University of Groningen

Statistical approach to dislocation dynamics

Limkumnerd, Surachate; van der Giessen, Erik

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Link to publication in University of Groningen/UMCG research database

Statistical approach to dislocation dynamics: From dislocation correlations to a multiple-slip continuum theory of plasticity

Surachate Limkumnerd[*]

Department of Physics, Faculty of Science, Chulalongkorn University, Phayathai Road, Patumwan, Bangkok 10300, Thailand

Erik Van der Giessen[†]

Zernike Institute for Advanced Materials, Nijenborgh 4, University of Groningen, 9747 AG Groningen, The Netherlands
(Received 26 October 2007; revised manuscript received 27 March 2008; published 14 May 2008)

Due to recent successes of a statistical-based nonlocal continuum crystal plasticity theory for single-glide in explaining various aspects such as dislocation patterning and size-dependent plasticity, several attempts have been made to extend the theory to describe crystals with multiple-slip systems using *ad hoc* assumptions. We present here a mesoscale continuum theory of plasticity for multiple-slip systems of parallel edge dislocations. We begin by constructing the Bogolyubov–Born–Green–Yvon–Kirkwood integral equations relating different orders of dislocation correlation functions in a grand canonical ensemble. Approximate pair correlation functions are obtained for single-slip systems with two types of dislocations and, subsequently, for general multiple-slip systems of both charges. The effect of the correlations manifests itself in the form of an entropic force in addition to the external stress and the self-consistent internal stress. Comparisons with a previous multiple-slip theory based on phenomenological considerations shall be discussed.

I. INTRODUCTION

Statistical mechanics provides an optimal framework and various tools for studying emergent phenomena from a complex conglomerate of bodies—may they be molecules of gases, polymer chains of rubber, or crystalline defects. The use of correlation functions in analyzing two-dimensional solids and their defects has been proven very successful in the past. For example, Mermin[1] showed that the two-dimensional crystals do not have conventional long-range order, but can have "directional long-range order." Nelson and co-worker[2,3] applied the technique to explain dislocation-assisted melting in two dimensions. Over a decade ago, Groma[4] proposed a theory to describe dislocations and their motions using distribution functions and probability arguments. Unlike the existing continuum theories at the time,[5] the formalism was physically motivated and it correctly incorporated the long-range nature of dislocation interactions. Several variations of this work—all of which reduce to the same two-dimensional theory—also exist for three-dimensional dislocation systems.[6–9]

Although having laid out the foundation for possible interactions of many-dislocation configurations, Groma's pioneering work did not investigate these correlated effects in detail. Zaiser *et al.*[10] explicitly considered the evolution of dislocation correlations by extending Groma's theory for systems of single-slip, parallel edge dislocations. They were able to qualitatively obtain the correct scaling behavior of the evolution equations for both single and pair correlation densities and explained some general properties of these functions. Their formulation, however, was limited to only one active slip system and the analytical forms of pair correlation functions were not derived. In a later work, Groma *et al.*[11] included the influence of dislocation correlations in the form of a local back stress. Yefimov *et al.*[12,13] connected this statistical description to a continuum crystal plasticity theory

and applied this to various boundary value problems. While the theory successfully captured most features observed in discrete dislocation simulations, its *ad hoc* extension to multiple-slip systems failed to explain the size effects in single-crystal thin films.[14] The main goals of this paper are (1) to correctly describe and obtain analytical expressions for dislocation pair correlations and (2) to systematically generalize the approach of Groma *et al.* to multiple-slip systems.

We begin in Sec. II by introducing ensembles of dislocations and deriving the partition function for multiple-slip systems. The nth-order dislocation densities and dislocation correlation functions are subsequently defined. We construct the Bogolyubov–Born–Green–Yvon–Kirkwood (BBGYK) integral equations in Sec. III. These equations link correlation functions of order n to those of order $n+1$ (a technique generally used in the study of dense gases and fluids). The integral equations are expanded in powers of interaction strength (the ratio between the interaction energy and "thermal" energy). We then obtain a set of approximate integral equations for pair ($n=2$) correlation functions after applying a closure approximation to truncate the series. These equations are valid regardless of the form of the interaction potential, and thus are applicable to other systems, provided that this pair interaction vanishes at a large distance.

By appealing to the Peach–Koehler interaction, analytical expressions for pair dislocation densities for single- and multiple-slip systems are derived in Secs. IV and V, respectively. Our single-slip solution agrees with the result from the study of induced geometrically necessary dislocations (GNDs) in terms of a single pinned dislocation by means of a variational approach.[15,16] The dislocation spacing $1/\sqrt{\rho}$ emerges as a natural length scale in this formulation in accordance with the scaling study by Zaiser *et al.*[10] Our analysis further shows long-range attractive correlations when more than one slip system are present, confirming the absence of dislocation patterning in single-glide systems as ob-

served in many discrete dislocation simulations[17–24] and explained in a recent three-dimensional continuum plasticity theory.[7,8]

In Sec. VI, we write down the transport equations for both total dislocation densities and GND densities on each slip system under the influence of the Peach–Koehler forces from both single and pair dislocation correlations. While the former gives a self-consistent, long-range internal stress contribution, the latter exerts an additional short-range, entropic force due to a deviation away from a preferred dislocation arrangement in the form of a back stress. The formulation is a direct extension of the work by Groma co-workers[10,11] for crystals with one active slip system. Using the knowledge of the pair correlation functions, we obtain a complete description of the back stress as a function of slip orientations—something that has not been achieved in the Groma–Zaiser approach but which had been previously incorporated in the multiple-slip theory using the *ad hoc* phenomenological considerations.[14,25]

Finally in Sec. VII, we contrast our theory with the multiple-slip theory of Yefimov and Van der Giessen.[14,25] While both theories propose that interactions among slip systems solely depend on relative angles of slip orientations, the functional forms are different. We attribute the failure of the earlier theory in explaining size effects in single-crystal thin films partly to this difference and partly to the treatment of dislocation nucleation in the theory.

II. DEFINITIONS OF THE BASIC QUANTITIES

Let us first consider the equation of motion of a dislocation, which drifts along its glide plane (taken for simplicity to be along the $\hat{x}$ direction) subject to the Peach–Koehler force $f(x,y) = -\partial_x u(x,y)$ generated by another dislocation at the origin and to random fluctuations in the form of the Gaussian white noise[26] $\xi(t)$ (also along $\hat{x}$) where $\langle \xi(t_1)\xi(t_2)\rangle = \delta(t_1 - t_2)$,

$$\dot{\vec{r}}(x,y,t) = \hat{x}[f(x,y) + \sqrt{2T}\xi(t)]. \qquad (1)$$

The form of the fluctuation amplitude $\sqrt{2T}$ is given afterward by the fluctuation-dissipation theorem. Thus, T in this theory is not physical temperature but a parameter measuring the amplitude of random fluctuations. The stationary state solution of the corresponding one-dimensional Smoluchowski equation,

$$\frac{\partial P_1}{\partial t} = \frac{\partial}{\partial x}\left[\left(f + T\frac{\partial}{\partial x}\right)P_1\right], \qquad (2)$$

which describes that the probability $P_1(\vec{r})$ of finding a dislocation at $\vec{r}$ can be described by the Boltzmann distribution $P_1 \sim e^{(-u/T)}$.

To generalize the above concept to a many-dislocation system, consider an arrangement of r species of dislocations and denote the coordinate of the ith dislocation of species s by $\vec{i}_s$. The dislocation configuration $\{\mathbf{N}\}$ is the set of the coordinates of all dislocations, where $\mathbf{N} \equiv (N_1, N_2; N_3, N_4; \dots; N_{r-1}, N_r)$ denotes the "collection" of dislocations of type s. In this convention, odd and even slots,

respectively, contain plus and minus dislocations on distinct slip systems.[27] We introduce the notation $\{\mathbf{N}+1_s\}$ to denote the addition of an extra dislocation of species s to $\{\mathbf{N}\}$, while similarly, a configuration $\{\mathbf{N}\}$ with coordinates of $\mathbf{n}$ removed is indicated by $\{\mathbf{N}-\mathbf{n}\}$.

The interacting Hamiltonian $U_\mathbf{N}$ of the system can be written as the sum of potentials $u(\vec{i}_{s_1}, \vec{j}_{s_2})$ of all pairs of dislocations,

$$U_\mathbf{N}(\{\mathbf{N}\}) = \sum_{s_1 \leq s_2} \sum_{i \leq j} u(\vec{i}_{s_1}, \vec{j}_{s_2}). \qquad (3)$$

We can define a canonical partition function of configuration $\mathbf{N}$ by

$$\mathcal{Z}_\mathbf{N} \equiv \int e^{-U_\mathbf{N}/T} d\{\mathbf{N}\}, \qquad (4)$$

where the integrations are taken over the "volume" measure $d\{\mathbf{N}\} \equiv \prod_{s=1}^r d^2\vec{1}_s d^2\vec{2}_s \cdots d^2\vec{N}_s$ of the dislocation configuration at $\{\mathbf{N}\}$. Consider the coordinates of a particular set $\{\mathbf{n}\}$, the probability of observing the configuration $\mathbf{n}$ in $d\{\mathbf{n}\}$ about the points in $\{\mathbf{n}\}$ irrespective of the remaining collection $\mathbf{N}-\mathbf{n}$ is

$$P_\mathbf{N}^{(\mathbf{n})}(\{\mathbf{n}\})d\{\mathbf{n}\} = \frac{d\{\mathbf{n}\}}{\mathcal{Z}_\mathbf{N}} \int e^{-U_\mathbf{N}(\{\mathbf{N}\})/T} d\{\mathbf{N}-\mathbf{n}\}, \qquad (5)$$

where $\int P_\mathbf{N}^{(\mathbf{n})}(\{\mathbf{n}\})d\{\mathbf{n}\} = 1$. The probability density of observing *any* statistically equivalent possible collection $\mathbf{n}$ within the volumes $d\{\mathbf{n}\}$ about the points $\{\mathbf{n}\}$ is therefore

$$\rho_\mathbf{N}^{(\mathbf{n})}(\{\mathbf{n}\}) = \prod_{s=1}^r \frac{N_s!}{(N_s - n_s)!} P_\mathbf{N}^{(\mathbf{n})}(\{\mathbf{n}\}). \qquad (6)$$

