied by investigating the set of distributions $\phi^{(i)};i=1,N$. In analogy with particle systems, see for example, Landau and Lifshitz[17] and Liboff,[18] one aims here at finding a set of kinetic equations which are satisfied by the distributions $\phi^{(i)}$. Zorski[19] formulated a problem which might be relevant; he considered a set of infinitesimal Somigliana defects.

In order to develop the kinetic equations, a fundamental invariant (or a conserved quantity) of the evolving dislocation system must be found. For a particle system, for example, the total number of particles in the system is invariant regardless of how the particles are distributed in the phase space. It is this fact which enables the derivation of kinetic equations in general, e.g., the plasma kinetic equation of Klimontovich or its collisionless version of Vlasov.[20,21]

Consider a large crystal of volume Ω which is bounded by the surface $\partial\Omega$ with unit normal $\mathbf{n}$. The condition of compatibility of the total distortion field in the crystal is written as: $\boldsymbol{\alpha}+\nabla\times\boldsymbol{\beta}^P=\mathbf{0}$, see Ref. 37. Upon integrating this condition over the entire volume, the following result is obtained

$$\mathcal{A}=\int_\Omega \boldsymbol{\alpha}\, d\Omega+\int_\Omega \nabla\times\boldsymbol{\beta}^P d\Omega=\mathbf{0}. \tag{7}$$

After lengthy algebraic manipulation, see the appendix, the second integral term can be cast in the form

$$\int_\Omega \nabla\times\boldsymbol{\beta}^P d\Omega$$

$$=\int_{-\infty}^{t} dt' \int_\theta d\theta \int_{\partial\Omega} \sum_{i=1}^{N} \mathbf{t}\otimes\mathbf{b}^{(i)}(\mathbf{n}\cdot\overline{\mathbf{v}})\,\varphi^{(i)}(\mathbf{x},\theta,t')\,dS, \tag{8}$$

in which $\overline{\mathbf{v}}\varphi^{(i)}(\mathbf{x},\theta,t')=\int_{\mathbf{v}}\mathbf{v}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t')\,d\mathbf{v}$. It is obvious that the integrand to the right-hand side of Eq. (8) is the sum of flux of $\boldsymbol{\alpha}$ at t' contributed by dislocations of orientation $\mathbf{t}$ on all slip systems. The integral term itself can be viewed as the accumulation of slip traces at the surface. It can be written in the form $\int_{\partial\Omega}\boldsymbol{\alpha}^s dS$, where $\boldsymbol{\alpha}^s=\mathbf{n}\times\boldsymbol{\beta}^P$ is known as the surface dislocation density tensor, or the slip trace tensor.[22]

Geometrically, Eq. (7) implies that a finite crystal undergoing plastic distortion has two effective dislocations, a bulk dislocation given by the volume integral and a surface dislocation given by the surface integral. The latter arises due to slip trace formation on the surface. The two effective dislocations are always of equal and opposite strength, and can vanish only simultaneously. Bulk dislocations are sources of internal stress, are the carriers of plastic distortion, and as they move they change their line length and sense. Surface dislocations are merely slip traces, once formed they do not move relative to the crystal, their line sense is defined by the contour of the intersection of slip planes and the crystal surface, and they are not associated with the stress field.

It can be easily argued that for every finite, reasonably large volume of a crystal undergoing a *statistically homogeneous* plastic distortion, the two sides of Eq. (8) vanish. This also means that the mean curvature of the crystal volume under consideration vanishes, which is the case considered in the present formulation. The general case, however, is a systematic extension. Mathematically, then, we consider

$$\mathcal{A}=\int_\Omega \boldsymbol{\alpha}\, d\Omega=\mathbf{0}, \tag{9}$$

which is also a property of a system of closed dislocation network. Consequently,

$$\frac{d\mathcal{A}}{dt}=\frac{d}{dt}\int_\Omega \boldsymbol{\alpha}\, d\Omega=\mathbf{0}. \tag{10}$$

The result (7) can be viewed as *the principle of invariance of the total Burgers vector* of the crystal in the general case, where both bulk and surface dislocations contribute. However, when the mean curvature vanishes, it takes the form (9) or (10).

The result (10) is valid for every dislocation population having the same Burgers vector (e.g., those on colinear slip systems), provided that reactions involving various Burgers vectors are not allowed to occur. This can be visualized by considering the fact that, in the absence of reactions, dislocations of the same Burgers vector can exist in either closed loop (not necessarily planar) or line (ending on the surface) configurations. In reality, however, it is possible that two segments of different Burgers vectors react to produce a segment of a third Burgers vector. These reactions lead to the destruction and creation of scalar dislocation densities. The result (10) can thus be specialized for individual slip systems provided that tensorial balance terms representing reactions among various slip systems and cross slip are added. In other words, for the ith slip system one obtains

$$\frac{d}{dt}\int_\Omega \boldsymbol{\alpha}^{(i)} d\Omega=\int_\Omega \sum \mathbf{S}^{(i)} d\Omega;\quad i=1,N. \tag{11}$$

$\Sigma\mathbf{S}^{(i)}$ includes all possible tensorial sources, mainly those resulting from Burgers vector reactions and cross slip. The tensorial source due to cross slip, which represents transfer of screw dislocations between colinear systems, must be of opposite sign for the two involved systems. Therefore, this source can only appear at the slip system level. Also, due to the fact that annihilating species must be of the opposite sense, the sources associated with these reactions appear only at the level of individual slip systems. The same argument extends to sources associated with reactions leading to production of segments of new Burgers vector. In other words, if Eq. (11) is summed over all slip systems, the tensor source terms cancel each other, and the result (10) is recovered.

C. The evolution in the phase space

The result (11) is now combined with the phase-space representation of dislocation densities. A minor notation adjustment is made; $d\Omega$ will be replaced by $d\mathbf{x}$. The right-hand side of Eq. (11) can be written in the form

$$\frac{d}{dt}\int_{\mathbf{x}} \boldsymbol{\alpha}^{(i)}(\mathbf{x},t)\, d\mathbf{x}=\frac{d}{dt}\int_{\mathbf{x}}\int_{\mathbf{v}}\int_\theta \mathbf{t}\otimes\mathbf{b}^{(i)}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\, d\mathbf{x}d\mathbf{v}d\theta, \tag{12}$$

in which d/dt is the total time derivative operator. The right-hand side can be broken into two integrals as below

$$\int_{\mathbf{x}}\int_{\mathbf{v}}\int_\theta \frac{d\mathbf{t}}{dt}\otimes\mathbf{b}^{(i)}\phi^{(i)}\, d\mathbf{x}d\mathbf{v}d\theta+\int_{\mathbf{x}}\int_{\mathbf{v}}\int_\theta \mathbf{t}\otimes\mathbf{b}^{(i)}\frac{d\phi^{(i)}}{dt}\, d\mathbf{x}d\mathbf{v}d\theta, \tag{13}$$

where the arguments of $\phi^{(i)}$ are dropped for simplicity. In the case of a finite deformation, the operators d/dt and $\int_{\mathbf{x}}$ may commute only in a material or Lagrangian frame, which will be considered in a future development. As previously mentioned, only infinitesimal deformation is considered here. The first integral in Eq. (13) can be evaluated as follows. Define $\varphi(\theta)=\int_{\mathbf{v}}\phi^{(i)}(\mathbf{v},\theta)d\mathbf{v}$, therefore, $\int_{\mathbf{v}}\int_{\theta}(d\mathbf{t}/dt)\otimes\mathbf{b}^{(i)}\phi^{(i)}d\mathbf{v}d\theta$ reduces to $\int_{\theta}(d\mathbf{t}/dt)\otimes\mathbf{b}^{(i)}\varphi(\theta)d\theta$. Since $\mathbf{t}=\mathbf{t}(\theta)$, then $d\mathbf{t}/dt=\dot{\theta}(\partial\mathbf{t}/\partial\theta)$. In addition, by using $(\partial\mathbf{t}/\partial\theta)\varphi=\partial/\partial\theta(\mathbf{t}\varphi)-\mathbf{t}(\partial/\partial\theta)\varphi$, one finally obtains

$$\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\frac{d\mathbf{t}}{dt}\otimes\mathbf{b}^{(i)}\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta = -\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\dot{\theta}\frac{\partial\phi}{\partial\theta}^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta, \tag{14}$$

where $[\mathbf{t}\otimes\mathbf{b}^{(i)}\varphi(\theta)]_0^{2\pi}=0$ was substituted, and the definition of φ was reversed. The second integral in Eq. (13) is systematically found to be

$$\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\frac{d\phi^{(i)}}{dt}\,d\mathbf{x}d\mathbf{v}d\theta=\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_v+\dot{\theta}\frac{\partial}{\partial\theta}\right)\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta. \tag{15}$$

