Scale-Free Phase Field Theory of Dislocations

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According to recent experimental and numerical investigations, if a characteristic length (such as grain size) of a specimen is in the submicron size regime, several new interesting phenomena emerge during the deformation. Since in such systems boundaries play a crucial role, to model the plastic response it is crucial to determine the dislocation distribution near the boundaries. In this Letter, a phase-field-type continuum theory of the time evolution of an ensemble of parallel edge dislocations with identical Burgers vectors, corresponding to the dislocation geometry near internal boundaries, is presented. Since the dislocation-dislocation interaction is scale free ($1/r$), apart from the average dislocation spacing the theory cannot contain any length scale parameter. As shown, the continuum theory suggested is able to recover the dislocation distribution near boundaries obtained by discrete dislocation dynamics simulations.

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Three-dimensional (3D) crystals [1] and different two-dimensional (2D) lattices, such as Abrikosov vortices [2,3], charge density waves [4,5], or Wigner solids [6], generically contain a large number of line-type topological defects called dislocations, greatly affecting the plastic response of these systems. Thus, studying the collective properties of interacting dislocations is of utmost relevance in material physics. Although the interaction and dynamical properties of individual dislocations are well known for a long time, in most cases the deformation properties of the crystalline materials are controlled by the collective evolution of a large number of dislocations. One approach to model the rather complex phenomena caused by the collective motion of dislocations is the numerical solution of the equation of motion of individual dislocations called discrete dislocation dynamics (DDD). During the past decades, numerous DDD simulation algorithms have been developed both in two [7–17] and three [18–22] dimensions, allowing us to study problems like hardening [14,18,20], size effect [15,21–24], jamming-flowing transition [10,25], relaxation [17] dislocation avalanches [9,16,25,26], etc.

One may expect, however, that for a large number of problems not all the details accounted for by DDD simulations are important; the response of the dislocation network can be well described on a continuum level. Although several such continuum theories of dislocations have been developed [27–37], most of them correspond either to mean field approximation or are based on completely phenomenological grounds. However, the role of dislocation-dislocation correlation, crucial because of the long-range nature of dislocation-dislocation interaction, is far from understood. Correlation effects are taken into account in a systematic manner only in the limit when the signed dislocation density κ [geometrically necessary dislocation (GND) density] is much smaller than the stored density ρ [38–42].

With the advance of nanotechnology, the characteristic size of the microstructure of crystalline materials has been reduced to the submicron level. As a consequence, the role of boundaries (grain boundary, sample surface) has become even more important than earlier. So, to model the plastic response of samples with features on the submicron scale, it is crucial to determine the dislocation distribution near the boundaries. Close to a boundary, the GND density is often comparable to the stored one, so the assumption $|\kappa| \ll \rho$ is not valid.

The dislocation distribution near a boundary is traditionally described by the one-dimensional pileup of the dislocations [43]. For many real dislocation configurations, however, the interaction between dislocations in different slip planes is important, requiring one to go up to modeling in a minimum of 2D. In this Letter, a phase-field-type theory is suggested for the simplest possible 2D dislocation arrangement consisting of straight parallel dislocations with single slip. The evolution equations of the dislocation densities are obtained from a functional of the dislocation densities and the stress potential. In contrast to other approaches suggested recently, where a set of walls of dislocations with equidistant slip distances is considered to model the dislocation configuration near the boundary [34,37], here we assume that the slip planes of the dislocations are arranged completely randomly. Because of the $1/r$, i.e., scale-free nature of dislocation-dislocation interaction, a key consequence of the random slip plane setup is that besides the coarse-grained local dislocation spacing no other parameter with a length scale can appear in the theory. As explained in detail below, this scale-free nature largely determines the possible form of the phase field potential. We speculate that the framework suggested could be applicable to other systems with scale-free interaction, such as gravitation.