Consider now an *open* system (which could be realized, say, by allowing for nucleation and annihilation of dislocations as the system relaxes); a grand canonical partition function is given by

$$\Xi = \sum_{\mathbf{N} \geq 0} \prod_{s=1}^r \frac{z_s^{N_s}}{N_s!} \mathcal{Z}_\mathbf{N}, \qquad (7)$$

where z_s is the activity of species s. The prefactor arises from integrating away the momentum degrees of freedom in the Hamiltonian, which are irrelevant to this problem. The probability $\mathcal{P}$ of the occurrence of configuration $\mathbf{N}$ in the open system is therefore

$$\mathcal{P}_\mathbf{N} = \prod_{s=1}^r \frac{z_s^{N_s}}{N_s!} \frac{\mathcal{Z}_\mathbf{N}}{\Xi}. \qquad (8)$$

Finally, the probability density of observing any n_1 dislocations of species 1, n_2 dislocations of species 2, etc., (any collection $\mathbf{n}$) in $d\{\mathbf{n}\}$ at $\{\mathbf{n}\}$ is

$$\rho^{(\mathbf{n})}(\{\mathbf{n}\}) = \sum_{\mathbf{N} \geq \mathbf{n}} \mathcal{P}_\mathbf{N} \rho_\mathbf{N}^{(\mathbf{n})}(\{\mathbf{n}\}). \qquad (9)$$

The summation is taken over all collections $\mathbf{N}$ greater than or

equal to **n**, i.e., for all $N_1 \geq n_1$, $N_2 \geq n_2$, etc. We take Eq. (9) as the *definition* of dislocation density of order (**n**). Explicitly, we have

$$\rho^{(\mathbf{n})}(\{\mathbf{n}\}) = \frac{1}{\Xi} \sum_{\mathbf{N} \geq \mathbf{n}} \left[\prod_{s=1}^{r} \frac{z_s^{N_s}}{(N_s - n_s)!} \right] \int e^{-U_{\mathbf{N}}(\{\mathbf{N}\})/T} d\{\mathbf{N} - \mathbf{n}\}. \tag{10}$$

This definition of an (**n**)th-order dislocation density is equivalent to the ones used by Groma[4] and Zaiser[10] in the realization of an open system.[28] Finally, we define the (**n**)th-order correlation function $g^{(\mathbf{n})}(\{\mathbf{n}\})$ through

$$\rho^{(\mathbf{n})}(\{\mathbf{n}\}) = \left[\prod_{s=1}^{r} \rho^{(1)}(\vec{1}_s)\rho^{(1)}(\vec{2}_s) \cdots \rho^{(1)}(\vec{n}_s) \right] g^{(\mathbf{n})}(\{\mathbf{n}\}). \tag{11}$$

III. DERIVATION OF THE BOGOLYUBOV–BORN–GREEN–YVON–KIRKWOOD INTEGRAL EQUATIONS

The Bogolyubov–Born–Green–Yvon–Kirkwood integral equations first appeared in the study of classical fluids with a total potential energy given by the sum of pair interactions.[29–32] They provided a set of relations between distribution functions of fluid density at different orders. Here, we extend the BBGYK formalism to include the noncentral interactions of dislocations in a multicomponent system.[33,34] We proceed in three steps: (1) take a derivative of the (**n**)th-order dislocation density with respect to the glide direction of one particle of the interested species; (2) express the result in terms of the next higher order densities; and (3) convert the integral equations of densities into those of correlation functions.

Differentiating $\rho^{(\mathbf{n})}(\{\mathbf{n}\})$ as expressed in Eq. (10) with respect to the glide direction of dislocation 1 of species 1 located, we find

$$\nabla_{\vec{1}_1} \rho^{(\mathbf{n})}(\{\mathbf{n}\}) = -\frac{1}{\Xi} \sum_{\mathbf{N} \geq \mathbf{n}} \left[\prod_{s=1}^{r} \frac{z_s^{N_s}}{(N_s - n_s)!} \right]$$
$$\times \int e^{-\bar{U}_{\mathbf{N}}(\{\mathbf{N}\})} \nabla_{\vec{1}_1} \bar{U}_{\mathbf{N}}(\{\mathbf{N}\}) d\{\mathbf{N} - \mathbf{n}\}, \tag{12}$$

where we absorb $1/T$ into the definition $\bar{U}_{\mathbf{N}} \equiv U_{\mathbf{N}}/T$. The derivative of the potential can be separated into two parts:

$$\nabla_{\vec{1}_1} \bar{U}_{\mathbf{N}} = \sum_{s=1}^{r} \sum_{\substack{i=1 \\ (i,s) \neq (1,1)}}^{n_s} \nabla_{\vec{1}_1} \bar{u}(\vec{1}_1, \vec{i}_s) + \sum_{s=1}^{r} \sum_{i=n_s+1}^{N_s} \nabla_{\vec{1}_1} \bar{u}(\vec{1}_1, \vec{i}_s). \tag{13}$$

Direct substitution of Eq. (13) into the integrand of Eq. (12) splits the expression into two integrals I_1 and I_2. Notice in the first integral that the derivative of the potential does not depend on coordinates $\{\mathbf{N} - \mathbf{n}\}$ and thus can be taken out of the integral, which yields

$$I_1 = -\rho^{(\mathbf{n})}(\{\mathbf{n}\}) \sum_{s=1}^{r} \sum_{\substack{i=1 \\ (i,s) \neq (1,1)}}^{n_s} \nabla_{\vec{1}_1} \bar{u}(\vec{1}_1 - \vec{i}_s), \tag{14}$$

with the aid of Eq. (10). The second integral I_2 requires a little more work,

$$I_2 = -\frac{1}{\Xi} \sum_{s=1}^{r} \sum_{\mathbf{N} \geq \mathbf{n}} \left[\prod_{s'=1}^{r} \frac{z_{s'}^{N_{s'}}}{(N_{s'} - n_{s'})!} \right] \int \sum_{i=n_s+1}^{N_s} \nabla_{\vec{1}_1} \bar{u}(\vec{1}_1, \vec{i}_s)$$
$$\times e^{-\bar{U}_{\mathbf{N}}(\{\mathbf{N}\})} d\{\mathbf{N} - \mathbf{n}\}. \tag{15}$$

The expression involves integrating $\vec{i}_s$ over the sample size. Since each integral over $\vec{i}_s$ between $n_s + 1 \leq i \leq N_s$ is equivalent in infinite space, the summation therefore gives a factor of $(N_s - n_s)$. The remaining integrals over all other dislocation coordinates are unaffected.

Equation (15) thus becomes

$$I_2 = -\sum_{s=1}^{r} \frac{1}{\Xi} \sum_{\mathbf{N} \geq \mathbf{n}} \left[\prod_{s'=1}^{r} \frac{z_{s'}^{N_{s'}}}{(N_{s'} - n_{s'})!} \right] (N_s - n_s) \int \nabla_{\vec{1}_1} \bar{u}[\vec{1}_1, \overrightarrow{(n_s+1)}_s] \{ \int e^{-\bar{U}_{\mathbf{N}}(\{\mathbf{N}\})} d[\{\mathbf{N} - \mathbf{n}\} \setminus \{\overrightarrow{(n_s+1)}_s\}] \} d^2 \overrightarrow{(n_s+1)}_s$$

$$= -\sum_{s=1}^{r} \int \nabla_{\vec{1}_1} \bar{u}[\vec{1}_1, \overrightarrow{(n_s+1)}_s] \left\{ \frac{1}{\Xi} \sum_{\mathbf{N} \geq \mathbf{n}} \left[\prod_{s'=1}^{r} \frac{z_{s'}^{N_{s'}}(N_s - n_s)}{(N_{s'} - n_{s'})!} \right] \int e^{-\bar{U}_{\mathbf{N}}(\{\mathbf{N}\})} d[\{\mathbf{N} - \mathbf{n}\} \setminus \{\overrightarrow{(n_s+1)}_s\}] \right\} d^2 \overrightarrow{(n_s+1)}_s$$

$$= -\sum_{s=1}^{r} \int \nabla_{\vec{1}_1} \bar{u}[\vec{1}_1, \overrightarrow{(n_s+1)}_s] \rho^{(\mathbf{n}+1_s)}(\{\mathbf{n}+1_s\}) d^2 \overrightarrow{(n_s+1)}_s. \tag{16}$$

The symbol $d[\{\mathbf{N} - \mathbf{n}\} \setminus \{\overrightarrow{(n_s+1)}_s\}]$ represents the volume measure of $\{\mathbf{N} - \mathbf{n}\}$ *without* $d^2 \overrightarrow{(n_s+1)}_s$. Collecting both I_1 and I_2 from Eq. (14) and Eq. (16), we arrive at the BBGYK equations for the (**n**)th-order dislocation density,

$$\vec{\nabla}_{\vec{1}_1}\rho^{(\mathbf{n})}(\{\mathbf{n}\}) = -\rho^{(\mathbf{n})}(\{\mathbf{n}\}) \sum_{(s,i)\neq(1,1)}^{(r,n_s)} \vec{\nabla}_{\vec{1}_1}\vec{u}(\vec{1}_1,\vec{i}_s)$$

$$-\sum_{s=1}^{r} \int \vec{\nabla}_{\vec{1}_1}\vec{u}[\vec{1}_1,\overrightarrow{(n_s+1)}_s]\rho^{(\mathbf{n}+1_s)}$$

$$\times(\{\mathbf{n}+1_s\})d^2\overrightarrow{(n_s+1)}_s. \qquad (17)$$

One can obtain a series of integrodifferential equations for the correlation functions $g^{(\mathbf{n})}$ from Eq. (17) by expanding out $\rho^{(\mathbf{n})}(\{\mathbf{n}\})$ using Eq. (11). All but two of the single-dislocation densities on the left-hand side (LHS) and right-hand side (RHS) of the equality cancel, which results in

$$\vec{\nabla}_{\vec{1}_1}[\rho(\vec{1}_1)g^{(\mathbf{n})}(\{\mathbf{n}\})] = -\rho(\vec{1}_1)g^{(\mathbf{n})}(\{\mathbf{n}\}) \sum_{(s,i)\neq(1,1)}^{(r,n_s)} \vec{\nabla}_{\vec{1}_1}\vec{u}(\vec{1}_1,\vec{i}_s)$$

$$-\rho(\vec{1}_1)\sum_{s=1}^{r} \int \vec{\nabla}_{\vec{1}_1}\vec{u}[\vec{1}_1,\overrightarrow{(n_s+1)}_s]\rho$$

$$\times[\overrightarrow{(n_s+1)}_s]g^{(\mathbf{n}+1_s)}(\{\mathbf{n}+1_s\})d^2\overrightarrow{(n_s+1)}_s. \qquad (18)$$