Substituting Eqs. (14) and (15) into Eq. (12), the latter simplifies to

$$\frac{d}{dt}\int_{\mathbf{x}}\boldsymbol{\alpha}^{(i)}(\mathbf{x},t)\,d\mathbf{x}=\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_v\right)\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta, \tag{16}$$

where the terms containing $\dot{\theta}(\partial/\partial\theta)$ cancel each other. The left-hand side of Eq. (12) can also be represented by a phase-space integral of scalar source functions

$$\int_{\mathbf{x}}\sum\mathbf{S}^{(i)}d\mathbf{x}=\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\sum S^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta. \tag{17}$$

By equating the right-hand sides of the last two equations and removing the integral signs, a partial differential equation for the distribution $\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)$ can be rewritten in the form

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_v\right)\phi^{(i)}=\sum S^{(i)};\quad i=1,N. \tag{18}$$

in which $\Sigma S^{(i)}$ is a superposition of all possible scalar sources contributing to the time rate of change of the distribution $\phi^{(i)}$. This set of equations will be subsequently called the *set of kinetic equations*.

The scalar dislocation densities can be created or destroyed by (1) annihilation reactions of elements of opposite sense, (2) cross slip of dislocations or annihilation via cross slip, (3) reactions between segments on two slip systems giving rise to a segment with a third different Burgers vector, and (4) multiplication. Annihilation of elements of opposite sense which have the same Burgers vector do not appear in a tensorial representation, since they cancel *a priori*. Cross slip and reactions involving different Burgers vectors result in nonvanishing tensorial contributions. Expressions for the scalar sources are given in Sec. II F.

D. The continuity equation for the dislocation density tensor

The continuity of the total dislocation density tensor $\boldsymbol{\alpha}$, see Refs. 38, 42, and 43, can be recovered in two steps; taking the zeroth-velocity-first-angular moment of the kinetic equation (18), then summing over all slip systems. Multiply Eq. (18) by $\mathbf{t}\otimes\mathbf{b}^{(i)}$ and integrate over the phase space,

$$\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_v\right)\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta = \int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\sum S^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta = \int_{\mathbf{x}}\sum\mathbf{S}^{(i)}d\mathbf{x}. \tag{19}$$

By definition, the integral over the phase space of $\mathbf{t}\otimes\mathbf{b}^{(i)}(\partial\phi/\partial t)^{(i)}$ yields $\dot{\boldsymbol{\alpha}}^{(i)}$; see Eq. (3). In order to manipulate the second term to the left-hand side of Eq. (19), the following identities are used: $\mathbf{v}\cdot\nabla\phi^{(i)}=\nabla\cdot(\mathbf{v}\phi^{(i)})-(\nabla\cdot\mathbf{v})\phi^{(i)}$; $\nabla\cdot\mathbf{v}=0$ since $\mathbf{x}$ and $\mathbf{v}$ are independent phase space coordinates; $\boldsymbol{\nabla}\times[\mathbf{t}\times(\mathbf{v}\phi^{(i)})\otimes\mathbf{b}^{(i)}]=\mathbf{t}\otimes\mathbf{b}^{(i)}(\mathbf{v}\cdot\boldsymbol{\nabla}\phi^{(i)})-\mathbf{v}\otimes\mathbf{b}^{(i)}(\mathbf{t}\cdot\boldsymbol{\nabla}\phi^{(i)})$; $\mathbf{t}\cdot\boldsymbol{\nabla}\phi^{(i)}=\boldsymbol{\nabla}\cdot(\mathbf{t}\phi^{(i)})-\phi^{(i)}\boldsymbol{\nabla}\cdot\mathbf{t}=0$; $\boldsymbol{\nabla}\cdot\mathbf{t}=0$, and since dislocation lines are continuous $\boldsymbol{\nabla}\cdot(\mathbf{t}\phi^{(i)})=0$. With this in mind, the second integral term becomes

$$\int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\mathbf{t}\otimes\mathbf{b}^{(i)}\mathbf{v}\cdot\boldsymbol{\nabla}\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta = \int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\boldsymbol{\nabla}\times\mathbf{t}\times\mathbf{v}\otimes\mathbf{b}^{(i)}\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta = \int_{\mathbf{x}}\int_{\mathbf{v}}\int_{\theta}\boldsymbol{\nabla}\times v\,\mathbf{n}^{(i)}\otimes\mathbf{b}^{(i)}\phi^{(i)}\,d\mathbf{x}d\mathbf{v}d\theta = \int_{\mathbf{x}}\boldsymbol{\nabla}\times\mathbf{J}^{(i)}\,d\mathbf{x}. \tag{20}$$

It can be easily verified that the third integral term to the left-hand side of Eq. (19) vanishes identically. To show this, first use $\dot{\mathbf{v}}\cdot\nabla_v\phi^{(i)}=\nabla_v\cdot(\dot{\mathbf{v}}\phi^{(i)})$. Then, $\mathbf{t}\otimes\mathbf{b}^{(i)}\int_{\mathbf{v}}\nabla_v\cdot(\dot{\mathbf{v}}\phi^{(i)})d\mathbf{v} = \mathbf{t}\otimes\mathbf{b}^{(i)}\nabla_v\cdot\int_{\mathbf{v}}(\dot{\mathbf{v}}\phi^{(i)})d\mathbf{v}=\mathbf{t}\otimes\mathbf{b}^{(i)}\nabla_v\cdot(\langle\dot{\mathbf{v}}\rangle\varphi^{(i)}(\theta))=0$, where $\varphi^{(i)}(\theta)=\int_{\mathbf{v}}\phi^{(i)}d\mathbf{v}$. Equation (19) therefore simplifies to

$$\int_{\mathbf{x}}\left(\frac{\partial\boldsymbol{\alpha}}{\partial t}^{(i)}+\nabla\times\mathbf{J}^{(i)}\right)d\mathbf{x}=\int_{\mathbf{x}}\mathbf{S}^{(i)}d\mathbf{x}, \tag{21}$$

for some arbitrary crystal volume. Upon summing over all slip systems, the source terms cancel. Furthermore, by localization one obtains

$$\frac{\partial\boldsymbol{\alpha}}{\partial t}+\boldsymbol{\nabla}\times\mathbf{J}=\mathbf{0}, \tag{22}$$

as predicted by the classic theory of dislocation fields. Equation (22) shows that the local density tensor can only change due to the motion of dislocations regardless of the dislocation reactions. Aifantis[7] argues that to derive the macroscopic balance law (22), various dislocation reactions must not be allowed. Mescheryakov and Prockuratova[13] have reported a nonvanishing right-hand side for the continuity condition (22). Anthony and Azirhi[23] made the same suggestion for the case of generation or annihilation reaction, see their Eq. (66). We remark here, without proof, that the right-hand side of Eq. (22) must remain zero, i.e., the only way of introducing additional contribution to the net Burgers vector contained by a Burgers circuit (fixed onto the crystal) is via motion of dislocation into this circuit.

E. Driving force and the dislocation equation of motion

Glide of dislocations is determined by the externally imposed stress, lattice resistance, short-range reactions, and the long-range stress. The intrinsic lattice resistance includes the Peierls resistance and electron and phonon drag. In body-centered-cubic (bcc) crystals, the Peierls barrier is significant and exhibits strong temperature dependence. In face-centered-cubic (fcc) crystals, the Peierls barrier gives rise to a small resistance to the dislocation motion. Jogs and energy radiation also result in dragging forces. For a review of these topics, the reader is referred to Refs. 24–26. Here only the drag mechanism is mentioned, which is relevant to fcc crystals. For a test dislocation line of velocity $\mathbf{v}$ and line direction $\mathbf{t}$, the induced drag force $\mathbf{f}_{d\mathbf{t}}$ is given by

$$\mathbf{f}_{d\mathbf{t}} = -B\mathbf{v} = -Bv\boldsymbol{\xi}, \tag{23}$$

where B is a drag coefficient and $\boldsymbol{\xi} = \boldsymbol{\xi}(\theta) = \mathbf{v}/v = \mathbf{n}^{(i)} \times \mathbf{t}$ is a unit vector along the direction of motion.

