Debye Screening of Dislocations

I. Groma,[1,*] G. Györgyi,[2,†] and B. Kocsis[1,*]

[1]*Department of General Physics, Eötvös University, 1117 Budapest, Pázmány sétány 1/a, Hungary*
[2]*Institute for Theoretical Physics, HAS Research Group, Eötvös University, 1117 Budapest, Pázmány sétány 1/a, Hungary*
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Debye-like screening by edge dislocations of some externally given stress is studied by means of a variational approach to coarse grained field theory. Explicitly given are the force field and the induced geometrically necessary dislocation (GND) distribution, in the special case of a single glide axis in 2D, for (i) a single edge dislocation and (ii) a dislocation wall. Numerical simulation demonstrates that the correlation in relaxed dislocation configurations is in good agreement with the induced GND in case (i). Furthermore, the result (ii) well predicts the experimentally observed decay length for the GND developing close to grain boundaries.

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Crystalline materials generically contain a large number of dislocations; thus the study of systems of interacting dislocations is of utmost relevance in material physics [1]. Beside 3D crystals, in several 2D lattices, like Abrikosov vortices [2] and Wigner solids [3] dislocations greatly affect the response of the system. At first sight it would be natural to assume that the dislocations are arranged completely randomly within the crystal. According to transmission electron microscopic studies, however, at high enough deformation level dislocations form different patterns [1]. Even at small deformations, completely randomly distributed dislocations would have properties contradicting experiments. First, the stored energy per unit volume, corresponding to complete randomness, would diverge logarithmically with the crystal size R [4]. In stored energy measurements, however, there is no evidence for this logarithmic size dependence [5]. A more precise experimental method is the x-ray Bragg peak profile analysis to determine some statistical parameters (like the average and the variance of the dislocation density) of dislocation systems [6]. As was theoretically shown by Krivoglaz [7] and Wilkens [8], for a completely random dislocation distribution, the width of a Bragg peak is also proportional to $\log(R)$. Experimentally, however, the width is found to be independent of the crystal size if the size is larger than a few micrometers. So these experiments indicate that real dislocation arrangements are not completely random. In other words, they are correlated so that the $\sigma \propto 1/r$ stress field of a dislocation is screened by the others. X-ray peak broadening enables the measurement of the screening length, which was found in the order of the average dislocation spacing [9]. In spite of several attempts to describe statistical properties of dislocation systems [10–15], to this date there is no commonly accepted theory for screening.

Recently, Berdichevsky proposed a variational approach to the thermal distribution of uniform-sign screw dislocations in 2D [16]. The next simplest model, where dislocations can already screen each other, is a system of parallel edge dislocations with single glide orientation and $\pm$ Burgers vectors. For this system, the screening of the elastic field of a disclination was analyzed by Sarafanov and Perevezentev [17]. On the other hand, the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy of the time evolution equations of different order dislocation density functions was constructed and numerically studied [18,19]. A key assumption of this theory is that the dislocation-dislocation correlation is short range.

In this Letter we address the static problem by a variational effective thermodynamics approach. This yields a screening equation, which we solve analytically, and compare results to discrete dislocation simulations and experimental results.

Variational principle for stress in equilibrium.—We start out from the coarse grained field equations of Kröner and Kosevich [20,21] for the stress field of a given dislocation system. The dislocation distribution can be characterized by Nye's density tensor $\hat{\alpha} = -\boldsymbol{\nabla} \times \hat{\beta}$, where the circumflex marks a tensor and $\hat{\beta}$ is the elastic distortion. If a volume element dV contains the dislocation line element $d\boldsymbol{s}$ then $\hat{\alpha}$ is related to the Burgers vector by $\hat{\alpha} dV = d\boldsymbol{s} \circ \boldsymbol{b}$. So as to automatically satisfy $\mathrm{div}\hat{\sigma} = 0$, one expresses the stress tensor $\hat{\sigma}$ in terms of the "stress function" tensor $\hat{\chi}$ as $\hat{\sigma} = \boldsymbol{\nabla} \times \hat{\chi} \times \boldsymbol{\nabla} = \mathrm{inc}\hat{\chi}$. Then one easily finds (see Refs. [20,21]) that $\hat{\chi}$ satisfies in a linear medium (subscript s means symmetric part)

$$\hat{\eta} = (\boldsymbol{\nabla} \times \hat{\alpha}^{\mathrm{T}})_s = \mathrm{inc}(\hat{\hat{S}}:\mathrm{inc}\hat{\chi}), \tag{1}$$

where $\hat{\hat{S}}$ is the compliance tensor of four indices.

