A line-tension model of dislocation networks on several slip planes

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Abstract

Dislocations in crystals can be studied by a Peierls-Nabarro type model, which couples linear elasticity with a nonconvex term modeling plastic slip. In the limit of small lattice spacing, and for dislocations restricted to planes, we show that it reduces to a line-tension model, with an energy depending on the local orientation and Burgers vector of the dislocation. This model predicts, for specific geometries, spontaneous formation of microstructure, in the sense that straight dislocations are unstable towards a zig-zag pattern. Coupling between dislocations in different planes can lead to microstructures over several length scales.

Keywords: Dislocation, Peierls-Nabarro model, Crystal plasticity, Relaxation

1. Introduction

Dislocations are topological defects in crystals, which are responsible for plastic deformation. They can be interpreted as discontinuity lines of the plastic slip. Geometrically, a dislocation may be seen as an oriented line with a multiplicity, which corresponds to the Burgers vector. The Burgers vector is a lattice vector of the crystal and is a conserved quantity, in the sense that it is constant on the parts of the dislocation line which have no intersections, and at intersection points the sum of the Burgers vectors of the dislocations entering must equal the sum of the Burgers vectors of the dislocations exiting the point.

For a more detailed description we refer for example to [1, 2, 3, 4].
Dislocations are accompanied by long-range elastic stresses. To make this precise, we consider the variational problem of linear elasticity

\[ \int_\Omega \frac{1}{2} C \nabla^s u \cdot \nabla^s u \, dx + \text{body forces} + \text{surface tractions} \]

with suitable boundary conditions. Here \( \Omega \subset \mathbb{R}^3 \) is the reference configuration, \( u : \Omega \to \mathbb{R}^3 \) is the (possibly discontinuous) elastic displacement, \( C \) the matrix of elastic coefficients, and \( \nabla^s u = (\nabla u + \nabla u^T)/2 \) the elastic strain. Assuming for simplicity that plastic slip only takes place on the plane \( \{x_3 = 0\} \), and denoting by \( v(x_1, x_2) \) the slip at the point \((x_1, x_2, 0)\), we require \( u \) to be continuous away from the plane and the limits of \( u \) on both sides of the plane to differ by \( v \),

\[ u^+(x_1, x_2, 0) - u^-(x_1, x_2, 0) = v(x_1, x_2). \]

Here \( u^+ \) and \( u^- \) denote the one-sided limits, taken on \( x_3 > 0 \) and \( x_3 < 0 \) respectively. A simple situation, corresponding to a straight dislocation with Burgers vector \( b \) along the \( x_1 \)-axis, would have \( v(x_1, x_2) = 0 \) for \( x_2 < 0 \) and \( v(x_1, x_2) = \varepsilon b \) for \( x_2 \geq 0 \). Here \( \varepsilon \) represents the lattice spacing. The elastic strain \( \nabla^s u \) necessarily diverges at least as \( \varepsilon |b|/\sqrt{x_2^2 + x_3^2} \) around the dislocation, and thus cannot be square integrable. In other words, all displacements \( u \) which obey the given jump condition have infinite elastic energy.

The singularity in the strain field is normally regularized at the atomic scale \( \varepsilon \), at which the continuum elasticity approach loses validity. For example, one can truncate the energy in the core region removing a cylinder of radius \( \varepsilon \) around the dislocation line from the domain. Alternatively, one can let the slip \( v \) pass continuously from 0 to \( \varepsilon b \) over a length of order \( \varepsilon \). In both cases the elastic energy scales as \( \varepsilon^2 \ln(1/\varepsilon) \), see for example [1].

In this paper we make this computation quantitative and rigorous, deriving a model for the line-tension energy of dislocations, in the more general case that dislocations are contained in several parallel planes and without restricting to straight lines. One main finding will be that certain dislocations are unstable towards formation of oscillations. This will require replacing the line-tension model by its relaxation, as explained below. To illustrate our result we need to
introduce a more precise notation. We denote the elastic energy by

\[ E_{3D}[u, \Omega] = \int_{\Omega} \frac{1}{2} C \nabla^s u \cdot \nabla^s u \, dx \]  

(3)

and characterize a distribution of dislocations by a set of curves \( \gamma^i \), with tangent vectors \( t^i \) and Burgers vectors \( b^i \). A line-tension model then takes the form

\[ E_{LT}[(\gamma^i, t^i, b^i)_i, \Omega] = \sum_i \int_{\Omega} \varphi(b^i, t^i) \, d\gamma^i \]  

(4)

where \( \varphi \) is the line-tension energy, depending on the Burgers vector \( b^i \) and the orientation \( t^i \) of the dislocation, and \( d\gamma^i \) denotes integration over the curve \( \gamma^i \), \( d\gamma^i = dH^1_{\gamma^i} \) (in (4) we only integrate over the part inside \( \Omega \)). We shall show that, in the limit of small lattice spacing \( \varepsilon \rightarrow 0 \), and if the displacement field \( u \) corresponds to the dislocation distribution \( (\gamma^i, t^i, b^i)_i \), the elastic energy \( E_{3D}[u, \Omega_\varepsilon] \) reduces, to leading order, to \( \varepsilon^2 \ln(1/\varepsilon) \, E_{LT}[(\gamma^i, t^i, b^i)_i, \Omega] \) for a suitable \( \varphi \). Here \( \Omega_\varepsilon \) denotes the set \( \Omega \) minus a tube of radius \( \varepsilon \) around the union of the dislocation lines \( \gamma^i \).