The long-range stress field of dislocations $\tilde{\boldsymbol{\sigma}}$ is strongly fluctuating since dislocations are discrete stress sources, and it can be approximated by a stochastic (fluctuating) component which accounts for the dislocation-dislocation correlation $\boldsymbol{\sigma}^f$, superimposed on a slowly varying (mean-field) component determined by the dislocation density tensor $\boldsymbol{\sigma}^\alpha$, that is $\tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^f + \boldsymbol{\sigma}^\alpha$. This superposition has been previously justified by other authors.[27–29] Here, a simplified argument is used to reveal the origin of the stochastic long-range field within the present framework.

A discrete dislocation system can be viewed as a set of lines each of which is a sequence of small segments gliding at discrete velocities $\mathbf{V}_k = \mathbf{V}_k(t)$, centered at discrete locations $\mathbf{X}_k = \mathbf{X}_k(t)$ and having line orientation described by the angle $\Theta_k = \Theta_k(t)$ in the phase space $(\mathbf{x}, \mathbf{v}, \theta)$. Hence, the phase-space distributions corresponding to a discrete dislocation system has the form $\tilde{\phi}^{(i)}(\mathbf{x}, \mathbf{v}, \theta, t) = \varrho^{(i)} \Sigma_k \delta(\mathbf{x} - \mathbf{X}_k)\,\delta(\mathbf{v} - \mathbf{V}_k)\,\delta(\theta - \Theta_k)$, where $\varrho^{(i)}$ can be regarded as a time-dependent normalization factor. These phase-space distributions must individually satisfy divergence conditions of the form $\boldsymbol{\nabla} \cdot [\mathbf{t}(\theta)\tilde{\phi}^{(i)}] = 0$. Obviously, in this representation, the summation must be replaced by a product operation if the spatial dislocation-dislocation correlation is to be effected, as was suggested by Kröner[11] (spatial correlations are not considered here). Following the procedure explained in Sec. II B, the following kinetic equation is obtained for the nonsmooth function $\tilde{\phi}^{(i)}(\mathbf{x}, \mathbf{v}, \theta, t)$

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \tilde{\dot{\mathbf{v}}} \cdot \nabla_v\right) \tilde{\phi}^{(i)} = \sum S^{(i)}; \quad i = 1, N, \tag{24}$$

in which the acceleration $\tilde{\dot{\mathbf{v}}}$ is also a nonsmooth function. By splitting $\tilde{\phi}^{(i)}$ into its mean (smooth) value $\phi^{(i)}$ plus a fluctuating term $\delta\phi^{(i)}$, similarly, writing $\tilde{\dot{\mathbf{v}}} = \dot{\mathbf{v}} + \delta\dot{\mathbf{v}}$ and carrying out ensemble averaging, Eq. (24) can be rewritten in the form

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \dot{\mathbf{v}} \cdot \nabla_v\right) \phi^{(i)} + \langle \delta\dot{\mathbf{v}} \cdot \nabla_v \delta\phi^{(i)} \rangle = \sum S^{(i)}; \quad i = 1, N. \tag{25}$$

If the dynamics of the system is such that $\tilde{\phi}^{(i)}$ remains close to $\phi^{(i)}$ at all times, the quantity $\langle \delta\dot{\mathbf{v}} \cdot \nabla_v \delta\phi^{(i)} \rangle$ should identically vanish for a large volume. In the classical kinetic theory, this quantity gives rise to the so-called collision term. It can be easily shown that the fluctuating stress field $\boldsymbol{\sigma}^f$ is determined by the fluctuations $\delta\phi^{(i)}$. Again, $\langle \boldsymbol{\sigma}^f \rangle$ vanishes for a large volume if $\tilde{\phi}^{(i)}$ remains close to $\phi^{(i)}$.

Upon ignoring the internal stress fluctuations, the glide force per unit length of the dislocation line $\mathbf{f}_{g\mathbf{t}}^{(i)}$ is given by the celebrated Peach-Koehler formula

$$\mathbf{f}_{g\mathbf{t}}^{(i)} = (\mathbf{b}^{(i)} \cdot [\boldsymbol{\sigma}^\circ + \boldsymbol{\sigma}^\alpha] \cdot \mathbf{n}^{(i)})\,\boldsymbol{\xi}, \tag{26}$$

in which $\boldsymbol{\sigma}^\circ$ is the applied stress field. A complete form of the equation of motion for a dislocation line can then be written as follows:

$$\mathbf{f}_{g\mathbf{t}}^{(i)} - B\mathbf{v} - \mathrm{sgn}(\mathbf{f}_{g\mathbf{t}}^{(i)}) f_P \boldsymbol{\xi} + \boldsymbol{\Gamma} = \boldsymbol{\Phi}(\dot{\mathbf{v}}, \mathbf{v}, \boldsymbol{\gamma}), \tag{27}$$

in which $\boldsymbol{\Phi}(\dot{\mathbf{v}}, \mathbf{v}, \boldsymbol{\gamma})$ is a vector function of its arguments, $\boldsymbol{\Gamma}$ is a stochastic force field associated with $\boldsymbol{\sigma}^f$, and $\boldsymbol{\gamma}$ denotes any other parameters on which the acceleration of dislocation lines might depend. Inverting the last equation for the acceleration

$$\dot{\mathbf{v}} = \boldsymbol{\Psi}(\mathbf{f}_{g\mathbf{t}}^{(i)}, \mathbf{v}, f_P, \boldsymbol{\Gamma}, \boldsymbol{\gamma}), \tag{28}$$

which provides the connection between the lattice stress field, applied plus long-range, and evolution of the distrubutions $\phi^{(i)}$ described by the kinetic equations (18).

F. Scalar source terms

To demonstrate how various contributions to the source term to the right-hand side of equation (18) are formulated, the primary slip systems in an fcc crystal are considered. The notation of Schmid and Boas[30] is used here, see also Francoisi and Zaoui.[31] The slip planes $(\bar{1}11), (111), (\overline{11}1), (1\bar{1}1)$ are labeled A, B, C, and D, and the slip directions $[011], [0\overline{11}], [101], [\bar{1}01], [\bar{1}10], [110]$ are labeled 1, 2, 3, 4, 5, and 6, respectively. The 12 slip systems are A2, A3, A6, B2, B4, B5, C1, C3, C5, D1, D4, D6. Slip systems sharing the same Burgers vector are called *colinear*, and those sharing the same slip plane are called *coplanar*. Therefore, in fcc crystals, there are six pairs of colinear systems, and four triplets of coplanar systems.

Throughout this subsection, the source terms will be subscripted by the initial letters of the process they represent. A constant R, with this subscript, along with a probability (cross-section-like) functions are used as proportionality coefficients. These coefficients can be obtained by modeling the behavior of individual dislocations. Hirth and Lothe[32] give a detailed account of dislocation-dislocation reaction at short range. Due to the size of this paper, only the mathematical form of reaction rate terms is shown, and formulas for these rate coefficients are kept for a future publication.

Cross slip: Cross slip is a process by which a screw dislocation changes its glide plane. According to Devincre,[33] the probability rate for cross slip, per unit length of a single screw dislocation, is given by $p_{cs}e^{-Q(\tau)/k_BT}$, where p_{cs} is a normalization factor, $Q(\tau)$ is an activation energy which is a function of the resolved shear stress τ on the cross slip plane, k_B is the Boltzmann constant, and T is the absolute temperature. With a phase-space representation of the dislocation species, cross slip from the ith to the jth slip system gives rise to the source term

$$S_{cs}^{(i)}(\mathbf{v},\theta)=-R_{cs}e^{-Q(\tau^{(j)})/k_BT}\delta(\theta-\theta_{cs})\phi^{(i)}(\mathbf{v},\theta_{cs}), \tag{29}$$

where $\delta(\theta)$ is the Dirac delta distribution. The angle θ_{cs} defines the line sense for cross slip; that is $\mathbf{t}(\theta)\cdot\mathbf{b}^{(i)}=\pm1$, which is satisfied by two values of θ. On the jth slip system, the source term is also localized at the cross slip angle. It is given by

$$S_{cs}^{(j)}(\mathbf{v},\theta)=R_{cs}e^{-Q(\tau^{(j)})/k_BT}\delta(\theta-\theta_{cs}) \times\int_{\mathbf{v}'}f(\mathbf{v},\mathbf{v}')\phi^{(i)}(\mathbf{v}',\theta_{cs})\,d\mathbf{v}', \tag{30}$$

in which $f(\mathbf{v},\mathbf{v}')$ refers to the probability that a cross-slipped element has velocity $\mathbf{v}$, and the integration over $\mathbf{v}'$ takes into account all cross slipping dislocation elements. Thus, cross slip results in linear coupling of the set of equations (18). Satisfaction of a cross slip criterion can be imposed for cross slip to occur from a particular slip system to another; see Ref. 33.