The first-order densities $\rho(\vec{1})$ that plague the expression can be removed by first using the product rule to the LHS, then dividing both sides by $\rho(\vec{1})$. The LHS becomes

$$\text{LHS} = \vec{\nabla}_{\vec{1}_1}g^{(\mathbf{n})}(\{\mathbf{n}\}) + g^{(\mathbf{n})}(\{\mathbf{n}\})\frac{\vec{\nabla}_{\vec{1}_1}\rho(\vec{1}_1)}{\rho(\vec{1}_1)}.$$

The ratio of the derivative of the first-order density with itself can be rewritten using Eq. (17) specialized to first order, which gives

$$\frac{\vec{\nabla}_{\vec{1}_1}\rho(\vec{1}_1)}{\rho(\vec{1}_1)} = -\sum_{s=1}^{r} \int \vec{\nabla}_{\vec{1}_1}\vec{u}(\vec{1}_1,\vec{\zeta}_s)\rho(\vec{\zeta}_s)g^{(2)}(\vec{1}_1,\vec{\zeta}_s)d^2\vec{\zeta}_s,$$

where $\vec{\zeta}_s \equiv \overrightarrow{(n_s+1)}_s$ is the position of the (n_s+1)th dislocation of species s and $g^{(2)}(\vec{1}_1,\vec{\zeta}_s)$ represents the pair correlation function between the first dislocation of species 1 at $\vec{1}_1$ and the (n_s+1)th dislocation of species s at $\vec{\zeta}_s$. This expression could be seamlessly incorporated into the right-hand side of Eq. (18). The final result is[35]

$$\vec{\nabla}_{\vec{1}_1}g^{(\mathbf{n})}(\{\mathbf{n}\}) = -g^{(\mathbf{n})}(\{\mathbf{n}\}) \sum_{(s,i)\neq(1,1)}^{(r,n_s)} \vec{\nabla}_{\vec{1}_1}\vec{u}(\vec{1}_1,\vec{i}_s)$$

$$-\sum_{s=1}^{r} \int \vec{\nabla}_{\vec{1}_1}\vec{u}(\vec{1}_1,\vec{\zeta}_s)\rho(\vec{\zeta}_s)[g^{(\mathbf{n}+1_s)}(\{\mathbf{n}+1_s\}) - g^{(\mathbf{n})}$$

$$\times(\{\mathbf{n}\})g^{(2)}(\vec{1}_1,\vec{\zeta}_s)]d^2\vec{\zeta}_s. \qquad (19)$$

For the remainder of this paper, we shall restrict our attention to the Peach–Koehler interaction. Recall that the interaction energy between two parallel edge dislocations of length L (over energy T due to random forces) in an infinite medium is[36]

$$\vec{u}(\vec{i}_s,\vec{j}_{s'}) = -\Gamma\psi(\vec{i}_s,\vec{j}_{s'}), \qquad (20)$$

where $\Gamma \equiv \frac{\mu b^2 L}{2\pi(1-\nu)T}$, and

$$\psi(\vec{i}_s,\vec{j}_{s'}) \equiv \begin{cases} (\hat{m}_{\vec{i}_s}\cdot\hat{m}_{\vec{j}_{s'}})\ln(|\vec{i}_s-\vec{j}_{s'}|) \\[2mm] +\dfrac{[\hat{m}_{\vec{i}_s}\cdot(\vec{i}_s-\vec{j}_{s'})][\hat{m}_{\vec{j}_{s'}}\cdot(\vec{i}_s-\vec{j}_{s'})]}{|\vec{i}_s-\vec{j}_{s'}|^2} \end{cases}. \qquad (21)$$

Here, $\hat{m}_{\vec{i}_s}$ denotes the slip-plane normal of species s. The relative strength Γ represents the ratio between dislocation interaction energy versus energy from random fluctuation due to noise. Note that the latter originates from the use of the Boltzmann distribution in Eq. (4) to describe the equilibrium configuration of systems with noise. As the dislocation configuration becomes more and more correlated, Γ becomes smaller.

For an explicit dependence on Γ to use as an expansion coefficient, we rescale the distance by the square root of the relative strength, $\sqrt{\Gamma}\vec{r}\mapsto\vec{r}$. Equation (19) specialized to second order gives

$$\vec{\nabla}_{\vec{1}}g^{(2)}(\vec{1},\vec{2}) = \Gamma g^{(2)}(\vec{1},\vec{2})\vec{\nabla}_{\vec{1}}\psi(\vec{1},\vec{2}) + \sum_{s=1}^{r} \int \vec{\nabla}_{\vec{1}}\psi(\vec{1},\vec{3}_s)\rho(\vec{3}_s)$$

$$\times[g^{(3)}(\vec{1},\vec{2},\vec{3}_s) - g^{(2)}(\vec{1},\vec{2})g^{(2)}(\vec{1},\vec{3}_s)]d^2\vec{3}_s. \qquad (22)$$

Here, we have simplified the notation even further by suppressing all irrelevant subscripts: vectors $\vec{1}$ and $\vec{2}$ simply denote the positions of dislocations 1 and 2 with their corresponding species. The summation Σ_r is taken over all s species present in the system.

We proceed by assuming that the correlation functions have the following forms:

$$g^{(2)}(\vec{1},\vec{2}) = 1 + \Gamma f^{(2)}(\vec{1},\vec{2}), \qquad (23a)$$

$$g^{(3)}(\vec{1},\vec{2},\vec{3}) = 1 + \Gamma[f^{(2)}(\vec{1},\vec{2}) + f^{(2)}(\vec{1},\vec{3}) + f^{(2)}(\vec{2},\vec{3})]$$

$$+ \Gamma^2 f^{(3)}(\vec{1},\vec{2},\vec{3}) \qquad (23b)$$

for any vectors $\vec{1}$, $\vec{2}$, and $\vec{3}$. The functions $f^{(2)}(\vec{1},\vec{2})$ and $f^{(3)}(\vec{1},\vec{2},\vec{3})$ should asymptotically vanish along the boundaries of the sample or as $|\vec{1}-\vec{2}|,|\vec{1}-\vec{3}|,|\vec{2}-\vec{3}|\rightarrow\infty$ for an infinite system. Note, in particular, that

$$g^{(3)}(\vec{1},\vec{2},\vec{3}) - g^{(2)}(\vec{1},\vec{2})g^{(2)}(\vec{1},\vec{3}) = \Gamma f^{(2)}(\vec{2},\vec{3})$$

$$+ \Gamma^2[f^{(3)}(\vec{1},\vec{2},\vec{3}) - f^{(2)}(\vec{1},\vec{2})f^{(2)}(\vec{1},\vec{3})]. \qquad (24)$$

So far, no approximation has been made. Equation (22) governing the second-order correlations naturally involves the third-order correlations. To systematically close the chain at the second order, we substitute Eqs. (23) and (24) into Eq. (22) to produce a set of integrodifferential equations of $f^{(2)}$ and $f^{(3)}$ for each power of Γ. This technique was introduced

by Bogolyubov[37] in the study of correlations in the Coulomb interactions and has been widely used in both high-energy and condensed matter communities in renormalization group theory. It should be mentioned that, in principle, Γ needs to be small for the expansion to be valid,[38] but this is not true here. The values of Γ in Secs. IV and V turn out to be greater than 1—as often happens in diagrammatic expansion calculations in high-energy physics. The validity of the approach can be judged by comparisons between the theory and numerical simulation results.

The equation of power Γ^0 gives an identity. After integrating away $\nabla_{\vec{1}}$ because $f^{(2)}$ and ψ vanish at infinity, the equation of power Γ becomes

$$f^{(2)}(\vec{1},\vec{2}) = \psi(\vec{1},\vec{2}) + \sum_{s=1}^{r} \int \psi(\vec{1},\vec{3}_s)\rho(\vec{3}_s)f^{(2)}(\vec{2},\vec{3}_s)d^2\vec{3}_s.$$

(25)

This equation is the key result of the analysis. We shall use it to obtain dislocation pair correlation functions for systems with one in Sec. IV and many in Sec. V active slip systems.