For a given dislocation distribution this yields the equilibrium stress field. For further considerations it is useful to note that the bulk Eq. (1) can be obtained via variation by $\hat{\chi}$ from the functional

$$E[\hat{\chi}, \hat{\eta}] = \int dV \left[-\frac{1}{2} \mathrm{inc}\hat{\chi}:\hat{\hat{S}}:\mathrm{inc}\hat{\chi} + \hat{\chi}:\hat{\eta} \right], \tag{2}$$

if surface terms are neglected. Here the negated first term is the elastic energy $\int \hat{\varepsilon}\,\hat{\sigma}/2$ and so is E itself for a given $\hat{\eta}$ if (1) holds. An advantage of the form (2) is that $\hat{\eta}$, characterizing the dislocation distribution, appears linearly, in the second term. This term actually represents the interaction energy of a dislocation system in a fixed stress field characterized by $\hat{\chi}$, whence from variation by the position of a given dislocation segment the Peach-Koehler formula follows [21]. We mention that it is a rough approximation to consider only the coarse grained elastic energy, while neglecting other energy terms like the core energy or contributions coming from coarse graining.

Edge dislocations in a 2D isotropic medium.—Let us consider a system of parallel edge dislocations, with tangent vector $\boldsymbol{t} = d\boldsymbol{s}/ds = (0, 0, -1)$ and single glide axis parallel to the x direction. Then the Burgers vector can be $\boldsymbol{b} = \pm b(1, 0, 0)$, where the + sign refers to $\perp$ dislocations. The respective (coarse grained) number densities are ϱ_+ and ϱ_-. The absolute density of the dislocations is $\varrho = \varrho_+ + \varrho_-$, while the density of the signed ones is $\kappa = \varrho_+ - \varrho_-$, commonly called the density of geometrically necessary dislocations (GNDs). The energy now depends only on χ_{33}, denoted henceforth by χ, and by definition the planar stress tensor components are

$$\sigma_{xx} = -\partial_y^2\chi, \qquad \sigma_{xy} = \partial_x\partial_y\chi, \qquad \sigma_{yy} = -\partial_x^2\chi. \quad (3)$$

The only nonzero element of $\hat{\eta}$ of (1) is $\eta_{33} = \partial_1\alpha_{32} - \partial_2\alpha_{31} = b\partial_y\kappa$. Assuming isotropy Eq. (2) becomes

$$E[\chi, \kappa] = \int dV\left[-\frac{D}{2}(\Delta\chi)^2 + b\chi\partial_y\kappa\right], \quad (4)$$

where D equals $(1-\nu)/2\mu$ for a 3D crystal, and $1/[2\mu(1+\nu)]$ in a 2D hexagonal lattice, respectively, with μ the shear modulus and ν Poisson's ratio. By varying functional (4) we get the equilibrium condition $D\Delta^2\chi = b\partial_y\kappa$. This can be solved by the Green function

$$G_0(\boldsymbol{r}) = (4\pi)^{-1} y \ln(r/r_0), \quad (5)$$

with r_0 an arbitrary constant, representing the stress function for $\kappa = D/b\,\delta(\boldsymbol{r})$ in an infinite system.

Effective free energy for screening.—In order to address the problem of screening, we add externally fixed (pinned) dislocations with GND density κ_{ext}. Then $E[\chi, \kappa + \kappa_{\text{ext}}]$ gives the elastic energy at extremum in χ. When dislocation dynamics is affected by thermal noise, this should be taken into account by an appropriate entropy. While it is often argued for that entropic effects are negligible in practical cases of plastic deformations, we shall see it below that, at least for small GND, an effective temperature parameter characterizes the relaxed equilibrium state of dislocations restricted to their glide axes. Next we consider the entropy of a gas of $\pm$ dislocations $S = \int s d^2r$ with

$$\begin{aligned} s &= -\varrho_+ \ln\frac{\varrho_+}{\varrho_0} - \varrho_- \ln\frac{\varrho_-}{\varrho_0} \\ &= -\frac{1}{2}[(\varrho+\kappa)\ln(\varrho+\kappa) + (\varrho-\kappa)\ln(\varrho-\kappa) \\ &\quad - 2\varrho\ln 2\varrho_0], \end{aligned} \quad (6)$$