Annihilation reactions: Two dislocation elements can annihilate each other if they have the opposite sense and the same Burgers vector. Dislocations on colinear (cross slip) systems annihilate if they are of screw character. If glide is to control this process, the two annihilating elements must move on their respective planes until they coincide with the line of intersection of these planes. In reality, cross slip can expedite the annihilation process. An annihilation rate term due to cross slip can be formulated as follows:

$$S_{acs}^{(i)}(\mathbf{v},\theta)=-R_{acs}\delta(\theta-\theta_{cs})\phi^{(i)}(\mathbf{v},\theta_{cs})\int_{\mathbf{v}'}\phi^{(j)}(\mathbf{v}',\theta_{cs})d\mathbf{v}'. \tag{31}$$

The expression remains the same if the superscripts (i) and (j) are switched. The line sense of the annihilating dislocations is determined by $\mathbf{t}(\theta_{cs}^{(i)})\cdot\mathbf{t}(\theta_{cs}^{(j)})=-1$. It is also clear that $\mathbf{t}(\theta_{cs}^{(i)}+\pi)\cdot\mathbf{t}(\theta_{cs}^{(j)}+\pi)=-1$.

Dislocation elements of the same Burgers vector which share the same glide plane annihilate by glide for all values of θ. A rate term representing this process can be cast in the form

$$S_{agl}^{(i)}(\mathbf{v},\theta)=-R_{agl}\phi^{(i)}(\mathbf{v},\theta)\int_{\mathbf{v}'}\phi^{(i)}(\mathbf{v}',\theta+\pi)d\mathbf{v}', \tag{32}$$

where the velocity integral has been previously explained. Dislocations on parallel glide planes can also annihilate if they are of pure edge or screw character, two edge elements can annihilate by climb, and two screw elements can annihilate by cross slip. For edge-type dislocation elements, the climb annihilation rate is

$$S_{acl}^{(i)}(\mathbf{v},\theta)=-R_{acl}\delta(\theta-\theta_{cl})\phi^{(i)}(\mathbf{v},\theta_{cl}) \times\int_{\mathbf{v}'}\phi^{(i)}(\mathbf{v}',\theta_{cl}+\pi)d\mathbf{v}'. \tag{33}$$

Within the same slip system, the cross-slip-assisted annihilation of screw dislocations is expressed by a rate term of the form

$$S_{acs}^{(i)}(\mathbf{v},\theta)=-R_{acs}\delta(\theta-\theta_{cs})\phi^{(i)}(\mathbf{v},\theta_{cs}) \times\int_{\mathbf{v}'}\phi^{(i)}(\mathbf{v}',\theta_{cs}+\pi)d\mathbf{v}'. \tag{34}$$

Reactions forming glissile segments: Based on experimental observations, dislocations in a deformed crystal form three-dimensional networks. In such networks, the intersections are in the form of junctions of variable length. Moreover, the junction can be either sessile or glissile. A detailed list of possible reactions in fcc crystals, determined by using the linear elasticity theory, was developed by Hirth.[34]

In fcc crystals, see Schmid and Boas notation above, (B2,B4)→B5, (B2,B5)→B4, and (B4,B5)→B2 are possible glissile-junction-forming reactions. However, for these reactions to occur, the reacting segments must be aligned in such a way that these reactions are *energetically* favorable. Ideally speaking, two parallel segments are in the most favorable configuration, but small deviations from this situation may not influence the outcome. Denote by the superscripts (i) and (j) the reacting species and by the superscript (k) the product species. For every orientation on the ith species, let Θ_{gj}^{j} be the range of orientation of dislocations on jth slip system within which glissile junction reactions with ith slip system is possible. Source terms associated with this reaction are represented as follows. For the kth slip system,

$$S_{gj}^{(k)}(\mathbf{v},\theta)=R_{gj}p(\theta)\int_{\Theta_{gj}^{i},\Theta_{gj}^{j}}d\theta'd\theta'' \times\int_{\mathbf{v}'}\int_{\mathbf{v}''}g\,\phi^{(i)}(\mathbf{v}',\theta')\phi^{(j)}(\mathbf{v}'',\theta'')d\mathbf{v}'d\mathbf{v}'', \tag{35}$$

in which $p(\theta)$ defines the orientation of the resulting segment and $g=g(\mathbf{v},\mathbf{v}',\mathbf{v}'')$ is a measure of the probability that the reaction product comes out with velocity $\mathbf{v}$. For the ith and jth slip systems,

$$S_{gj}^{(i)}(\mathbf{v},\theta)=-R_{gj}\phi^{(i)}(\mathbf{v},\theta)\int_{\Theta_{gj}^{j}}\int_{\mathbf{v}'}\phi^{(j)}(\mathbf{v}',\theta')d\mathbf{v}'d\theta'$$

$$S_{gj}^{(j)}(\mathbf{v},\theta)=-R_{gj}\phi^{(j)}(\mathbf{v},\theta)\int_{\Theta_{gj}^{i}}\int_{\mathbf{v}'}\phi^{(i)}(\mathbf{v}',\theta')d\mathbf{v}'d\theta'. \tag{36}$$

Noncoplanar systems such as pairs (B5,A2) and (B4,A2) can also interact in a similar fashion to produce glissile segments. It is also possible that the product segment dissociates, which can be easily accounted for.

It is important to notice that annihilation or glissile-junction-forming reactions yield binary collision source terms, leading to quadratic coupling of the system of kinetic equations (18). These reactions lead to destruction of the reacting species as opposed to just a change in velocity.

Sessile junctions: Dislocation on slip system pairs such as (B5,A3) can form locks, a form of sessile junction, which can be destroyed if the stress acting on a junction arm exceeds a certain value. The formation of locks reduces the velocities of the reacting species to zero without annihilating them. If the ith and jth species form sessile junctions, the source term can be written as follows:

$$S_{sj}^{(i)}(\mathbf{v},\theta)=-R_{sj}\phi^{(i)}(\mathbf{v},\theta)\int_{\Theta_{sj}^{j}}\int_{\mathbf{v}'}\phi^{(j)}(\mathbf{v}',\theta')d\mathbf{v}'d\theta' + R_{sj}\kappa\delta(\mathbf{v})\phi^{(i)}(\mathbf{v},\theta)\int_{\Theta_{sj}^{j}}\int_{\mathbf{v}'}\phi^{(j)}(\mathbf{v}',\theta')d\mathbf{v}'d\theta', \tag{37}$$

in which κ is an adjustible coefficient and Θ_{sj}^{j} is the orientation range within which a sessile junction formation is possible. The first term to the right-hand side of equation (37) expresses reduction at all other velocities, and the second expresses the density increase at $\mathbf{v}=\mathbf{0}$, notice $\delta(\mathbf{v})$. A similar term can be written for the jth slip system.

Multiplication: At small strains, which is the case considered here, the increase in the scalar dislocation density occurs mainly due to operation of Frank-Read sources. The density of these sources is essentially proportional to the amount of strain or the area swept by gliding dislocations.[35] A multiplication source term can be written in the form

$$S_{m}^{(i)}(\mathbf{v},\theta)=R_{m}q(\mathbf{v})\int_{\mathbf{v}'}\int_{\theta}v'\phi^{(i)}(\mathbf{v}',\theta')d\mathbf{v}'d\theta', \tag{38}$$

in which the function $q(\mathbf{v})$ determines the velocity distribution of the source. This source term is considered here to be isotropic with respect to θ. In a bcc crystal deforming at low temperature, the Frank-Read source is anisotropic, leading to forming more screw dislocation lines than edge-type lines. This anisotropy can be easily accounted for using a simple geometric argument.