Let us consider a system of parallel edge dislocations with line vectors $\vec{l} = (0, 0, 1)$ and Burgers vectors

$\vec{b}_\pm = \pm(b,0,0)$. The force in the slip plane acting on a dislocation is $b\tau$ where τ is the shear stress generated by the other dislocations plus the external shear. It is commonly assumed that the velocity of a dislocation is proportional to the shear stress at the dislocation (overdamped dynamics) [39]. So the equation of the motion of the ith dislocation positioned at point $\vec{r}_i$ is

$$\frac{dx_i}{dt} = \frac{b}{B}\tau(\vec{r}_i) = \frac{b_i}{B}\left(\sum_{j=1,j\neq i}^{N} s_j \tau_{\mathrm{ind}}(\vec{r}_i - \vec{r}_j) + \tau_{\mathrm{ext}}\right) \quad (1)$$

where B is the dislocation drag coefficient, τ_{ind} is the stress field generated by a dislocation, τ_{ext} is the external stress, and $s_i = b_i/b = \pm 1$. The coupled system of equations of motion can be solved numerically (DDD simulation).

As was shown in detail in Refs. [40–42], the equation of motion of the dislocations Eq. (1) can be obtained from the variational "plastic" potential

$$P_d[\chi,\rho^d] = \int \left[-\frac{D}{2}(\Delta\chi)^2 + b\chi\partial_y(\rho_+^d - \rho_-^d)\right] dxdy \quad (2)$$

as

$$\frac{\delta P_d}{\delta\chi} = -D\Delta^2\chi + b\partial_y(\rho_+^d - \rho_-^d) = 0, \quad \dot{\vec{r}}_i = \frac{\vec{b}_i}{B}\frac{\partial P_d}{\partial \vec{r}_i} \quad (3)$$

where D is a constant depending on the elastic moduli, χ is the stress function with $\tau = \partial_x\partial_y\chi$, and $\rho_\pm^d(\vec{r}) = \sum_{i=1}^{N_\pm}\delta(\vec{r} - \vec{r}_i)$ in which the summation has to be taken for the positive or negative signed dislocations, respectively. So $\rho_+^d(\vec{r})$ and $\rho_-^d(\vec{r})$ are the "discrete" dislocation densities with the corresponding signs.

One may expect, however, that for many problems not all the details represented by the discrete description are needed. So with appropriate coarse graining one can obtain a continuum theory suitable to model the evolution of inhomogeneous dislocation systems. In order to derive a continuum theory from the discrete evolution equation, as a first step, one can replace in P_d given by Eq. (2) the "discrete" $\rho_\pm^{\mathrm{d}}$ fields by their local averages $\rho_\pm$, leading to the form

$$P_{\mathrm{sc}}[\chi,\rho_\pm] = P_d[\chi,\rho_\pm]. \quad (4)$$

Although by applying the standard formalism of phase field theories from P_{sc} one can derive evolution equations for the fields $\rho_\pm$ in a systematic manner (see below), as it is explained in detail in Refs. [40,41], P_{sc} corresponds to the mean (self-consistent) field approximation; i.e., dislocation-dislocation correlation effects are completely neglected. Because of the long-range nature of dislocation-dislocation interaction, correlation effects are extremely important. Therefore, terms accounting for correlations have to be added to P_{sc} to arrive at a physically relevant model.

As explained in detail in Refs. [40–42], because of the stress screening observed by DDD simulations for close to neutral systems ($\kappa = \rho_+ - \rho_-$ is much smaller than $\rho = \rho_+ + \rho_-$), correlations can be well accounted for by adding a quadratic term in κ to P_{sc}. With this term, the potential reads as

$$P[\chi,\rho_\pm] = P_{\mathrm{sc}}[\chi,\rho_\pm] + P_{\mathrm{corr}}^{\pm}[\chi,\rho_\pm] \quad (5)$$

where

$$P_{\mathrm{corr}}^{\pm}[\chi,\rho_\pm] = \int \frac{T_0}{2}\frac{\kappa^2}{\rho}dxdy, \quad (6)$$

in which T_0 is a constant (with the dimension of force) determined by the dislocation-dislocation correlation function [41]. With the phase field formalism for conserved quantities, the evolution equations for the fields $\rho_\pm$ take the form

$$\dot{\rho}_\pm + \partial_x j_\pm = 0 \quad \text{with} \quad j_\pm = \mp B^{-1}\rho_\pm\partial_x\frac{\delta P}{\delta\kappa}. \quad (7)$$