IV. PAIR CORRELATION FUNCTIONS FOR SINGLE SLIP

To illustrate the use of Eq. (25), we first apply it to the case of one slip system containing two species of dislocations (denoted as $+$ and $-$). According to Eq. (21) valid for an infinite sample, $\psi(\vec{1},\vec{2})=\psi(\vec{1}-\vec{2})=\psi(\vec{2}-\vec{1})$ which implies that $f^{ab}(\vec{1},\vec{2})=f^{ab}(\vec{1}-\vec{2})=f^{ab}(\vec{2}-\vec{1})$. Without loss of generality, we can take the origin to be at $\vec{2}$ and thus, from Eq. (25), we obtain the following set of integral equations:

$$f^{++}(\vec{r}) = \psi_1(\vec{r}) + \int d^2\vec{r}'\,\psi_1(\vec{r}-\vec{r}')[\rho^+(\vec{r}')f^{++}(\vec{r}')$$
$$-\rho^-(\vec{r}')f^{+-}(\vec{r}')],$$

(26a)

$$f^{+-}(\vec{r}) = -\psi_1(\vec{r}) - \int d^2\vec{r}'\,\psi_1(\vec{r}-\vec{r}')[\rho^-(\vec{r}')f^{--}(\vec{r}')$$
$$-\rho^+(\vec{r}')f^{-+}(\vec{r}')],$$

(26b)

$$f^{--}(\vec{r}) = \psi_1(\vec{r}) + \int d^2\vec{r}'\,\psi_1(\vec{r}-\vec{r}')[\rho^-(\vec{r}')f^{--}(\vec{r}')$$
$$-\rho^+(\vec{r}')f^{-+}(\vec{r}')],$$

(26c)

$$f^{-+}(\vec{r}) = -\psi_1(\vec{r}) - \int d^2\vec{r}'\,\psi_1(\vec{r}-\vec{r}')[\rho^+(\vec{r}')f^{++}(\vec{r}')$$
$$-\rho^-(\vec{r}')f^{+-}(\vec{r}')].$$

(26d)

In the current context, Eq. (21) reduces to

$$\psi_1(\vec{r}) = \psi^{++}(\vec{r}) = -\psi^{+-}(\vec{r}) = \ln(|\vec{r}|) + \frac{y^2}{|\vec{r}|^2},$$

(27)

where we orient our (x,y) coordinate system in such a way that the slip direction points along the x direction. The minus

signs in Eqs. (26a)–(26d) arise from a sign difference in the interactions between plus-plus dislocations versus plus-minus dislocations, as shown in Eq. (27). By comparing Eq. (26a) against Eq. (26d) and Eq. (26b) against Eq. (26c), we find that $f^{++}(\vec{r})=-f^{-+}(\vec{r})$ and $f^{+-}(\vec{r})=-f^{--}(\vec{r})$. These symmetries further imply that $f^{++}(\vec{r})=f^{--}(\vec{r})$. Finally, we obtain

$$f^{++}(\vec{r}) = \psi_1(\vec{r}) + \int \psi_1(\vec{r}-\vec{r}')f^{++}(\vec{r}')[\rho^+(\vec{r}') + \rho^-(\vec{r}')]d^2\vec{r}'.$$

(28)

Our general formulation in Sec. III allows for spatial variation of an uncorrelated density $\rho(\vec{r}_s)$. Without externally applied force, $\rho(\vec{r}_s)=\langle N_s\rangle/A$ is constant in space. An analytical solution to Eq. (28) can be obtained for constant ρ^+ and ρ^-. The dimensionless nature of the interaction potential ψ_1 suggests a change in variable $\sqrt{\rho^+ + \rho^-}\,\vec{r} \mapsto \vec{r}$ (note that ρ^+ and ρ^- are always positive). The resulting dimensionless integral equation

$$f^{++}(\vec{r}) = \psi_1(\vec{r}) + \int \psi_1(\vec{r}-\vec{r}')f^{++}(\vec{r}')d^2\vec{r}'$$

(29)

can be directly solved by applying $\Delta^2 \equiv (\partial_x^2+\partial_y^2)^2$ on both sides of the equation and using the identity

$$\Delta^2\psi_1(\vec{r}) = 2\pi\Delta\delta(\vec{r}) + 2\pi(\partial_y^2 - \partial_x^2)\delta(\vec{r}) = 4\pi\partial_y^2\delta(\vec{r}).$$ (30)

Equation (29) then becomes

$$\Delta^2 f^{++} = 4\pi\partial_y^2[f^{++} + \delta(\vec{r})],$$

(31)

whose explicit solution is

$$f^{++} = \frac{y}{r}\sinh(\sqrt{\pi}y)K_1(\sqrt{\pi}r) - \cosh(\sqrt{\pi}y)K_0(\sqrt{\pi}r),$$ (32)

where $K_0(\cdot)$ and $K_1(\cdot)$ are the zeroth- and first-order modified Bessel functions of the second kind. With the aid of Eqs. (23a) and (23b), the correlation functions $g^{(++)}=g^{(--)}$ and $g^{(+-)}=g^{(-+)}$, correct to $\mathcal{O}(\Gamma^2)$, can be expressed in the original coordinates,

$$g^{(++)}(\vec{r}) = 1 + \Gamma\left[\frac{y}{r}\sinh(k_0 y)K_1(k_0 r) - \cosh(k_0 y)K_0(k_0 r)\right],$$

(33a)

$$g^{(+-)}(\vec{r}) = 1 - \Gamma\left[\frac{y}{r}\sinh(k_0 y)K_1(k_0 r) - \cosh(k_0 y)K_0(k_0 r)\right],$$

(33b)

where $k_0 \equiv \sqrt{\pi\Gamma(\rho^+ + \rho^-)}$ gives an inverse "Debye radius" of the dislocation cloud. The third-order correlation functions correct up to $\mathcal{O}(\Gamma^2)$ straightforwardly follow from Eq. (23b). The validity of Eq. (32) can be verified by comparing $g^{(++)}(\vec{r}) - g^{(+-)}(\vec{r})$ to the dislocation difference, or GND, field $\kappa(\vec{r})$ in Eq. (15) of Ref. 15. In this latter work, the *same* expression is obtained for the induced GND due to a single pinned dislocation, which was interpreted by the authors as the pair correlation of dislocations in a relaxed system.

The values of $g^{(++)}$ and $g^{(+-)}$ in Eq. (32) diverge—and hence are unphysical—at very small radii. The reason arises

from the omission of a core energy term in Eqs. (20) and (27) which would otherwise offset the logarithmic divergence. Physically speaking, when two dislocations approach each other, if they are of the same sign, they merge into one dislocation; otherwise they cancel. In both cases, nothing is diverging. Note also that the pair correlation functions depend only on the scaled space coordinate $\sqrt{\rho}\vec{r}$ ($\rho \equiv \rho^+ + \rho^-$ being the total dislocation density) in agreement with the scaling argument given by Zaiser *et al.*[10] This dependence also holds in the multiple-slip case to be discussed in Sec. V.

V. PAIR CORRELATION FUNCTIONS FOR MULTIPLE SLIP

The procedure to obtain the correlation functions for a system with multiple slips follows the same types of arguments and expansions as those for single slip. We shall further develop the integral of Eq. (25) for a system of N slip systems, each with two charges, and subsequently give an explicit analytical solution for the pair correlation function in the case wherein the difference in slip-orientation angle between adjacent slip planes is constant.

For an N-slip system with both types of charges, we have $4N^2$ coupled integral equations for different pairs of $\vec{1}$ and $\vec{2}$ in Eq. (25). To reduce the number of equations, and essentially decouple them, some symmetry arguments can be employed. For an infinite system,

$$\psi_{ij}^{++} = \psi_{ij}^{--} = -\psi_{ij}^{+-} = -\psi_{ij}^{-+}, \quad \psi_{ij}^{ab} = \psi_{ji}^{ab},$$

where the superscripts denote the charges of the first and second dislocations, while the subscripts show the slip systems in which they live. Equation (25) can be recast by using the convolution operator $*$ and the symmetry of ψ_{ij}^{ab} as

$$f_{ij}^{ab} = \psi_{ij}^{ab} + \sum_{k=1}^{N} \psi_{ik}^{a+} * [\rho_k^+ f_{jk}^{b+} - \rho_k^- f_{jk}^{b-}]. \quad (34)$$

By direct substitution of $+$ and $-$ into a and b, it is immediate that $f_{ij}^{++}(\vec{r}) = -f_{ij}^{-+}(\vec{r})$ and $f_{ij}^{--}(\vec{r}) = -f_{ij}^{+-}(\vec{r})$, which further implies that

$$f_{ij}^{++} = f_{ij}^{--} = \psi_{ij}^{++} + \sum_{k=1}^{N} \psi_{ik}^{++} * [\rho_k^+ f_{jk}^{++} + \rho_k^- f_{jk}^{--}]. \quad (35)$$

With this, Eq. (34) reduces to

$$f_{ij} = \psi_{ij} + \sum_{k=1}^{N} \psi_{ik} * [\rho_k f_{jk}], \quad (36)$$

where the superscripts have been omitted and $\rho_k \equiv \rho_k^+ + \rho_k^-$ is the total dislocation density of both types on slip k. We thus effectively reduce the number of coupled equations to N^2. Also note that because of $\psi_{ij} = \psi_{ji}$, there are only $N(N+1)/2$ independent ψ_{ij}'s.

As seen from the single-slip case, Eq. (36) subjected to an arbitrary distribution of the local density $\rho_k(\vec{r})$ cannot be analytically solved. For spatially independent ρ_k, however, these equations can be decoupled. Let λ_k be the relative population of density in slip system k relative to the total density ρ, i.e.,

$\rho_k = \lambda_k \rho$, where $\sum_{k=1}^{N} \lambda_k = 1$. We can then perform a change in variable $\sqrt{\rho}\vec{r} \mapsto \vec{r}$ to absorb the ρ dependence. In addition, in the Fourier space (indicated by a superposed $\sim$), a convolution becomes a product. We can solve the Fourier transform of Eq. (36) for $\tilde{f}_{ij}$ by essentially performing a matrix inversion on

$$\tilde{\psi}_{ij} = \sum_{m,n} (\delta_{im}\delta_{jn} - \lambda_n \tilde{\psi}_{in}\delta_{jm})\tilde{f}_{mn}. \quad (37)$$

The Fourier representation of ψ_{ij} in Eq. (21) can be very simply expressed in polar coordinates (k, ϕ_k),

$$\tilde{\psi}_{ij} = -\frac{4\pi}{k^2}\sin(\phi_k - \theta_i)\sin(\phi_k - \theta_j) = -\frac{4\pi}{k^4}(\hat{m}_i \cdot \vec{k})(\hat{m}_j \cdot \vec{k}), \quad (38)$$

where θ_i is the angle that slip plane i makes with the x axis (which can be arbitrarily chosen, so that $\theta_i = i\pi/N$). Owing to the simple form of Eq. (38), the solution to Eq. (37) is[39]

$$\tilde{f}_{ij} = \frac{\tilde{\psi}_{ij}/\lambda_j}{1 - \sum_n \tilde{\psi}_{nn}}, \quad (39)$$

where we have used $\sum_n \tilde{\psi}_{in}\tilde{\psi}_{nj} = \tilde{\psi}_{ij}\sum_n \tilde{\psi}_{nn}$. Equation (39) shall be used in the derivation of the evolution law for parallel edge dislocations in a multislip system in Sec. VI.