G. The kinetic equations

In the system (18), the dependence on the angular variable θ is both implicit and explicit. In the left-hand side, no partial derivatives with respect to θ appear, but $\mathbf{v}$ and $\dot{\mathbf{v}}$ depend on θ. The source terms (29) through (38) bring in the angular dependence explicitly. In particular, the terms (35), (36), (37), and (38) involve integrals with respect to θ. The system (18) is thus an integro-differential equation system.

The final form of the system of kinetic equations (18) is expressed as follows:

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\mathbf{\Psi}\cdot\nabla_{v}\right)\phi^{(i)}=\Upsilon^{(i)}(\boldsymbol{\phi});\quad i=1,N, \tag{39}$$

in which $\boldsymbol{\phi}$ is the set of phase-space distributions, and $\mathbf{\Upsilon}^{(i)}(\boldsymbol{\phi})$ is a functional of $\phi^{(i)}$ and the subset of $\boldsymbol{\phi}$ contributing to its source, and the expression (28) for the acceleration has been used. The set of kinetic equations (39) is nonlinear since the driving force for dislocation motion is a functional of all phase-space distributions. Further detailed investigation is needed to determine the functional $\mathbf{\Phi}$ (or $\mathbf{\Psi}$) and the stochastic force term $\mathbf{\Gamma}$.

III. A SPECIAL CASE

The excercise presented in this section shows how macroscopic transport equations can be derived from the kinetic equations developed in Sec. II. A formal treatment of the three-dimensional case will be published in the future.

Aiming at investigating the effect of the long-range nature and the spatial angular dependence of the interaction force between dislocations, Groma[36] used some statistical physics concepts to develop a model of a system of parallel edge dislocations in a single slip configuration. In doing so, he focused on the spatial correlation between dislocations, up to the two-dislocation correlation, without consideration of velocity dependence. In this section, the final results of his model are recovered as a special case.

A Cartesian frame with basis $(\mathbf{e}_x,\mathbf{e}_y,\mathbf{e}_z)$ is considered. The slip plane is the $zx-$plane, with normal $\mathbf{n}=\mathbf{e}_y$. The Burgers vector is $\mathbf{b}=b\mathbf{e}_x$. Two groups of edge-type dislocations extending along the z axis with line vectors $\mathbf{t}_1=\mathbf{e}_z$ and $\mathbf{t}_2=-\mathbf{e}_z$ are considered. Dislocations are assumed to be randomly distributed in the xy plane. In this case, the only available distribution function $\phi(\mathbf{x},\mathbf{v},\theta,t)$ and its source $S(\mathbf{x},\mathbf{v},\theta,t)$ are written as follows:

$$\phi(\mathbf{x},\mathbf{v},\theta,t)=\phi_1(\mathbf{x},\mathbf{v},t)\delta(\theta-\pi/2)+\phi_2(\mathbf{x},\mathbf{v},t)\delta(\theta-3\pi/2),$$
$$S(\mathbf{x},\mathbf{v},\theta,t)=S_1(\mathbf{x},\mathbf{v},t)\delta(\theta-\pi/2)+S_2(\mathbf{x},\mathbf{v},t)\delta(\theta-3\pi/2), \tag{40}$$

indicating two distributions and two sources localized on the angular coordinate. In this representation θ is measured clockwise, relative to the x axis, in the slip plane when viewed downward the y axis. The kinetic equation system (18) reduces to

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_{v}\right)\phi(\mathbf{x},\mathbf{v},\theta,t)=S(\mathbf{x},\mathbf{v},\theta,t). \tag{41}$$

The governing equations for the two distributions ϕ_1 and ϕ_2, in terms of their respective sources S_1 and S_2, can be developed by integrating equation (41) with respect to θ twice over arbitrary intervals enclosing $\theta=\pi/2$ and $\theta=3\pi/2$, and using the filtering property of the Dirac delta function. This leads to separation of the two populations. The governing equations are found to be

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_{v}\right)\phi_1(\mathbf{x},\mathbf{v},t)=S_1(\mathbf{x},\mathbf{v},t),$$

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\dot{\mathbf{v}}\cdot\nabla_v\right)\phi_2(\mathbf{x},\mathbf{v},t)=S_2(\mathbf{x},\mathbf{v},t). \tag{42}$$

Multiplying the above two equations by $d\mathbf{v}$ and integrating with respect to $\mathbf{v}$, we arrive at

$$\frac{\partial \varrho_1(\mathbf{x},t)}{\partial t}+\nabla\cdot(\overline{\mathbf{v}_1}\varrho_1(\mathbf{x},t))=g_1(\mathbf{x},t),$$

$$\frac{\partial \varrho_2(\mathbf{x},t)}{\partial t}+\nabla\cdot(\overline{\mathbf{v}_2}\varrho_2(\mathbf{x},t))=g_2(\mathbf{x},t), \tag{43}$$

where $\varrho_i(\mathbf{x},t)=\int_{\mathbf{v}}\phi_i(\mathbf{x},\mathbf{v},t)d\mathbf{v}$, $g_i(\mathbf{x},t)=\int_{\mathbf{v}}S_i(\mathbf{x},\mathbf{v},t)d\mathbf{v}$, and $\overline{\mathbf{v}_i}(\mathbf{x},t)=\int_{\mathbf{v}}\mathbf{v}\phi_i(\mathbf{x},\mathbf{v},t)d\mathbf{v}/\int_{\mathbf{v}}\phi_i(\mathbf{x},\mathbf{v},t)d\mathbf{v}$; $i=1,2$. $\overline{\mathbf{v}_1}$ and $\overline{\mathbf{v}_2}$ are the mean velocities. A linear velocity law of the form (23) is used to bring the resolved shear stress (Peach-Koehler force) into the above equations. Furthermore, upon adding and subtracting the these two equations, the governing equations for the sum and difference are found to be

$$\frac{\partial \varrho(\mathbf{x},t)}{\partial t}+b\frac{\partial}{\partial x}(\tau(\mathbf{x},t)\zeta(\mathbf{x},t))=g_\varrho(\mathbf{x},t),$$

$$\frac{\partial \zeta(\mathbf{x},t)}{\partial t}+b\frac{\partial}{\partial x}(\tau(\mathbf{x},t)\varrho(\mathbf{x},t))=g_\zeta(\mathbf{x},t), \tag{44}$$

in which $\varrho=\varrho_1+\varrho_2$, $\zeta=\varrho_1-\varrho_2$, $g_\varrho=g_1+g_2$, $g_\zeta=g_1-g_2$, and the substitutions $\overline{\mathbf{v}_1}=v\mathbf{e}_x$, $\overline{\mathbf{v}_2}=-v\mathbf{e}_x$, $v=bB\tau$ were made. The time t is replaced by Bt, and only $\partial/\partial x$ is considered since the dislocation motion is restricted to be in the slip plane. The shear stress τ is given by $\tau=|\tau^\circ+\tau^\zeta|$; τ° is externally applied and τ^ζ is obtained in terms of the dislocation density tensor $\boldsymbol{\alpha}=(\varrho_1-\varrho_2)\mathbf{e}_z\otimes b\mathbf{e}_x=\zeta\mathbf{e}_z\otimes b\mathbf{e}_x$, see Eq. (2). As shown in Sec. II F, for the present special case, the source terms include annihilation via glide and climb and production. The set of equations (44), with an equation governing the long-range stress,[37] constitute the final set of equations of the model summarized in Ref. 36. The linear stability analysis conducted by Groma shows that if $dg_\varrho/d\varrho$ is positive, a homogeneous stationary solution is unstable and density perturbations grow, leading to pattern formation. By enforcing certain simplifications about the problem dimensionality and the characteristics of the dislocation system, other models such as those developed by Aifantis,[7,8] Walgraef and Aifantis,[9] and Kratochvil and co-workers[10] are readily recoverable as special cases.