where ϱ_0 is a normalizing constant. From (4) and (6) the following free energy can be constructed

$$F = E[\chi, \kappa + \kappa_{\text{ext}}] - TS[\varrho, \kappa], \quad (7)$$

where T is an effective temperature. Since in this Letter our goal is to study screening by the GND density κ, we assume that the absolute density ϱ is given, so, only the GND together with the stress field is allowed to relax. Thus the condition of equilibrium reads as

$$\frac{\delta F}{\delta\chi} = -D\Delta^2\chi + b\partial_y(\kappa + \kappa_{\text{ext}}) = 0, \quad (8a)$$

$$\frac{\delta F}{\delta\kappa} = -b\partial_y\chi + T\tanh^{-1}(\kappa/\varrho) = 0. \quad (8b)$$

Green's function for Debye screening of pinned dislocations.—We shall consider the case of an infinite medium, which turns out to be solvable in the limit of small GND density, $|\kappa| \ll \rho$, if ϱ is constant in space. In leading order Eq. (8b) yields

$$b\partial_y\chi = T\kappa/\varrho. \quad (9)$$

Differentiating by y, keeping ϱ constant, from (8a) we get

$$\Delta^2\chi = 4k_0^2\partial_y^2\chi + q\partial_y\kappa_{\text{ext}}, \quad (10)$$

with the notation $q = b/D$, $k_0 = \sqrt{b^2\varrho/4DT}$. The equation for the Green function corresponding to (10) reads

$$\Delta^2 G(\boldsymbol{r}) = 4k_0^2\partial_y^2 G(\boldsymbol{r}) + \partial_y\delta(\boldsymbol{r}). \quad (11)$$

Its solution decaying at infinity is

$$G(\boldsymbol{r}) = -(4\pi k_0)^{-1}\sinh(k_0 y)K_0(k_0 r), \quad (12)$$

where K_0 is the zeroth modified Bessel function of the second kind. One can check directly for $r > 0$ that (12) solves (11). Near the origin, the asymptote $K_0(z) \approx -\ln z$ yields $G(\boldsymbol{r}) \approx G_0(\boldsymbol{r})$ of (5) with $r_0 = 1/k_0$. Since for small r we have $k_0^2\partial_y^2 G_0 \ll \Delta^2 G_0$, thus Eq. (11) becomes the unscreened ($k_0 = 0$) equation. This is indeed solved by $G_0(\boldsymbol{r})$, so we can conclude that (12) satisfies (11) also around the origin. The emergence of $G_0(\boldsymbol{r})$ for small r means that, as one expects, screening is ineffective near a pinned dislocation. Furthermore, for $k_0 \to 0$, the high-T limit, $G_0(\boldsymbol{r})$ is recovered for any $\boldsymbol{r}$. We can now express the stress function χ induced by an arbitrary external dislocation field κ_{ext} as

$$\chi(\boldsymbol{r}) = q\int d^2r' G(\boldsymbol{r} - \boldsymbol{r}')\kappa_{\text{ext}}(\boldsymbol{r}'), \quad (13)$$

whence by (3) the stress tensor follows. Thus by Eq. (9) the density of the induced GND is

$$\kappa(\boldsymbol{r}) = 4k_0^2 q^{-1} \partial_y \chi(\boldsymbol{r}). \tag{14}$$

Screening of a single pinned dislocation: induced GND and stress field.—It follows from the above considerations that a positive edge dislocation fixed at the origin induces the stress function $\chi = qG(\boldsymbol{r})$, whence by (14)

$$\kappa(\boldsymbol{r}) = \frac{k_0^2}{\pi}\left[\frac{y\sinh(k_0 y)}{r}K_1(k_0 r) - \cosh(k_0 y)K_0(k_0 r)\right]. \tag{15}$$

This function is displayed on a contour plot in Fig. 1. The Peach-Koehler force [21] acting on a dislocation with positive Burgers vector is $\boldsymbol{f} = b(\sigma_{xy}, -\sigma_{xx})$. If we define the potential V via $\boldsymbol{f} = -b\nabla V$, from (3) and (14) we find $V(\boldsymbol{r}) = -\partial_y \chi(\boldsymbol{r}) = -q\kappa(\boldsymbol{r})/4k_0^2$. Hence follows the remarkable feature that κ also plays the role of the induced potential felt by a negative edge dislocation.