To verify that Eq. (39) is applicable in glide-controlled systems, we consider an ensemble of 1500 relaxed configurations of 64 plus and 64 minus dislocations randomly placed on a 1 μm^2 square and restricted to move along their glide directions. The simulations were performed with periodic boundary conditions in the absence of thermal noise. The glide constraint helps prevent dislocation annihilation, and thus, to fix the total number of dislocations and to maintain the finite effective temperature. As an example, Fig. 1 shows (b) the density plot of the theoretical correlation function f_{12}^{++} between plus dislocations on 60° and 120° slip systems against (a) the simulation result. The erroneous oscillations in Fig. 1(b) along 0° and 90° lines are caused by the numerical inverse Fourier transform operation of Eq. (39). (The general closed form solution of a double-slip pair correlation function does not exist for an arbitrary pair of slip-orientation angles.) Overall, the theory gives accurate angular predictions except along the two slip directions where it underpredicts the same-sign anticorrelation due to the suppression of climb. The plot of the correlation function along the $\hat{x}$ axis is shown in Fig. 2. Very close to the origin, the function logarithmically diverges as does the unscreened potential. About one dislocation spacing from the core, the correlation function decays as $1/x^2$.

The real-space solution to Eq. (39) is possible if we assume that *the angle between each adjacent pair of slip planes is constant*. For any $N \in \mathbf{Z}^+$ and $N > 1$,
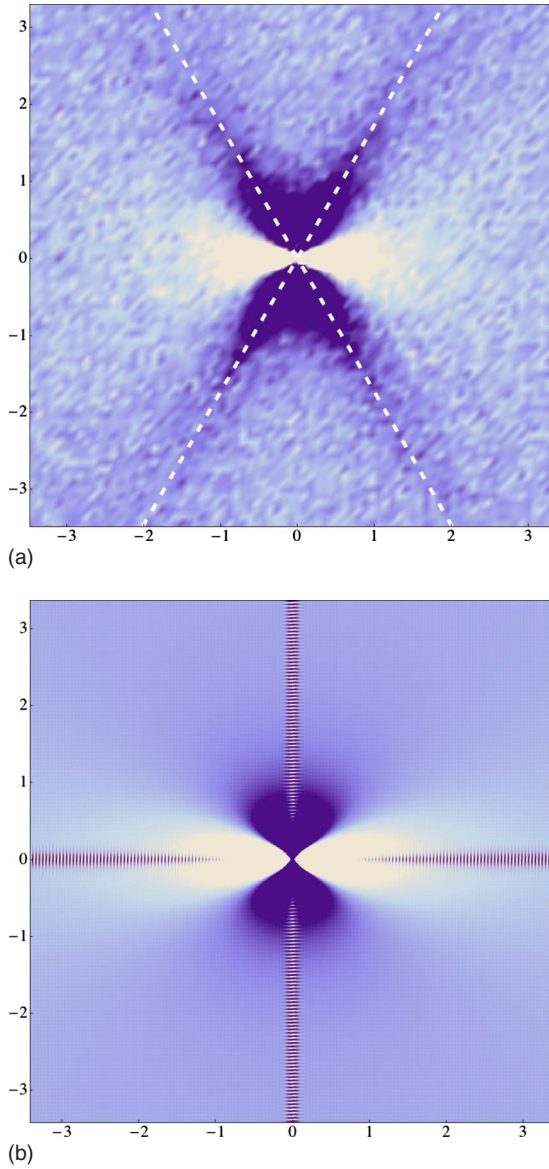
(a)

(b)

FIG. 1. (Color online) (a) Discrete dislocation result and (b) theoretical prediction of the correlation function f_{12}^{++} between plus dislocations on 60° and 120° slip systems. The values increase toward brighter regions. The coordinates are measured in units of $1/\sqrt{\rho}$. The dashed lines indicate the two slip directions where the plus-plus anticorrelation is underpredicted due to the glide constraint of the discrete dislocation simulations. The fitting parameter due to rescalings of length was found to be $k_0 \simeq 22\sqrt{\rho}$.

$$\sum_{n=1}^{N} \sin^2\left(\phi_k - \frac{n\pi}{N}\right) = \frac{N}{2} \tag{40}$$

regardless of ϕ_k. With the above identity, the denominator of $\tilde{f}_{ij}$ becomes angular independent and can be directly integrated. The final result, with

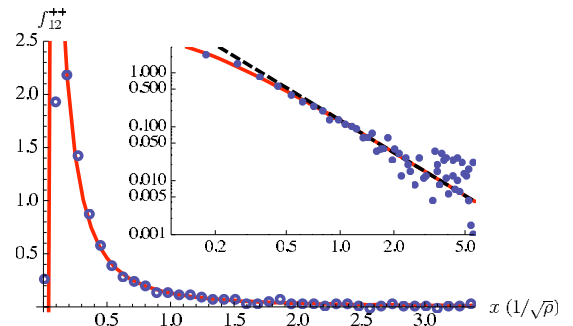$$k_0 \equiv \sqrt{2\pi N\Gamma\rho},$$

reads

FIG. 2. (Color online) Cross-sectional plot of the data points versus theoretical curves of the pair correlation function (Fig. 1) along the $\hat{x}$ axis. After a short distance away from the core, the function has a power law decay of $1/x^2$, as shown with the dashed line in the log-log plot in the inset.

$$f_{ij}(r,\phi) = \frac{-2}{\lambda_j}\left\{\frac{\cos(2\phi - \theta_i - \theta_j)}{(k_0 r)^2} - \frac{\cos(\theta_i - \theta_j)}{k_0 r}K_1(k_0 r)\right.$$
$$\left. - \sin(\phi - \theta_i)\sin(\phi - \theta_j)K_2(k_0 r)\right\}. \tag{41}$$

At large distances, the first term dominates and the pair correlation decays like $1/r^2$ (except along the directions where the argument of the cosine is $\pi/2$, $3\pi/2$, etc.). Compared to the single-slip case [Eq. (32)] where the pair correlation exponentially diminishes (except along the dislocation wall direction), the presence of extra slip(s) suppresses the Debye screening. It should be noted that $-f_{ij}(\vec{r})$ can be thought of as the effective interaction potential due to screening. More precisely, $\vec{F}^{PK} \sim \vec{\nabla}f_{ij}$ is the Peach–Koehler force felt by a positive dislocation on slip system i due to the induced screening of dislocations on slip system j. It has been shown[15] that, for single-slip system, the attractive parabolic potential in the glide direction (taken to be along $\hat{x}$) falls off with a prefactor of $1/|y|^{5/2}$ along the wall direction. Series expansion of ϕ in Eq. (41) about θ_i and θ_j reveals that, for multiple-slip system, the prefactor of the parabolic potential about the glide directions decays as $1/r^2$—slightly more slowly than the single-slip case. This could explain the necessity to include more than one slip system to see the formation of cell walls and grain boundaries in two-dimensional discrete dislocation simulations prohibiting climb motion.[17–24] The analysis also confirms the "directional long-range order" of two-dimensional crystals as rigorously proven by Mermin.[1]

VI. DERIVATION OF A MULTIPLE-SLIP EVOLUTION LAW

To arrive at a set of transport equations for an ensemble of multiple-slip dislocation systems, we extend the treatments of Groma and co-workers in Refs. 4, 10, and 40. The evolution equations for the uncorrelated single-dislocation densities on slip system i read

$$\partial_t \rho_i^+(\vec{r}_i, t) = -(\vec{b}_i \cdot \vec{\nabla})\left\{+\rho_i^+(\vec{r}_i, t)\tau_i^{ext} + \sum_j \int d^2\vec{r}_j[\rho_{ij}^{++}(\vec{r}_i, \vec{r}_j, t)\right.$$
$$\left. - \rho_{ij}^{+-}(\vec{r}_i, \vec{r}_j, t)]\tau_{ij}^{ind}\right\}, \tag{42a}$$

$$\partial_t \rho_i^-(\vec{r}_i,t) = -(\vec{b}_i \cdot \vec{\nabla})\{-\rho_i^-(\vec{r}_i,t)\tau_i^{\text{ext}} + \sum_j \int d^2\vec{r}_j[\rho_{ij}^{--}(\vec{r}_i,\vec{r}_j,t)$$

$$-\rho_{ij}^{-+}(\vec{r}_i,\vec{r}_j,t)]\tau_{ij}^{\text{ind}}\}, \qquad (42b)$$

where the dislocation mobility has been absorbed into the rescaling of time t. With the assumption that all dislocations have the same magnitude b, the Burgers vector can be written as $\vec{b}_i = b\hat{s}_i$ ($\hat{s}_i$ and $\hat{m}_i$, respectively, are the slip direction and slip-plane normal direction of slip system i). $\tau_{ij}^{\text{ind}}(\vec{r}_i - \vec{r}_j)$ is the resolved shear stress exerted on a dislocation at $\vec{r}_i$ on slip i by a dislocation at $\vec{r}_j$ on slip j and can be written as

$$\tau_{ij}^{\text{ind}}(\vec{r}) = \hat{s}_i \cdot \boldsymbol{\sigma}_j \cdot \hat{m}_i = Gb(\hat{s}_i \cdot \vec{\nabla})(\hat{m}_i \cdot \vec{\nabla})(\hat{m}_j \cdot \vec{\nabla})[r^2 \ln r].$$

$$(43)$$

Here, $G \equiv \mu/[2\pi(1-\nu)] = E/[4\pi(1-\nu^2)]$, where E, μ, and ν are the Young modulus, the shear modulus, and the Poisson ratio, respectively.