IV. THE INITIAL-BOUNDARY-VALUE PROBLEM

A. The mechanical boundary conditions

The kinetic behavior of a dislocation system in a deforming crystal is analogous to the behavior of ion-electron plasmas. One important aspect of similarity is that, for both systems, the kinetic equations describing the evolution in the phase space must be complemented by another set of equations describing the long-range interactions and the background force field. In the case of a plasma, the kinetic equations are complemented by the famous set of Maxwell's equations in free space. In the case of dislocations, the lattice stress field is obtained by solving the stress equilibrium equations.

A crystal can be subjected to either stress or displacement boundary condition, or both (mixed). When stress boundary conditions are applied, the total stress field is computed as a superposition of the applied stress and the long-range stress. The former satisfies the applied boundary condition while the latter satisfies traction-free boundary condition. In satisfying a displacement boundary condition, however, both the elastic and plastic distortions must be combined to match the boundary displacement. Here, remarks are given on converting the displacement (or mixed) boundary value problem into a stress boundary value problem. The latter is then summarized in more detail in the following subsection.

Consider a crystal volume Ω with boundary $\partial\Omega$ which is subjected to a displacement $\mathbf{u}^b(\mathbf{x},t);\mathbf{x}\in\partial\Omega$ for all t. Hence, the surface displacement gradient $\nabla_s\mathbf{u}^b=\mathbf{n}\times\nabla\mathbf{u}^b$, with six independent components, is known. It can be easily shown that $\mathbf{n}\times\nabla\mathbf{u}^b=\mathbf{n}\times(\boldsymbol{\beta}^\circ+\delta\boldsymbol{\beta}+\delta\boldsymbol{\beta}^P)$, in which $\boldsymbol{\beta}^\circ$ is the elastic distortion associated with the boundary traction, and $\delta\boldsymbol{\beta}$ and $\delta\boldsymbol{\beta}^P$ are the changes in the elastic distortion due to dislocations and the plastic distortion, respectively, over time t. By using $\boldsymbol{\beta}^\circ=\mathbf{C}^{-1}:\boldsymbol{\sigma}^\circ$, one may write

$$\mathbf{n}\times\mathbf{C}^{-1}:\boldsymbol{\sigma}^\circ=\nabla_s\mathbf{u}^b-\mathbf{n}\times\delta\boldsymbol{\beta}-\mathbf{n}\times\delta\boldsymbol{\beta}^P;\quad \mathbf{x}\in\partial\Omega, \tag{45}$$

in which $\boldsymbol{\sigma}^\circ$ is the boundary value of the stress field equivalent to the traction needed to sustain the boundary displacement field $\mathbf{u}^b(\mathbf{x},t)$ in the presence of evolving dislocation field. The term $\mathbf{n}\times\delta\boldsymbol{\beta}$ is the accumulated change in the (nonintegrable) elastic surface displacement gradient, consistent with the long-range stress of dislocations, from the onset of loading to time t. It is dependent only on the initial and final states of the dislocation field. Similarly, $\mathbf{n}\times\delta\boldsymbol{\beta}^P$ is the accumulated change in the (nonintegrable) plastic surface gradient over the same period of time. It depends on the history of the dislocation flux at the boundary. From Eq. (45), the six given components of $\nabla_s\mathbf{u}^b$ can be used to determine the six components of $\boldsymbol{\sigma}^\circ$ or, rather, the equivalent boundary traction

$$\mathbf{t}^\circ=\mathbf{n}\cdot\boldsymbol{\sigma}^\circ. \tag{46}$$

In what follows the stress boundary value problem is stated and, for simplicity, the lattice inertia is ignored.

B. The dislocation-dynamics boundary value problem: Traction boundary condition

Upon loading, the crystal responds elastically until dislocations start to move somewhere in the crystal. However, unless the density of dislocations is nonzero, the local plastic distortion rate remains zero. Hence, for a nontrivial plastic disortion rate, the following conditions must be simultaneously satisfied:

$$\mathbf{f}_{g\mathbf{t}}>\mathbf{R}_\mathbf{t}\quad\text{and}\quad \phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)>0, \tag{47}$$

in which $\mathbf{R}_\mathbf{t}$ includes all resistive forces. It is obvious that if no dislocations are present, the stress alone cannot cause plasticity.

The applied stress boundary value problem. The applied stress field is the solution to the following boundary value problem:

$$\nabla\cdot\boldsymbol{\sigma}^\circ(\mathbf{x},t)=\mathbf{0};\quad \mathbf{x}\in\Omega\quad\text{for all}\quad t,$$

$$\mathbf{n}\cdot\boldsymbol{\sigma}^{\circ}(\mathbf{x},t)=\mathbf{t}^{\circ}(\mathbf{x},t);\quad \mathbf{x}\in\partial\Omega \quad \text{for all} \quad t, \tag{48}$$

where $\mathbf{t}^{\circ}(\mathbf{x},t)$ is the prescribed boundary traction.

The long-range stress boundary value problem. In a bounded crystal, the nonfluctuating component of the long-range stress field $\boldsymbol{\sigma}^{\alpha}$ is given by

$$\boldsymbol{\sigma}^{\alpha}=\boldsymbol{\sigma}^{s}+\boldsymbol{\sigma}^{i}, \tag{49}$$

where $\boldsymbol{\sigma}^{s}$ is the field of dislocations when Ω is embedded in an infinite medium, and $\boldsymbol{\sigma}^{i}$ is the image field. For an infinite crystal, the long-range stress field has only one component, $\boldsymbol{\sigma}^{s}$, which is generally nonvanishing prior to loading. The stress field $\boldsymbol{\sigma}^{s}$ is the solution to the following boundary value problem:

$$\nabla\cdot\boldsymbol{\sigma}^{s}(\mathbf{x},t)=\mathbf{0};\quad \mathbf{x}\in\Omega \quad \text{for all} \quad t$$

$$\boldsymbol{\sigma}^{s}(\mathbf{x},t)\to\mathbf{0};\quad \text{as} \quad |\mathbf{x}|\to\infty \quad \text{for all} \quad t,$$

$$\boldsymbol{\sigma}^{s}=\mathbf{C}:(\boldsymbol{\beta}^{s}-\boldsymbol{\beta}^{P}),\quad \boldsymbol{\beta}^{s}=\nabla\mathbf{u}^{s}, \tag{50}$$

in which $\boldsymbol{\beta}^{s}$ is the total distortion in the unloaded dislocated crystal, and $\mathbf{u}^{s}$ is a corresponding displacement field. It can be easily verified that the solution for $\boldsymbol{\sigma}^{s}$ depends only on the dislocation state in the crystal, i.e., on $\nabla\times\boldsymbol{\beta}^{P}$, but not on $\boldsymbol{\beta}^{P}$ itself.[38] When the crystal is finite the image field $\boldsymbol{\sigma}^{i}$ is needed to satisfy the traction-free boundary condition for the overall long-range stress field. This field is found by solving the boundary value problem

$$\nabla\cdot\boldsymbol{\sigma}^{i}(\mathbf{x},t)=\mathbf{0};\quad \mathbf{x}\in\Omega \quad \text{for all} \quad t,$$

$$\mathbf{n}\cdot\boldsymbol{\sigma}^{i}(\mathbf{x},t)=-\mathbf{n}\cdot\boldsymbol{\sigma}^{s}(\mathbf{x},t);\quad \mathbf{x}\in\partial\Omega \quad \text{for all} \quad t. \tag{51}$$

The image field $\boldsymbol{\sigma}^{i}$ is also dependent on the dislocation state in the crystal.

The dislocation field: kinetic equations. The evolving dislocation field satisfies the set of kinetic equations

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\boldsymbol{\Psi}\cdot\nabla_{v}\right)\phi^{(i)}=\Upsilon(\boldsymbol{\phi});\quad i=1,N. \tag{52}$$

The short-range interactions determine the functional $\boldsymbol{\Upsilon}(\boldsymbol{\phi})$, see Sec. IV F. Rules for cross slip, short-range interactions, and internal stress fluctuations (or stochastic force field) can be specified. As previously mentioned, the set (52) consists of nonlinearly coupled integrodifferential equations.