Whereas for small $\boldsymbol{r}$ screening is negligible, farther from the pinned dislocation, however, screening becomes important. We obtain essentially exponential asymptotes for large $|x|$ with constant y as $\kappa \propto e^{-k_0 r}/\sqrt{r}$. In the neighborhood of the y axis, however, we get for $|y| \to \infty$ a power law as

$$\kappa \approx \sqrt{\frac{k_0}{32\pi}} \frac{1}{|y|^{3/2}}\left(1 - \frac{3}{2}\frac{k_0 x^2}{|y|}\right), \tag{16}$$

thus screening is weak in the direction perpendicular to the Burgers vector. Furthermore, we see that the attractive parabolic potential in x for a positive dislocation survives screening, with a prefactor $|y|^{-5/2}$ decaying only slightly more slowly than the unscreened $|y|^{-2}$ [21]. This means that the stability of dislocation walls is hardly affected by screening.

The stress-free positions also change due to screening. While for small r the $|y| = |x|$ stable and $x = 0$ unstable positions are recovered for a negative dislocation, characterizing unscreened interaction, for larger distances the lines of the stable position bend, and asymptotically they satisfy $|y| \approx x^2/3$.

Correlations in relaxed dislocation systems.—Based on analogy with Coulomb plasma, one naturally expects that screening of a single pinned dislocation also characterizes correlations in many-dislocation systems. In order to test this assumption we performed simulation of overdamped dislocations, bound to randomly placed, parallel, glide axes, with periodic boundary conditions. Starting out from random initial configurations we allowed the system to relax. The number of positive and negative dislocations was equal, totaling 128, and an ensemble of 1000 such systems was considered. In the relaxed configurations the correlation functions $\varrho_{\sigma\sigma'}(\boldsymbol{r})$ were computed, characterizing dislocations of signs σ, σ' at relative position $\boldsymbol{r}$. Then $\varrho_{++} - \varrho_{+-}$ measures the signed density with respect to positive dislocations. Since on average this should equal the formula with inverted subscripts, for better statistics we consider $\kappa_{\text{corr}} = \varrho_{++} - \varrho_{+-} + \varrho_{--} - \varrho_{-+}$. This is expected to be represented by the appropriately scaled GND distribution from our theory. We were able to compare our theory with simulation near the y axis, where by (16) the GND decays the slowest. Figure 2 shows the comparison of $\kappa_{\text{corr}}(\boldsymbol{r})$ obtained by discrete dislocation dynamics simulation and $\kappa(\boldsymbol{r})$ given by (15). The only fitting parameter k_0 was found to be $k_0 = 4.2\sqrt{\rho}$.

We emphasize that the above simulation was done in the absence of thermal noise. Remarkably, the constraint to the glide axes, keeping dislocations apart, turned out to act as a finite effective temperature. Furthermore, the fixed glide axes prevent annihilation exempting the total density ρ from the condition of thermal equilibrium, justifying our treatment of ρ as externally given. We speculate that the temperature parameter $TD/b^2 = 0.014$ may characterize the relaxed states of most, moderately inhomogeneous dislocation systems with a single glide axis, too.

Screening of a dislocation wall.—The screening of a dislocation wall aligning perpendicular to the Burgers vector (low angle grain boundary), can be straightforwardly calculated based on the findings above. We consider a finite wall of length $2L$, centered at the origin, and

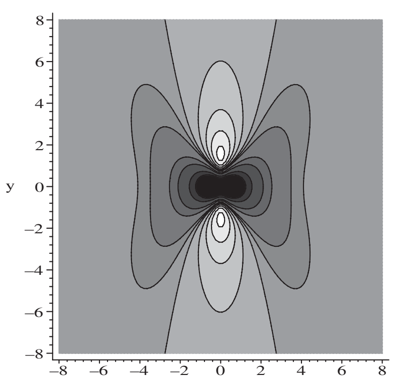

FIG. 1. Induced GND by a single pinned dislocation. Shading lightens towards increasing values, the only open contours indicate the zero level, and the coordinates are in units of $1/k_0$.