Addition and subtraction of Eqs. (42a) and (42b) give the evolution equations for the total dislocation density $\rho_i \equiv \rho_i^+ + \rho_i^-$ and the GND density $\kappa_i \equiv \rho_i^+ - \rho_i^-$,

$$\partial_t \rho_i = -(\vec{b}_i \cdot \vec{\nabla})\kappa_i \tau_i^{\text{ext}} + \sum_j \int d^2\vec{r}_j \underbrace{(\rho_{ij}^{++} + \rho_{ij}^{--} - \rho_{ij}^{+-} - \rho_{ij}^{-+})}_{\equiv \kappa_{ij}^{(2)}(\vec{r}_i,\vec{r}_j,t)}\tau_{ij}^{\text{ind}},$$

$$(44a)$$

$$\partial_t \kappa_i = -(\vec{b}_i \cdot \vec{\nabla})\left[\rho_i \tau_i^{\text{ext}} + \sum_j \int d^2\vec{r}_j \underbrace{(\rho_{ij}^{++} - \rho_{ij}^{--} - \rho_{ij}^{+-} + \rho_{ij}^{-+})}_{\equiv \rho_{ij}^{(2)}(\vec{r}_i,\vec{r}_j,t)}\tau_{ij}^{\text{ind}}\right].$$

$$(44b)$$

In accordance with Eq. (11), the dislocation-dislocation density can be written as

$$\rho_{ij}^{ss'} = \rho_i^s(\vec{r}_i)\rho_j^{s'}(\vec{r}_j)g_{ij}^{ss'}(\vec{r}_i - \vec{r}_j) = \rho_i^s(\vec{r}_i)\rho_j^{s'}(\vec{r}_j)[1 + d_{ij}^{ss'}(\vec{r}_i - \vec{r}_j)],$$

$$(45)$$

where $s, s' \in \{+,-\}$ and, according to Eq. (23a) and (23b), $d_{ij}^{ss'} = \Gamma f_{ij}^{ss'}$. In terms of the single and pair correlation functions, the total dislocation density and GND are

$$\rho_{ij}^{(2)} = \rho_i(\vec{r}_i)\rho_j(\vec{r}_j) + \frac{1}{2}\{-\rho_i(\vec{r}_i)\rho_j(\vec{r}_j)d_{ij}^a + \rho_i(\vec{r}_i)\kappa_j(\vec{r}_j)[d_{ij}^p + d_{ij}^s]$$

$$+ \kappa_i(\vec{r}_i)\rho_j(\vec{r}_j)[d_{ij}^p - d_{ij}^s] + \kappa_i(\vec{r}_i)\kappa_j(\vec{r}_j)d_{ij}^a\}, \qquad (46a)$$

$$\kappa_{ij}^{(2)} = \kappa_i(\vec{r}_i)\kappa_j(\vec{r}_j) + \frac{1}{2}\{\rho_i(\vec{r}_i)\rho_j(\vec{r}_j)[d_{ij}^p - d_{ij}^s] + \rho_i(\vec{r}_i)\kappa_j(\vec{r}_j)d_{ij}^a$$

$$- \kappa_i(\vec{r}_i)\rho_j(\vec{r}_j)d_{ij}^a + \kappa_i(\vec{r}_i)\kappa_j(\vec{r}_j)[d_{ij}^p + d_{ij}^s]\}, \qquad (46b)$$

where $d_{ij}^p = d_{ij}^{++}$, $d_{ij}^s = (1/2)(d_{ij}^{+-} + d_{ij}^{-+})$, and $d_{ij}^a = (1/2)(d_{ij}^{+-} - d_{ij}^{-+})$. After substitution of Eq. (45) and (46), Eq. (44) becomes

$$\partial_t \rho_i = -(\vec{b}_i \cdot \vec{\nabla})[\kappa_i(\tau_i^{\text{ext}} + \tau_i^{\text{sc}} - \tau_i^f - \tau_i^b) + \rho_i \tau_i^a], \quad (47a)$$

$$\partial_t \kappa_i = -(\vec{b}_i \cdot \vec{\nabla})[\rho_i(\tau_i^{\text{ext}} + \tau_i^{\text{sc}} - \tau_i^f - \tau_i^b) + \kappa_i \tau_i^a], \quad (47b)$$

in which

$$\tau_i^{\text{sc}} = \sum_j \int \kappa_j(\vec{r}_j)\tau_{ij}^{\text{ind}}(\vec{r}_i - \vec{r}_j)d^2\vec{r}_j, \qquad (48a)$$

$$\tau_i^b = -\frac{1}{2}\sum_j \int \kappa_j(\vec{r}_j)d_{ij}^t\tau_{ij}^{\text{ind}}(\vec{r}_i - \vec{r}_j)d^2\vec{r}_j, \qquad (48b)$$

$$\tau_i^f = \frac{1}{2}\sum_j \int \rho_j(\vec{r}_j)d_{ij}^a\tau_{ij}^{\text{ind}}(\vec{r}_i - \vec{r}_j)d^2\vec{r}_j, \qquad (48c)$$

$$\tau_i^a = \frac{1}{2}\sum_j \int \rho_j(\vec{r}_j)[d_{ij}^p - d_{ij}^s]\tau_{ij}^{\text{ind}}(\vec{r}_i - \vec{r}_j)$$

$$+ \kappa_j(\vec{r}_j)d_{ij}^a\tau_{ij}^{\text{ind}}(\vec{r}_i - \vec{r}_j)d^2\vec{r}_j. \qquad (48d)$$

The term $d_{ij}^t \equiv (1/4)(d_{ij}^{++} + d_{ij}^{--} + d_{ij}^{+-} + d_{ij}^{-+})$ in Eq. (48b) involves averaging over pairs of correlation functions.

Terms involving τ_i^a in Eqs. (47) can be cast away by going into a "comoving" frame of ρ_i and κ_i, respectively. Although $d_{ij}^{++} = d_{ij}^{--} = -d_{ij}^{+-} = -d_{ij}^{-+}$ and hence d_{ij}^t should vanish by definition, this is hardly the case when, e.g., the system is strained through external loading. Only one of these correlation functions locally dominates, which results in a nonzero d_{ij}^t. Similarly, the contribution from flow stress, τ_i^f, is greatest in regions with equal population of plus and minus dislocations; in most regions, its effect is negligible. We shall therefore focus only on the contribution from back stress τ_i^b. The validity of this assumption is supported by the success of the recent single-slip theory.[12,13]

Although $d_{ij}^t(\vec{r})$ is long range, the magnitude of the back stress τ_i^b is still considerably smaller than that of the self-consistent internal stress τ_i^{sc} when r is large compared to mean dislocation spacing. We are therefore interested in the contribution of $d_{ij}^t(\vec{r})$ to the stress only at short distances where its effect is much more pronounced. Consider a dislocation at $\vec{r}_i$, we can Taylor expand $\kappa_j(\vec{r}_j)$ about this point, $\kappa_j(\vec{r}_j) \simeq \kappa_j(\vec{r}_i) + (\vec{r}_j - \vec{r}_i) \cdot \vec{\nabla}\kappa_j|_{\vec{r}_i} +$ terms of higher orders. Because $d_{ij}^t(\vec{r})$ is symmetric while $\tau_{ij}^{\text{ind}}(\vec{r})$ is antisymmetric under $\vec{r} \mapsto -\vec{r}$, the first term in the expansion vanishes. We then make a change in variable to the scaled coordinate $\sqrt{\rho}\vec{r} \mapsto \vec{x}$, where ρ represents the mean total dislocations of the system. To second order, this yields

$$\tau_i^b(\vec{r}_i) = \sum_{j=1}^N \int \frac{\vec{\nabla}\kappa_j}{\rho} \cdot \int \vec{x}d_{ij}^t(\vec{x})\tau_{ij}^{\text{ind}}(\vec{x})d^2\vec{x}. \qquad (49)$$

Using the Fourier transform expression of d_{ij}^t, the integral in Eq. (49) can be directly evaluated by using Parseval's theorem,

$$\vec{I}_{ij} \equiv \int \vec{x} d_{ij}^t(\vec{x}, \theta) \tau_{ij}^{\mathrm{ind}}(\vec{x}) d^2\vec{x} = \int \tilde{d}_{ij}^t(\vec{k}) \mathcal{F}[\vec{x}\tau_{ij}^{\mathrm{ind}}] \; ![\vec{k}] d^2\vec{k}. \tag{50}$$

The Fourier transform of $\vec{x}\tau_{ij}^{\mathrm{ind}}$ can be directly computed from Eq. (43),

$$\mathcal{F}[\vec{x}\tau_{ij}^{\mathrm{ind}}][\vec{k}] = -4\pi Gb\vec{\nabla}_{\vec{k}}\left[\frac{(\hat{s}_i \cdot \vec{k})(\hat{m}_i \cdot \vec{k})(\hat{m}_j \cdot \vec{k})}{k^4}\right]$$

$$= -Gb\vec{\nabla}_{\vec{k}}[(\hat{s}_i \cdot \vec{k})\tilde{\psi}_{ij}]. \tag{51}$$

Owing to the connection $d_{ij}^t(\vec{x}) = \Gamma f_{ij}(\vec{x})$, Eq. (50) becomes, from Eqs. (39) and (51),

$$\vec{I}_{ij} = \frac{\Gamma^2 Gb}{\lambda_j} \int \frac{\tilde{\psi}_{ij}\vec{\nabla}_{\vec{k}}[(\hat{s}_i \cdot \vec{k})\tilde{\psi}_{ij}]}{1 - \sum_n \tilde{\psi}_{nn}} d^2\vec{k}. \tag{52}$$