The dislocation field: equation of motion. The equation of motion

$$\mathbf{f}_{g\mathbf{t}}^{(i)}-B\mathbf{v}-\mathrm{sgn}(\mathbf{f}_{g\mathbf{t}}^{(i)})f_{P}\boldsymbol{\xi}+\boldsymbol{\Gamma}=\boldsymbol{\Phi}(\dot{\mathbf{v}},\mathbf{v},\boldsymbol{\gamma}), \tag{53}$$

couples the elastic stress field with the evolution of distributions $\phi^{(i)}$. Ignoring the crystal inertia, in a sense, implies that the dislocation acceleration may be ignored. Thus, the equation of motion (53) can be used to determine the velocity of dislocations in terms of the local mean force field. Also, the term $\dot{\mathbf{v}}\cdot\nabla_{v}\phi^{(i)}$ drops from the kinetic equation.

The dislocation field: initial and boundary conditions. Prior to loading, the initial dislocation system is under mechanical equilibrium, and the initial phase-space densities can be expressed as follows:

$$\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,0)=\delta(\mathbf{v})\varphi^{(i)}(\mathbf{x},\theta);\quad i=1,N. \tag{54}$$

Obviously, the distributions $\phi^{(i)}$ are periodic with respect to θ. For first-order partial differential equations of the form (52), boundary condition may or may not be specified. In a bounded crystal, if dislocation emission is not permitted at its surface, neither the flux nor scalar density of dislocation needs to be specified on the boundary. If the crystal space is a representative volume element of a large crystal undergoing statistically homogeneous plastic distortion, the inward dislocation flux must be specified.[22]

The plastic distortion and slip trace fields. The rate of plastic distortion is given by Eqs. (5) and (6). Its time integral,

$$\boldsymbol{\beta}^{P}=\int_{-\infty}^{t}\dot{\boldsymbol{\beta}}^{P}dt, \tag{55}$$

is needed to determine the boundary traction, see Eqs. (45) and (46), the long-range stress field, see Eqs. (50) and (51), and the intensity of slip trace formation on the surface, $\boldsymbol{\alpha}^{s}=\mathbf{n}\times\boldsymbol{\beta}^{P}$.

V. DISCUSSION

A kinetic framework for the evolution of the dislocation density and plastic distortion fields in a single crystal is formulated. The formulation is based on two aspects of the dislocation system, the statistics and dynamics, which generally suffice to apply the statistical mechanics concepts. Dislocations are viewed as reacting-diffusing-multiplying species in an otherwise linear elastic crystal, which is consistent with the notion of multiple natural configurations introduced and elaborated in Refs. 39–41. This notion is also implied in computer simulation models.[14,15] The integral of the dislocation density tensor over the crystal volume is found to be a conserved quantity. From the invariance of this integral, the set of kinetic equations governing the evolution of the phase-space distributions is derived. The kinetic equations are strongly nonlinear. This nonlinearity arises in two ways, through the quadratic reaction terms and through the dependence of the long-range stress field (driving force for motion) on the overall dislocation density in the crystal. The plastic distortion, defining the irreversible plastic strain and lattice rotation, is readily determined from the transport of the dislocations in the crystal, Eqs. (5) and (6).

The kinetic formulation presented here represents an important step in developing further theoretical formulations for the problem of crystal plasticity. For example, similar to the development of fluid models of plasmas or the Navier-Stokes equations of fluids, a systematic development of the macroscopic transport equations should lead to defining the properties of single crystals which are relevant to plastic deformation. These properties will appear naturally as coefficients in the macroscopic transport equations and can be conveniently computed via numerical treatment of the kinetic equations, for example, by a lattice Boltzmann or a kinetic Monte Carlo technique. The transport properties normally embody the characteristic length and time scales for the spatiotemporal evolution of the dislocation field in the crystal.

Certain aspects of the role of plastic strain gradients in crystal plasticity may also be investigated through the kinetic treatment presented here. A single dislocation line represents the gradient of plastic distortion in its immediate neighborhood. Hence, integrals of the form $\varphi^{(i)}=\int_{\mathbf{v}}\phi^{(i)}d\mathbf{v}$ are angularly dependent shear strain gradients on various crystal slip systems. In a macroscopic transport framework, the Orowan's equation for the shear strain rate on a particular slip system becomes $\dot{\gamma}^{(i)}(\mathbf{x},t)=b^{(i)}\int_{\theta}\overline{v}\,\varphi^{(i)}(\mathbf{x},\theta,t)\,d\theta$, in which $\overline{v}=\overline{v}(\theta)$ is the mean glide velocity at orientation θ. This representation asserts that the rate of plastic distortion is linearly depedent on the shear strain gradient.

Other theoretical developments can be made possible if the present formulation is extended to deal with finite deformation cases. Under such situations, the difference between the Eulerian (spatial) and Lagrangian (material) form of the kinetic equations will become significant and the deformation kinematics must be introduced into the formulation. Also, at high dislocation densities, it will be required to account for the dislocation-dislocation correlations in order to capture the effects of dislocation multipoles. Some of these issues are currently under investigation.

ACKNOWLEDGMENTS

The work was performed as part of internal research and development at the Pacific Northwest National Laboratory, operated by Battelle for the U. S. Department of Energy. The financial support received from Lawrence Livermore National Laboratory under Grant No. B339033 at the University of California, Los Angeles is also acknowledged. The discussions with Ladislas Kubin, Michael Zaiser, John Gilman, Greg Schenter, John Jaffe, James Belak, K.R. Rajagopal, Arun Sirinivasa, Janet Jones-Oliveira, and Joseph Oliveira are greatly appreciated. The author would also like to thank Ladislas Kubin, Michael Glazov, Ekkehart Kröner, Michael Zaiser, Istvan Groma, and Jan Kratochvil for reviewing this work and providing valuable comments.

APPENDIX

Referring to Eqs. (5) and (6), the rate of the plastic distortion can be rewritten in the form

$$\dot{\boldsymbol{\beta}}^{P}=\sum_{i=1}^{N}\int_{\theta}\mathbf{t}\times\overline{\mathbf{v}}\otimes\mathbf{b}^{(i)}\varphi^{(i)}(\mathbf{x},\theta,t)\,d\theta, \tag{A1}$$

where $\overline{\mathbf{v}}$ is the mean velocity at orientation θ which is defined by

$$\overline{\mathbf{v}}=\frac{\int_{\mathbf{v}}\mathbf{v}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}}{\int_{\mathbf{v}}\phi^{(i)}(\mathbf{x},\mathbf{v},\theta,t)\,d\mathbf{v}}. \tag{A2}$$

In the right-hand side of Eq. (A2), the denominator is itself $\varphi^{(i)}(\mathbf{x},\theta,t)$. By taking the curl of Eq. (A1) and integrating over the volume, one obtains

$$\int_{\Omega}\nabla\times\dot{\boldsymbol{\beta}}^{P}(\mathbf{x},t)\,d\Omega=\int_{\Omega}d\Omega\sum_{i=1}^{N}\int_{\theta}\nabla\times\mathbf{j}^{(i)}(\mathbf{x},\theta,t)\,d\theta, \tag{A3}$$

in which the partial flux tensor $\mathbf{j}^{(i)}$ is defined by $\mathbf{t}\times(\overline{\mathbf{v}}\varphi^{(i)})\otimes\mathbf{b}^{(i)}$. The following identity can be easily verified:

$$\begin{aligned}\nabla\times\mathbf{j}^{(i)}&=\nabla\times[\mathbf{t}\times(\overline{\mathbf{v}}\varphi^{(i)})\otimes\mathbf{b}^{(i)}]\\&=(\mathbf{t}\otimes\mathbf{b}^{(i)})(\boldsymbol{\xi}\cdot\nabla(\overline{v}\,\varphi^{(i)}))-(\boldsymbol{\xi}\otimes\mathbf{b}^{(i)})(\mathbf{t}\cdot\nabla(\overline{v}\,\varphi^{(i)})),\end{aligned} \tag{A4}$$

where $\boldsymbol{\xi}$ is a unit vector along $\overline{\mathbf{v}}$, that is $\overline{\mathbf{v}}=\overline{v}\,\boldsymbol{\xi}$. After using the following identities:

$$\boldsymbol{\xi}\cdot\nabla(\overline{v}\,\varphi^{(i)})=\frac{\partial(\overline{v}\,\varphi^{(i)})}{\partial\boldsymbol{\xi}},$$

$$\boldsymbol{\xi}\cdot\nabla(\overline{v}\,\varphi^{(i)})=\nabla\cdot(\boldsymbol{\xi}\overline{v}\,\varphi^{(i)})-(\overline{v}\,\varphi^{(i)})\nabla\cdot\boldsymbol{\xi}=\nabla\cdot(\boldsymbol{\xi}\overline{v}\,\varphi^{(i)}),$$

$$\nabla\cdot\boldsymbol{\xi}=0,$$

$$\nabla\cdot(\boldsymbol{\xi}\overline{v}\,\varphi^{(i)})=\frac{\partial(\overline{v}\,\varphi^{(i)})}{\partial\boldsymbol{\xi}}+\frac{\partial(\overline{v}\,\varphi^{(i)})}{\partial\mathbf{t}}+\frac{\partial(\overline{v}\,\varphi^{(i)})}{\partial\mathbf{n}^{(i)}},$$

$$\frac{\partial(\overline{v}\,\varphi^{(i)})}{\partial\mathbf{t}}=0=\mathbf{t}\cdot\nabla(\overline{v}\,\varphi^{(i)}),\quad(\text{no flux along }\mathbf{t}),$$

$$\frac{\partial(\overline{v}\,\varphi^{(i)})}{\partial\mathbf{n}^{(i)}}=0,\quad(\text{no climb flux}). \tag{A5}$$