It should be mentioned that since the dislocation system is not a thermodynamical one there is no *a priori* reason a phase field approach should be applied. Thus, the correctness of the above form has to be justified. Comparing it with the field equations obtained earlier [39] by a systematic coarse-graining procedure of the discrete system of evolution equations (3), one can see that the phase field equation given by Eq. (7) is indeed justified if $|\kappa|/\rho \ll 1$ [41].

For many configurations, such as those close to a grain boundary, however, the $|\kappa|/\rho \ll 1$ condition, a key assumption in the microscopic derivation of the continuum theory, is not fulfilled. Therefore, a new concept is needed to construct the correlation term. The primary aim of the present Letter is to formulate a phase field theory if only one type of dislocation is present (say ρ_+), representing the other extreme case $|\kappa|/\rho = 1$.

Since $P_{\mathrm{sc}}[\chi,\rho_+]$ represents the mean field (i.e., correlationless) term, it is not affected by the $|\kappa|/\rho$ ratio. The real nontrivial question is the possible form of $P_{\mathrm{corr}}[\chi,\rho_+]$ in this case. As a first possible approximation, one can look for a term that does not contain the spatial derivatives of ρ_+. From simple dimensionality considerations, the general form of such a term is

$$P_{\mathrm{corr}}[\rho_+] = \int T\rho_+ f(\rho_+/\rho_0)dxdy, \quad (8)$$

where T is a constant, $f(x)$ is an arbitrary function, and ρ_0 is a parameter with inverse length square dimension. For the following consideration, a key point to notice is that since the dislocation-dislocation interaction is scale free, i.e., it does not contain any length scale parameter, the evolution equation of ρ_+ also cannot contain any parameter with a length dimension but the local dislocation spacing. As a consequence of this, the form of $f(x)$ has to be chosen

so that ρ_0 does not appear in the phase field equation (7). To fulfill this condition, the only possibility is if $f(x) \propto \ln(x)$. With the above form of $f(x)$, Eq. (7) takes the form

$$\dot{\rho}_+ + B^{-1} b \partial_x \left\{ \rho_+ \left[\tau_{\rm sc} - \frac{T}{b\rho_+} \partial_x \rho_+ \right] \right\} = 0, \qquad \tau_{\rm sc} = \partial_x \partial_y \chi \tag{9}$$

where $\tau_{\rm sc}$ is the "self-consistent" or "mean field" shear stress with χ determined from the relation $\delta P/\delta\chi = 0$ [42]. The evolution equation (9) has to be supplemented with appropriate boundary conditions. This depends on the actual properties of the boundaries, but it is quite a common case that the boundary is impenetrable for the dislocations, so the dislocation current has to vanish at the boundaries if the Burgers vector is not parallel to the surface.

One can easily see, however, that the above "diffusive-like" evolution equation is not satisfactory. Namely, let us consider a channel with surfaces perpendicular to the dislocation glide direction embedded into an infinite medium with the same elastic constants. This setup mimics a grain with boundaries impenetrable by dislocations. After randomly placing dislocations with the same Burgers vectors into the channel [Fig. 1(a)] and allowing the system to relax, a DDD simulation shows that the system does not remain homogeneous and boundary layers develop at the surfaces [Fig. 1(b)]. It is mentioned that due to the anisotropy of the dislocation-dislocation interaction, walls are naturally formed with an average distance proportional to the dislocation spacing [44]. The dislocation density obtained by averaging 5000 different realizations is plotted in Fig. 2.