The vector $\vec{I}_{ij}$ is most conveniently expressed in the coordinate system of slip j. Substitution of Eq. (38) into Eq. (52), while projecting $\hat{s}_i$ and $\hat{m}_i$ onto $(\hat{s}_j, \hat{m}_j)$, gives

$$\vec{I}_{ij} = (4\pi)^2 \frac{\Gamma^2 Gb}{\lambda_j} \hat{s}_j$$
$$\times \left\{ \int_0^{2\pi}\int_\epsilon^\infty \frac{-1}{k} \frac{\sin^2(\phi_k)\sin(\phi_k + \theta_{ij})\sin(3\phi_k + 2\theta_{ij})}{k^2 + 4\pi\sum_n \sin^2(\phi_k - \theta_n)} \right.$$
$$\times dk d\phi_k + \hat{m}_j \int_0^{2\pi}\int_\epsilon^\infty \frac{1}{2k}$$
$$\left. \times \frac{\sin(\phi_k)\sin(\phi_k + \theta_{ij})\sin(4\phi_k + 2\theta_{ij})}{k^2 + 4\pi\sum_n \sin^2(\phi_k - \theta_n)} dk d\phi_k \right\}, \tag{53}$$

where $\theta_{ij} = (j - i)\pi/N$ is the angle between slip planes i and j. We impose a cutoff ϵ at small k to prevent the logarithmic divergence due to the long-range nature of the pair correlation functions.

Under the assumption of equal interval of successive slip orientation, as in Sec. V, we can very straightforwardly carry out the above integrals, which give

$$\vec{I}_{ij} = \frac{GDb}{\lambda_j}\cos(\theta_{ij})\hat{s}_j, \tag{54}$$

where $D = 2\pi^2\Gamma^2|\ln \epsilon|/N$ serves as a fitting parameter. The factor λ_j nicely combines with ρ in the denominator of Eq. (55) to make $\rho_j = \lambda_j\rho$. For physical reasons, we are going to replace ρ_j with its local density $\rho_j(\vec{r})$. In Secs. II–V, we calculated the pair correlation functions of an ensemble of *spatially constant* single-dislocation densities in thermal equilibrium. When the distributions of single-dislocation densities are nonuniform in space as is the case for systems out of equilibrium, the back stress response should depend on how much the densities locally vary.

The final result is amazingly simple,

$$\tau_i^{\mathrm{b}}(\vec{r}) = GD\sum_{j=1}^N \cos(\theta_{ij})\frac{(\vec{b}_j \cdot \vec{\nabla})\kappa_j(\vec{r})}{\rho_j(\vec{r})}. \tag{55}$$

The above form for the back stress nicely converges to the single-slip theory of Groma *et al.*[11–14,25] The $\cos(\theta_{ij})$ coupling between slip systems should come as no surprise. The angular dependence of the back stress must emerge from the symmetry of the potential. The angular average of ψ_{ij} in Eq. (21) selects out $\cos(\theta_{ij})$ as the only possibility. It is also interesting to note that the same coupling also appears in the strain gradient theory for continuum crystal plasticity by Gurtin.[41–43]

VII. COMPARISON WITH THE EARLIER MULTISLIP PLASTICITY THEORY

Recently, Yefimov *et al.*[14,25] have proposed an extension of their single-slip continuum plasticity theory[12,13] to incorporate systems with more than one slip. In their theory, each slip system j contributes some amount of back stress, which is given in our notation by

$$\tau_j^{\flat}(\vec{r}) = GD\frac{(\vec{b}_j \cdot \vec{\nabla})\kappa_j(\vec{r})}{\rho_j(\vec{r})} \tag{56}$$

to the total back stress of slip system i according to

$$\tau_i^{\mathrm{tot}} = \sum_{j=1}^N S_{ij}\tau_j^{\mathrm{b}}, \tag{57}$$

with slip-orientation dependent weight factor S_{ij} acting as a projection matrix. For symmetry reason, three variations were postulated:[14,25]

$$S_{ij}^1 = (\hat{m}_i \cdot \hat{m}_j)(\hat{s}_i \cdot \hat{s}_j) = \cos^2(\theta_{ij}), \tag{58a}$$

$$S_{ij}^2 = \hat{m}_i \cdot (\hat{s}_j \otimes \hat{m}_j + \hat{m}_j \otimes \hat{s}_j) \cdot \hat{s}_i = \cos(2\theta_{ij}), \tag{58b}$$

$$S_{ij}^3 = \hat{s}_i \cdot \hat{s}_j = \cos(\theta_{ij}). \tag{58c}$$

Note that possibility (58c) is consistent with the expression for the back stress we have derived in Eq. (55).

To select among these choices, Yefimov *et al.*[25] successively used all three laws to numerically analyze the problem of simple shearing of a crystalline strip containing two slip systems with impenetrable walls. The results of each case were compared against that from the discrete dislocation simulations of Shu *et al.*[44] The best match was achieved with Eqs. (58b). Other choices underpredicted the amount of plastic strain. The chosen interaction law was then tested against the problem of bending of a single-crystal strip with satisfactory agreement with discrete dislocation results of Cleveringa *et al.*[45]

We believe that the success of their continuum theory in the shearing problem despite the incorrect choice of interaction law is due to a different reason. The amount of plastic strain is controlled by (i) the fitting parameter D and (ii) the number density of nucleation sites in the film. By adjusting these values, different interaction laws could be altered to

obtain the desired fit. In their analysis, Yefimov et al.[12] used the value of D from their previous single-slip theory without any readjustment. There is no a priori reason why this value should stay unaltered. The density of nucleation sources in their continuum theory was chosen to match that in the discrete dislocation simulations. The discrepancy could also arise from different ways in which the discrete dislocation theory and the continuum theory handle dislocation nucleation.

In a later publication, Yefimov and Van der Giessen[14] applied their formalism to the problem of stress relaxation in single-crystal thin films on substrates subjected to thermal loading. Due to the difference in thermal expansion coefficients between film and substrate, high tensile stresses can develop in the films as the temperature decreases. Contrary to the discrete dislocation simulations by Nicola et al.,[46,47] which show increasing stress built up inside a film with decreasing film thickness, the results from the continuum theory show a size-dependent hardening only during the early stage of cooling. Moreover, the theory gives identical results between some pair of slip orientations (e.g., when the angle between the two slip planes θ_{12} is either 60° or 120°), whereas the discrete dislocation simulations and our theory predict otherwise. Finally, in the previous continuum theory,[25] dislocations nucleate when the sum of the external stress τ^{ext}, the self-consistent long-range stress τ^{sc}, and back stress τ^b exceed a certain value. From our analysis, we believe that, in a more correct treatment of dislocation nucleation, this back stress should be supplemented by flow stress τ^f [Eqs. (48c)] which is dominant in a nucleation region where plus and minus dislocations are equally populated. Applications of the current theory to the shearing problem and the thin film problem, which shows the size-dependent hardening, will shortly appear following this publication.

VIII. DISCUSSION AND CONCLUSIONS

We have described nth-order dislocation densities and dislocation pair correlation functions in a grand canonical ensemble and obtained the relationships between different orders of the correlation functions in the form of a hierarchy of integral equations. By using the Bogolyubov ansatz instead of the more customary Kirkwood approximation, we have closed the chain of the equations at second order and solved for approximate expressions of the pair correlation functions—valid at all distances—for systems with one slip and multiple active slip systems. These solutions are invariant under simultaneous transformations $\vec{r} \mapsto \vec{r}/\sqrt{\rho}$ and $\rho \mapsto \rho^2$. The transformations suggest that any emergent dislocation pattern should exhibit a length scale given by $1/\sqrt{\rho}$ as pointed out by Holt[48] and in agreement with the "law of similitude."[49] For a complete analysis of scaling relations, the reader is referred to Ref. 10.

Recently, Groma et al.[15] have developed a mean-field variational approach to study the screening of dislocations, which is similar in spirit to the Debye–Hückel theory in the study of classical plasmas.[50–52] This method is based on approximating the system's total density matrix as a product of single-particle density matrices ρ_i with the free energy given by $F = \langle \mathcal{H} \rangle + T \Sigma_i \text{Tr} \, \rho_i \ln \rho_i$. Although this technique provides a complimentary approach and results in the same pair correlation expressions for a single-slip system (after some interpretation), its generalization to multiple-slip system is not obvious. In particular, one would have to supply additional cross couplings between different slips by hand. These couplings should automatically emerge from a complete theory.

In Sec. IV, we have formulated transport equations for the total dislocation and GND densities for general multiple slip. Interactions among dislocation pairs produce an additional (relatively) short-ranged "back stress" contribution to the long-range internal stress of individual dislocations. Most of the complexities of the correlation functions were integrated away, which leave only the $\cos(\theta_{ij})$ coupling between slip systems i and j [see Eq. (55)]. This dependence was also proposed by Gurtin[42,43] in his strain gradient plasticity theory, but it was abandoned by Yefimov et al.[14,25] We have argued in Sec. VII that this refusal was based on an unfair comparison with discrete dislocation simulations for the way in which dislocation nuncleation was treated.

There is an important issue regarding the use of dislocation correlations f_{ij} for d_{ij}^t in Sec. V. The formalism developed in Sec. III assumes that dislocations relax along the directions dictated by the Peach–Koehler forces. This implies dislocation glide, as included in the transport equations developed in Sec. VI, but also climb which is not considered a mechanism of plastic flow here. Mathematically speaking, Eq. (17) is *not* the stationary state of Eqs. (42a) and (42b). Early attempts in numerically describing dislocation correlations in glide-only, multiple-slip systems failed to produce noticeable patterns due to the need for large number of dislocations; the role of climb (or cross slip) was suggested to help overcome this difficulty.[53,54] The original motivation for our approach was to find the orientation dependence of the back stress in the most straightforward way. Extracting the angular dependence from a climb-assisted relaxed state gave us a quick input to use in the glide-only, multiple-slip theory. The validity of the continuum theory will always be vindicated by comparisons against discrete dislocation results.