$\boldsymbol{\nabla}\times\mathbf{j}^{(i)}$ reduces to $\boldsymbol{\nabla}\cdot(\overline{\mathbf{v}}\varphi^{(i)})\mathbf{t}\otimes\mathbf{b}^{(i)}$. In the above, $(\mathbf{t},\boldsymbol{\xi},\mathbf{n}^{(i)})$ form a right-handed orthogonal set of unit vectors. Equation (A3) can be recast in the form

$$\int_{\Omega}\nabla\times\dot{\boldsymbol{\beta}}^{P}(\mathbf{x},t)\,d\Omega=\int_{\Omega}d\Omega\sum_{i=1}^{N}\int_{\theta}\nabla\cdot(\overline{\mathbf{v}}\varphi^{(i)}(\mathbf{x},\theta,t))\mathbf{t}\otimes\mathbf{b}^{(i)}d\theta. \tag{A6}$$

By integrating with respect to time and applying the Gauss theorem, Eq. (A6) can be rewritten as follows:

$$\int_{\Omega}\nabla\times\boldsymbol{\beta}^{P}d\Omega=\int_{-\infty}^{t}dt'\int_{\theta}d\theta\int_{\partial\Omega}\sum_{i=1}^{N}\mathbf{t}\otimes\mathbf{b}^{(i)}(\mathbf{n}\cdot\overline{\mathbf{v}})\varphi^{(i)}(\mathbf{x},\theta,t')\,dS, \tag{A7}$$

which is Eq. (8) of Sec. II B.

*FAX: (509)372-4725. Electronic address: Anter.El-Azab@pnl.gov

[1] L.P. Kubin, in *Stability of Materials*, Vol. 355 of *NATO Advanced Study Institute, Series B: Physics*, edited by A. Gonis, P. Turchi, and J. Kudrnovsky (Plenum, New York, 1996), p. 99.

[2] L.P. Kubin, in *Materials Science and Technology, A Comprehensive Treatment, Vol. 6: Plastic Deformation and Fracture of Materials*, edited by Hael Mughrabi (VCH, Verlagsgesellschaft, 1993), p. 137.

[3] David L. Holt, J. Appl. Phys. **41**, 3197 (1970).

[4] D. Kuhlmann-Wilsdorf, Scr. Metall. Mater. **27**, 951 (1992).

[5] D. Kuhlmann-Wilsdorf, Mater. Sci. Eng., A **113**, 1 (1989).

[6] D. Kuhlmann-Wilsdorf, Philos. Mag. A **79**, 955 (1999).

[7] E. Aifantis, Int. J. Plast. **3**, 211 (1987).

[8] E. Aifantis, Int. J. Eng. Sci. **33**, 2161 (1995).

[9] D. Walgraef and E. Aifantis, J. Appl. Phys. **58**, 688 (1985).

[10] A. Franek, R. Kalus, and J. Kratochvil, Philos. Mag. A **64**, 491 (1991).

[11] E. Kröner, in *Inelastic Behavior of Solids*, edited by M.F. Kanninen, W.F. Adler, A.R. Rosenberg, and R.I. Jaffee (McGraw-Hill, New York, 1969), p. 137.

[12] R.B. Stout, Cryst. Lattice Defects **9**, 47 (1980).

[13] Yu I. Mescheryakov and E.I. Prockuratova, Int. J. Solids Struct. **32**, 1711 (1995).

[14] L.P. Kubin, G. Canova, M. Condat, B. Devincre, V. Pontikis, and Y. Bréchet, in *Non-Linear Phenomena in Materials Science II, Solid State Phenomena, Vol. 23* & *24*, edited by G. Martin and L. Kubin (Trans Tech Publications, Vaduz, Liechtenstein, 1992), p. 455.

[15] N.M. Ghoniem, S. Tong, and L. Sun, Phys. Rev. B **61**, 913 (2000).

[16] L.P. Kubin, B. Devincre, and M. Tang, J. Comput.-Aided Mater. Des. **5**, 31 (1998).

[17] L.D. Landau and E.M. Lifshitz, *Statistical Physics, Part 1*, 3rd ed. (Pergamon, New York, 1980).

[18] R.L. Liboff, *Kinetic Theory: Classical, Quantum and Relativistic Descriptions* (Prentice-Hall, Englewood Cliffs, NJ, 1990).

[19] H. Zorski, Int. J. Solids Struct. **4**, 959 (1968).

[20] D.R. Nicholson, *Introduction to Plasma Theory* (Wiley, New York, 1983).

[21] Nicholas A. Krall and Alvin W. Trivelpiece, *Principles of Plasma Physics* (McGraw-Hill, New York, 1973).

[22] A. El-Azab, Modell. Simul. Mater. Sci. Eng. **8**, 37 (2000).

[23] K.-H. Anthony and A. Azirhi, Int. J. Eng. Sci. **33**, 2137 (1995).

[24] F.R.N. Nabarro, *Theory of Crystal Dislocations* (Dover, New York, 1987).

[25] V.L. Indenbom and J. Lothe, *Elastic Strain Fields and Dislocation Mobility* (North-Holland, Amsterdam, 1992).

[26] T. Suzuki, S. Takeuchi, and H. Yoshinaga, *Dislocation Dynamics and Plasticity* (Springer-Verlag, Berlin, 1991).

[27] B. Bakó and I. Groma, Modell. Simul. Mater. Sci. Eng. **7**, 181 (1999).

[28] I. Groma and B. Bakó, Phys. Rev. B **58**, 2969 (1998).

[29] P. Hähner, in *Continuum Models and Discrete Systems*, edited by K. Z. Markov (World Scientific, Singapore, 1996), p. 514.

[30] R. Schmid and I.W. Boas, *Plasticity of Crystals* (Chapman & Hall, London, 1968).

[31] P. Francoisi and A. Zaoui, Acta Metall. **30**, 1627 (1982).

[32] John Price Hirth and Jens Lothe, *Theory of Dislocations* (Wiley, New York, 1982).

[33] B. Devincre, in *Computer Simulation in Materials Science*, edited by H.O. Kirchner, L.P. Kubin, and V. Pontikis (Kluwer, Dordrecht, 1996), p. 309.

[34] J.P. Hirth, J. Appl. Phys. **32**, 700 (1961).

[35] L.P. Kubin (private communication).

[36] I. Groma and B. Bakó, Phys. Rev. B **56**, 5807 (1997).

[37] Ekkehart Kröner, in *Physics of Defects* (North-Holland, Amsterdam, 1981), p. 217.

[38] Toshio Mura, *Micromechanics of Defects in solids* (Martinus Nijhoff, Dordrecht, 1987).

[39] Carl Eckart, Phys. Rev. **73**, 373 (1948).

[40] K.R. Rajagopal and A.R. Srinivasa, Int. J. Plast. **14**, 945 (1998).

[41] K.R. Rajagopal and A.R. Srinivasa, Int. J. Plast. **14**, 969 (1998).

[42] E. Kossecka and R. de Wit, Arch. Mech. **29**, 633 (1977).

[43] A.M. Kosevich, in *Dislocations in Solids, Volume 1*, edited by F.R.N. Nabarro (North-Holland, Amsterdam, 1979), p. 33.