On the other hand, however, in case of zero external shear stress, the homogeneous ρ_+ is a stable solution of Eq. (9) obtained above. So one can conclude that Eq. (9) is not able to reproduce the dislocation configuration developing in a channel. As the form of $P_{\rm corr}$ is dictated by the scale-free nature of dislocation-dislocation interaction, to resolve the discrepancy between the DDD simulation results and the prediction of Eq. (9) one has to introduce gradient terms in ρ_+ into $P_{\rm corr}$. Again, to avoid the appearance of length scale parameters in the evolution equation, the possible form of $P_{\rm corr}$ depending on $\nabla\rho_+$ is

$$P_{\rm corr} = \int_D T\rho_+ \left[\ln\left(\frac{\rho_+}{\rho_0}\right) + u\left(\frac{\nabla\rho_+ \hat{S} \nabla\rho_+}{2\rho_+^3}\right) \right] dxdy, \tag{10}$$

where $\hat{S}$ is a symmetric dimensionless 2×2 matrix and $u(x)$ is an arbitrary function. If $|\nabla\rho_+/\rho_+^{3/2}| \ll 1$, one can take the leading linear term in $u(x) = u_0 x$, so $P_{\rm corr}$ used in the considerations below is quadratic in $\nabla\rho_+$.

Because of the gradient terms introduced in $P_{\rm corr}$, the phase field equation (7) is a fourth-order partial differential equation in $\vec{r}$. In order to get a unique solution, further boundary conditions have to be introduced besides the one introduced earlier for the dislocation current $\vec{j}_+$. A dislocation wall developing next to a boundary has an extra surface energy, which can be accounted for by adding a surface term to $P_{\rm corr}$. For dimensionality reasons, the surface energy density has to be proportional to $\sqrt{\rho_+}$, but as above, parameters with length scale should not be introduced in the evolution equation of the dislocations, so the only possible form of the surface (∂D) contribution to the potential P is

$$P_{\rm sf}[\rho_+] = \oint_{\partial D} \alpha_{\rm sf} T \sqrt{\rho_+} \vec{n} d\vec{A} \tag{11}$$

where the $\vec{n} = \vec{b}/b$ term takes into account that in the surface energy only the surface projection perpendicular to the slip plane has contribution, and $\alpha_{\rm sf}$ is a constant. (One may consider an appropriate $\nabla\rho_+$ dependence of $\alpha_{\rm sf}$ but in this Letter only the leading term independent from $\nabla\rho_+$ is taken.) Since the relaxation of the dislocation configuration next to the surface is expected to be much faster than that in

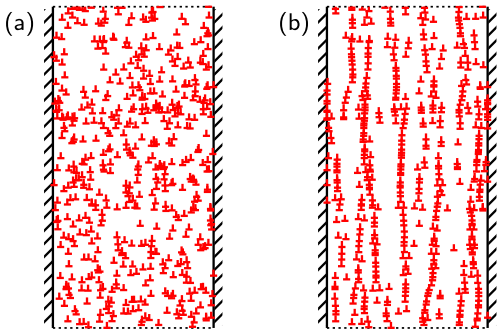

FIG. 1 (color online). (a) Random initial configuration of dislocations in a channel. (b) Relaxed dislocation configuration. The boundaries in the x direction are impenetrable, and periodic boundary condition is used in the y direction. We point out that the channel is embedded in a medium infinite in the x direction. The total number of dislocations is 512.

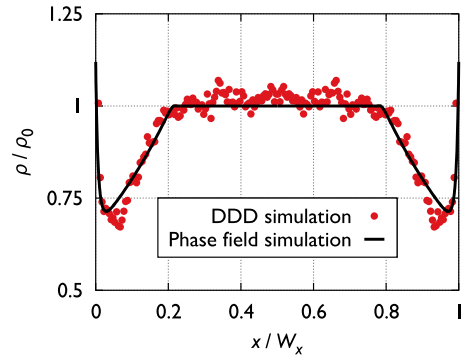

FIG. 2 (color online). Dislocation density profiles (relative to the initial density), averaged in the direction perpendicular to the slip direction, developing between two impenetrable walls obtained by DDD simulation (circles) and the numerical solution of the phase field model proposed (full line). Relevant simulation parameters are $u_0 = 0.26$, $\alpha_{\rm sf} = 5.5$, $\alpha_m = 0.02$.