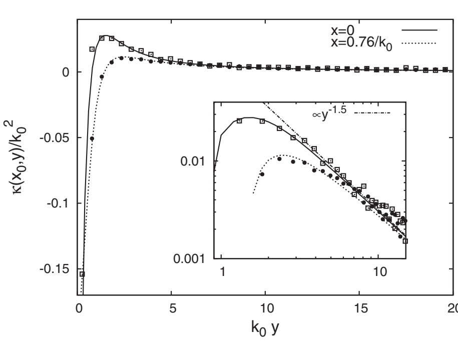

FIG. 2. Induced GND near the y axis ($x = 0$ and $x = 0.76/k_0$) and the theoretical prediction. The inset shows part of the curves with log-log scales, demonstrating the power decay predicted by (16).

consisting of N pinned positive dislocations. This corresponds to the external density

$$\kappa_{\rm ext}(\boldsymbol{r}) = \frac{N}{2L}\delta(x)[\theta(L+y) - \theta(y-L)], \tag{17}$$

where $\theta(x)$ is the Heaviside function. Substituting this into Eq. (13) we get the stress function, whence by (14) the GND is

$$\kappa(\boldsymbol{r}) = -\frac{k_0 N}{2\pi L}\{\sinh[k_0(L+y)]K_0(k_0 r_+) + \sinh[k_0(L-y)]K_0(k_0 r_-)\}, \tag{18}$$

with $r_\pm = \sqrt{x^2 + (y \pm L)^2}$. Again, screening causes exponential suppression in x; (18) decays essentially within a few $1/k_0$ lengths.

For a long wall we expect a quasi-1D GND distribution. Indeed, in the large $k_0 L$ limit, while $L \gg r$, we get

$$\kappa(\boldsymbol{r}) \approx -\frac{N}{2L}\sqrt{\frac{k_0}{2\pi L}}\exp\left(-\frac{x^2 k_0}{2L}\right), \tag{19}$$

which is independent of y. Since x may be in the region $k_0^{-1} \ll |x| \ll L$, the exponent need not be small. Note that, in the units of the linear density $N/2L$ of dislocations in the wall, the induced GND is small, because of the extra $1/\sqrt{L}$ factor. Remarkably, the quasi-1D approximation is good at $y = 0$ even if the condition $L \gg x$ is not met, e.g., for $k_0 L = 2$ the deviation from the exact function (18) is less than 10% of the peak value for all x. This means that near a small angle grain boundary the decay of the induced GND is characterized by the length $l = \sqrt{L/k_0} \propto \sqrt{L/\sqrt{\rho}}$. In order to test this prediction we compared it to the experimentally observed GND distribution of El-Dasher *et al.* [22]. There the dislocation distributions were displayed (Fig. 3 in Ref. [22]) in the proximity of a small angle grain boundary. The relaxation of the GND is apparent with characteristic length of about 10 μm. This is much larger than the dislocation spacing, the length one would expect by traditional arguments. If, however, we take a typical value $\rho \approx 10^{14}$ m^{-2}, with $L \approx 1$ mm extracted from the figure, l is in the order of magnitude of 10 μm. Although the slip configuration is obviously more complex in the experimental system than the one considered in our analysis, the order of magnitude of the surprisingly weak relaxation can be explained by our proposition that $\sqrt{L/\sqrt{\varrho}}$ is the relevant characteristic length.

The screening of a disclination studied in Ref. [17] corresponds in our framework to the external GND density $\kappa_{\rm ext}(\boldsymbol{r}) \propto \theta(y)$. From (11) and (12) one concludes that $\kappa(\boldsymbol{r}) \propto G(\boldsymbol{r})$, the very same result obtained in Ref. [17].

In conclusion, the effective free-energy functional proposed accounts for the screening phenomenon observed by discrete dislocation dynamics simulations. Furthermore, it predicts the right order of magnitude for the experimentally observed characteristic decay length of the GND density next to a grain boundary. We add that the meaning of the effective free energy at zero physical temperature is, in fact, the coarse grained energy, corrected by a term accounting for correlations. One of the most important consequences of screening of the stress field of a single dislocation is that the energy does not diverge with the system size. We suggest that other elastic screening problems can also be analyzed within our framework. The static theory is reinforced by the fact that from our free-energy functional one can obtain gradient dynamics [23], consistent with the ones derived from the equation of motion of individual dislocations in Ref. [19].

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*Electronic address: groma@metal.elte.hu
†Electronic address: gyorgyi@glu.elte.hu

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