Finally, we believe that our multiple-slip formulation provides a framework to address a long standing challenge in explaining dislocation patterning. For single-slip systems, short-range correlations occur between two dislocations except along directions normal to their glide plane (taken to be along $\hat{y}$). It has been shown that for a small deviation away from this "dislocation wall" direction, an attractive parabolic potential produced by the correlated dislocations decays as $|y|^{-5/2}$, which is compared to $|y|^{-2}$ in the unscreened case.[15] We have found in Sec. V, however, that when one or more extra slips are introduced, the effect of Debye-type screening diminishes. In this case, the attractive potential, in fact, decays like r^{-2} as if it was unscreened. This could explain the necessity to introduce extra slips to see the formation of walls in discrete dislocation simulations,[17–24] *unless* further aided by climb motions.[53,55] The latter suggests the existence of a critical exponent of the attractive potential below which structure formation cannot occur, as is the case in single-slip systems restricted to glide. A more detailed investigation of this is left for future work.

---

*surachate@sc.chula.ac.th

†e.van.der.giessen@rug.nl

[1] N. D. Mermin, Phys. Rev. **176**, 250 (1968).

[2] D. R. Nelson, Phys. Rev. B **18**, 2318 (1978).

[3] D. R. Nelson and B. I. Halperin, Phys. Rev. B **19**, 2457 (1979).

[4] I. Groma, Phys. Rev. B **56**, 5807 (1997).

[5] For a summary of various continuum theories, see, e.g., Ref. 56 and references therein.

[6] A. El-Azab, Phys. Rev. B **61**, 11956 (2000).

[7] S. Limkumnerd and J. P. Sethna, Phys. Rev. Lett. **96**, 095503 (2006).

[8] S. Limkumnerd and J. P. Sethna, J. Mech. Phys. Solids **56**, 1450 (2008).

[9] A. Roy and A. Acharya, J. Mech. Phys. Solids **53**, 143 (2005).

[10] M. Zaiser, M. Carmen Miguel, and I. Groma, Phys. Rev. B **64**, 224102 (2001).

[11] I. Groma, F. F. Csikor, and M. Zaiser, Acta Mater. **51**, 1271 (2003).

[12] S. Yefimov, I. Groma, and E. Van der Giessen, J. Mech. Phys. Solids **52**, 279 (2004).

[13] S. Yefimov, I. Groma, and E. Van der Giessen, Modell. Simul. Mater. Sci. Eng. **12**, 1069 (2004).

[14] S. Yefimov and E. Van der Giessen, Eur. J. Mech. A/Solids **24**, 183 (2005).

[15] I. Groma, G. Györgyi, and B. Kocsis, Phys. Rev. Lett. **96**, 165503 (2006).

[16] I. Groma, G. Györgyi, and B. Kocsis, Philos. Mag. **87**, 1185 (2007).

[17] A. A. Benzerga, Y. Bréchet, A. Needleman, and E. Van der Giessen, Modell. Simul. Mater. Sci. Eng. **12**, 159 (2004).

[18] A. A. Benzerga, Y. Bréchet, A. Needleman, and E. Van der Giessen, Acta Mater. **53**, 4765 (2005).

[19] R. Fournet and J. M. Salazar, Phys. Rev. B **53**, 6283 (1996).

[20] D. Gómez-García, B. Devincre, and L. P. Kubin, Phys. Rev. Lett. **96**, 125503 (2006).

[21] I. Groma and B. Bakó, Phys. Rev. Lett. **84**, 1487 (2000).

[22] I. Groma and G. S. Pawley, Philos. Mag. A **67**, 1459 (1993).

[23] I. Groma and G. S. Pawley, Mater. Sci. Eng., A **164**, 306 (1993).

[24] A. N. Gullouglu and C. S. Hartly, Modell. Simul. Mater. Sci. Eng. **1**, 383 (1993).

[25] S. Yefimov and E. Van der Giessen, Int. J. Solids Struct. **42**, 3375 (2005).

[26] We assume that the noise is weak enough that dislocation climb is not possible.

[27] Note that this limits the analysis to two-dimensional systems of dislocations.

[28] One distinction due to the choice of an ensemble type can be seen from the normalization condition. In the grand canonical ensemble, according to Eqs. (8) and (9), $\int \rho^{(\mathbf{n})}(\{\mathbf{n}\})d\{\mathbf{n}\} = \Sigma_{\mathbf{N} \geq \mathbf{n}} \mathcal{P}_{\mathbf{N}}[\Pi_{s=1}^{r} \frac{N_s!}{(N_s-n_s)!}] = \langle \Pi_{s=1}^{r} \frac{N_s!}{(N_s-n_s)!} \rangle$, where $\langle \cdot \rangle$ denotes an av-

erage over all statistically equivalent ensembles. In particular, the density of a single dislocation of species s in a system with no external shear, $\rho^{(1)}(\vec{1}_s)$, is independent of $\vec{1}_s$, thus, $\int \rho^{(1)}(\vec{1}_s)d^2\vec{1}_s = \rho_s^{(1)}A = \langle N_s \rangle$. In other words, $\rho^{(1)} = \langle N_s \rangle/A$ depends on the *average* number of dislocation of species s. If one were to carry a similar analysis in a canonical ensemble where the number of dislocations of each species is fixed, $\rho_s^{(1)}$ would have to be replaced by N_s/A, where N_s is fixed. For higher order density, the expression becomes quite cumbersome. For example, $\rho_{ss'}^{(2)} = N_s N_s'/A^2$ for $s \neq s'$, while for $s=s'$, it is $N_s(N_s-1)/A^2$. In thermodynamic limit ($N_s \to \infty$ and $A \to \infty$ while keeping the ratio fixed), these two expressions reduce to the same thing. In this sense, it is cleaner to work in the grand canonical ensemble.

[29] J. G. Kirkwood, J. Chem. Phys. **3**, 300 (1935).

[30] J. Yvon, *Actualités Scientifiques et Industrielles* (Hermann, Paris, 1935).

[31] M. Born and H. S. Green, *A General Kinetic Theory of Liquids* (Cambridge University Press, Cambridge, UK, 1949).

[32] H. S. Green, *Molecular Theory of Liquids* (North–Holland, Amsterdam, The Netherlands, 1952).

[33] I. Z. Fisher, *Statistical Theory of Liquids* (The University of Chicago Press, Chicago, IL, 1964).

[34] T. L. Hill, *Statistical Mechanics: Principles and Selected Applications* (McGraw-Hill, New York, 1956).

[35] In the presence of an external *conservative* force, it can be shown that both Eqs. (17) and (19) remain valid provided that an additional term representing the applied external force, $\vec{F}(\vec{1}_1) \equiv -(1/T)\nabla_{\vec{1}_1} \Phi(\vec{1}_1)$ generated by the external potential $\Phi(\vec{1}_1)$ which acts on $\vec{1}_1$, is added to their RHS. Qualitatively speaking, the original expression is nothing but the sum of all the Peach–Koehler interactions on the dislocation at $\vec{1}_1$ due to all other dislocations in the collection **n**.

[36] J. P. Hirth and J. Lothe, *Theory of Dislocations*, 2nd ed. (Wiley, New York, 1982).

[37] N. N. Bogolyubov, *Problems of Dynamical Theory in Statistical Physics* (State Technical, Moscow, 1946).

[38] There are some systems where climb is typical and Γ is naturally small such as dislocations in vortex lattices of type II superconductor where the values of elastic moduli can be small at suitably applied magnetic field (Ref. 57). By modifying the form of the interaction potential, the present analysis can be carried over straightforwardly.

[39] The form of the solution is not surprising; it suggests that the solution can be written as a sum of diagrams due to the expansion $1/(1-x) = 1+x+x^2+\cdots$, which is often encountered in a many-body theory.

[40] I. Groma and P. Balogh, Acta Mater. **47**, 3647 (1999).

[41] M. E. Gurtin, J. Mech. Phys. Solids **48**, 898 (2000).

[42] M. E. Gurtin, J. Mech. Phys. Solids **50**, 5 (2002).

[43] M. E. Gurtin, Int. J. Plast. **19**, 47 (2003).

[44] J. Y. Shu, N. A. Fleck, E. Van der Giessen, and A. Needleman, J. Mech. Phys. Solids **49**, 1361 (2001).

[45] H. H. M. Cleveringa, E. Van der Giessen, and A. Needleman, Int. J. Plast. **15**, 837 (1999).

[46] L. Nicola, E. Van der Giessen, and A. Needleman, J. Appl. Phys. **93**, 5920 (2003).

[47] L. Nicola, E. Van der Giessen, and A. Needleman, Philos. Mag. **85**, 1507 (2005).

[48] D. L. Holt, J. Appl. Phys. **41**, 3197 (1970).

[49] S. V. Raj and G. M. Pharr, Mater. Sci. Eng. **81**, 217 (1986).

[50] P. Debye and E. Hückel, Z. Phys. **24**, 185 (1923).

[51] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, New York, 1960).

[52] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley, Reading, MA, 1969).

[53] B. Bakó, I. Groma, G. Györgyi, and G. T. Zimányi, Comput. Mater. Sci. **38**, 22 (2006).

[54] B. Bakó, I. Groma, G. Györgyi, and G. T. Zimányi, Phys. Rev. Lett. **98**, 075701 (2007).

[55] D. B. Barts and A. E. Carlsson, Philos. Mag. A **75**, 541 (1997).

[56] N. M. Ghoniem, E. P. Busso, N. Kioussis, and H. Huang, Philos. Mag. **83**, 3475 (2003).

[57] G. Blatter, M. V. Feigel'man, V. B. Geshkenbein, A. I. Larkin, and V. M. Vinokur, Rev. Mod. Phys. **66**, 1125 (1994).