the bulk, the boundary condition can be obtained from the total plastic potential

$$P[\chi,\rho_+] = P_{\rm sc}[\chi,\rho_+] + P_{\rm corr}[\rho_+] + P_{\rm sf}[\rho_+] \tag{12}$$

given by Eqs. (4), (10), (11) as

$$\left.\frac{\delta P}{\delta \rho_+}\right|_{\partial D} = \left.\vec{C}\nabla\rho_+ - \rho_+^{3/2}\right|_{\partial D} = 0 \tag{13}$$

where $\vec{C}$ is a dimensionless constant 2D vector depending on $\hat{S}$, $\alpha_{\rm sf}$, and the surface direction.

The system of Eqs. (7) and (13) together with the condition that $\vec{j}_+$ vanishes at the system surface represent a closed set of equations with unique solution. As discussed below, however, it is not able to account for the dislocation density evolution obtained by DDD simulation for the channel problem mentioned above. Namely, for this geometry due to the translation symmetry in the y direction, Eq. (7) has an equilibrium solution satisfying the condition

$$\frac{\delta P}{\delta \rho_+} = \mu_0, \tag{14}$$

where μ_0 is a parameter (analogous to the chemical potential) depending on the initial average dislocation density. After substituting the actual form of $P[\chi,\rho_+]$ given by Eqs. (4), (10), (11) into Eq. (14), we arrive at a second-order ordinary differential equation for $\rho_{+,\rm eq}(x)$ in equilibrium. With the analysis of the structure of the equation, one can find that within the channel this $\rho_{+,\rm eq}(x)$ is either completely convex or concave depending on the actual value of the parameters; i.e., it is not able to recover the shape seen in Fig. 2, even for a general $u(x)$.

To resolve the problem, we recall that due to the constrained motion of dislocations the system cannot reach its absolute energy minimum; rather, it gets trapped in a local minimum, resulting a history dependence of the response of the system. So it is natural to assume that a system of dislocations with identical sign has an "internal rigidity" meaning that if the internal shear stress

$$\begin{aligned}\tau_{\rm int} &= -\partial_x \frac{\delta P}{\delta \rho_+} - \tau_{\rm sc} = -\partial_x \frac{\delta P_{\rm corr}}{\delta \rho_+} \\ &= -T\frac{\partial_x \rho^+}{\rho_+} + Tu_0\partial_x\left[\frac{\nabla\rho_+\hat{S}\nabla\rho_+}{\rho_+^3} + \nabla\frac{\hat{S}\nabla\rho_+}{\rho_+^2}\right]\end{aligned} \tag{15}$$

is smaller than a critical value the system cannot rearrange itself. This is somewhat similar to the "flow stress" of neutral systems but for a single signed system the flow stress is obviously zero since under an external stress the whole system can move rigidly. Although the "internal rigidity" (that is, history dependence) is a dislocation-dislocation correlation effect (like the flow stress introduced in Ref. [39] for neutral systems), there is no trivial way to take it into account by adding an appropriate term to $P[\chi,\rho_+]$, since the equilibrium density profile will be always determined by Eq. (14). Within the phase field framework, however, one has some freedom in defining the relation between the currents and the chemical potential. It is possible to introduce history dependence via a mobility function giving the dislocation current as

$$j_+ = B^{-1}b\rho_+[M(\tau_{\rm int}) + \tau_{\rm sc}] \tag{16}$$

with

$$M(\tau) = \begin{cases} 0, & \text{if } \tau < \tau_0, \\ \tau - \tau_0, & \text{if } \tau > \tau_0. \end{cases} \tag{17}$$

Since there is no other length scale but the dislocation spacing, from a simple dimensionality consideration $\tau_0 = \alpha_m b D^{-1}\sqrt{\rho_+}$. The quantity α_m and the shape of the mobility function $M(x)$ may depend on the possible different dimensionless combinations of the dislocation density and its derivatives, but in our analysis it was kept constant. As it is seen in Fig. 2 for the channel problem, the numerical solution of the evolution equation with Eqs. (7), (16), and (17) recovers the characteristic feature of the spatial variation of the dislocation density obtained by DDD. The phase field theory properly describes the intermediate time evolution of the density profile, too [45]. It should be noted, however, that before reaching equilibrium, the phase field solution (see in Fig. 2) has two points with sharp corner type of characters indicating that one might have to refine the mobility law, e.g., to allow higher order terms in $\alpha_{\rm m}$.

According to the discussion explained above, we have at hand continuum theories of dislocations in two extreme cases: if $|\kappa/\rho| \ll 1$ and if $|\kappa/\rho| = 1$. In the following speculations on linking, the two regimes are presented. It is natural to assume that the general κ/ρ case can be obtained by a smooth interpolation between the limits. (Since the mean field part of the plastic potential $P_{\rm sc}$ is valid for any κ we have to consider only the correlation part of P.) As a first step, let us simply take the sum $P^t_{\rm corr}[\rho_+,\rho_-] = P_{\rm corr}[\rho_+] + P_{\rm corr}[\rho_-]$. If $|\kappa/\rho| \ll 1$, apart from the terms depending on the derivatives of the dislocation densities (see below), one obtains that $P_{\rm sc} + P^t_{\rm corr}$ recovers the form of $P^{\pm}_{\rm corr}$ given by Eq. (6) if $T = T_0$. Since, however, T and T_0 are determined by the dislocation-dislocation correlation functions [40,41] that depend on the κ/ρ ratio [44], one cannot expect that $T = T_0$. To account for this, it is useful to rewrite the two logarithmic terms in $P^t_{\rm corr}$ into the form

$$\begin{aligned}&T\rho_+\ln(\rho_+/\rho_0) + T\rho_-\ln(\rho_-/\rho_0) \\ &\quad = \frac{T}{2}\rho\ln\left[\frac{\rho^2-\kappa^2}{4\rho_0^2}\right] + \frac{T'}{2}\kappa\ln\left[\frac{\rho+\kappa}{\rho-\kappa}\right]\end{aligned} \tag{18}$$

(with $T = T'$). For a general κ/ρ the coefficient T' can have a weak κ^2/ρ^2 dependence in the form of $T'(x) = T + (T_0 - T)(x-1)^2/2$. (Since in the evolution

equations the functional derivative has to be taken only with respect to κ, terms depending only on ρ can be dropped from P^{t}_{corr}.) Two things that should be mentioned at this point are that (i) the $(dT'/dx)(1) = 0$ condition ensures that no extra terms appears in $\delta P/\delta\kappa$ at $|\kappa| = \rho$ discussed above and (ii) the coefficient in front of the first term in the right hand side of Eq. (18) has to remain κ^2/ρ^2 independent to ensure that ρ_0 does not appear in the evolution equation of the dislocation densities. Without going into the details, we mention that in the plastic potential the gradient terms can be treated in a similar way. Certainly the actual values of the parameters appearing in the general form of P_{corr} have to be determined from DDD simulations corresponding to different system geometries.

In summary, a continuum theory of straight parallel dislocations is proposed that takes into account dislocation-dislocation correlation effects. It is obtained from a functional of the dislocation densities by applying the formalism of phase field theories. It has to be stressed that the form of the phase field functional proposed is the simplest possible one (containing only the leading order terms) that is able to recover the characteristic feature of the DDD simulation results. In order to recover the fine details of the DDD simulation results, one may have to introduce higher order terms. Furthermore, certainly the 2D dislocation geometry the continuum theory is corresponding to is a strong simplification of the real much more complex 3D ones. In the 3D continuum theory, however, the structure of the terms corresponding to the correlation between dislocation loops should have rather similar forms.

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