Let us now address the line-tension energy \( \varphi \) entering (4). A straightforward computation, based on the assumption that dislocations are straight, infinite lines, gives an expression for the line-tension energy, which we call \( \varphi_0 \), in terms of the elastic constants \( C \) of the crystal, as given for example in [1], see also Section 3 below. We shall show below that \( \varphi \neq \varphi_0 \). The difference can be understood on the basis of relaxation theory. Depending on the geometry, it may be energy-efficient for dislocations to spontaneously develop microstructures, which reduce the total energy. The integrand \( \varphi \) entering (4) should then take into account that possibility, and indeed the appropriate function is the one that minimizes over all possible microstructures. This decay is related to the decay of dislocations into Shockley partials, but in our setting only “full” dislocations are present and there are no stacking faults involved.

We shall use a Peierls-Nabarro-type model, as developed by Koslowski, Cuitiño and Ortiz [5, 6, 7] for the case of dislocations on a given slip plane, and generalize it to the case that more slip planes are active. Mathematically, the analysis of these models was initiated in the scalar case by Garroni and
Müller [8, 9], the vectorial case was then studied in [10, 11], an extension to three dimensions was initiated in [12, 13]. A general discrete model for dislocations was introduced in [14], its mathematical analysis is however not yet complete and in particular convergence to line-tension models has not yet been proven. In the simple case of screw dislocations in two dimensions both a discrete model [15] and a nonlinear regularization with subquadratic energy [16] have been shown to lead to the same $\varepsilon^2 \ln(1/\varepsilon)$ scaling of the energy.

This paper is organized as follows. In Section 2 we introduce our model for dislocations in a single plane, in Section 3 we study straight dislocations, in Section 4 we discuss the abstract theory of relaxation for dislocations, in Section 5 we extend the analysis to multiple planes, and finally in Section 6 we discuss some examples and predictions of our theory.

2. Peierls-Nabarro model

We start from the two-dimensional extension of the Peierls-Nabarro model that was introduced in [5, 6, 7]. We denote by $B$ the lattice of (normalized) Burgers vectors, which in the simple cases coincides with $\mathbb{Z}^N$, $N = 2$ or 3, and is assumed to be a subset of $\mathbb{R}^3$ (extending the vectors by 0 in the third component if $B = \mathbb{Z}^2$). We assume for simplicity the reference configuration to have the form $\Omega = \omega \times (-H, H) \subset \mathbb{R}^3$, where $H > 0$ and $\omega \subset \mathbb{R}^2$ is bounded, connected, with Lipschitz boundary. The key variable is the plastic slip $v_\varepsilon: \omega \to \mathbb{R}^N$.

The local energy term penalizes the deviations of the plastic slip from the set of Burgers vectors, which correspond to the distance of $v_\varepsilon$ from $\varepsilon B$. This allows for smooth transitions from one Burgers vector to another. Adding the elastic energy $E_{3D}$ we obtain the functional

$$\frac{1}{\varepsilon} \int_\omega \text{dist}^2(v_\varepsilon, \varepsilon B) dx + \min_u \{ E_{3D}[u, \Omega] : u^+ - u^- = v_\varepsilon \}.$$  \hspace{1cm} (5)

Here $u^+ - u^- = v_\varepsilon$ means that the jump of $u$ over the plane $x_3 = 0$ equals $v_\varepsilon$, in the sense specified in (2). The elastic displacement $u: \Omega \to \mathbb{R}^3$ is chosen as the one with the smallest elastic energy, among all those with the appropriate
jump. The minimization in $u$ in (5) is a linear problem, that can be solved explicitly if one knows the Green’s function of the relevant domain. If the domain is large, one can replace the Green’s function with the fundamental solution (corresponding to the case $\omega = \mathbb{R}^2, H = \infty$), up to boundary terms which do not modify the leading-order behavior of the energy. One then replaces (5) by the energy

$$F_\varepsilon[v, \omega] = \frac{1}{\varepsilon} \int_{\omega} \text{dist}^2(v, \varepsilon B) + \int_{\omega} \int_{\omega} (v_i(x) - v_i(y)) \Gamma_{ij}(x-y)(v_j(x) - v_j(y))$$

where we implicitly sum over $i, j = 1, \ldots, N$, $N$ being the dimension of the linear space spanned by $B$. The kernel $\Gamma : \mathbb{R}^2 \to \mathbb{R}^{N \times N}$ can be determined explicitly in Fourier space from the matrix of elastic constants $C$ and has the form

$$\Gamma(z) = \frac{1}{|z|^3} \hat{\Gamma} \left( \frac{z}{|z|^3} \right)$$

where $\hat{\Gamma}(s)$ is uniformly bounded and positive definite, in the sense that there is $c > 0$ such that

$$\frac{1}{c} |\xi|^2 \leq \xi \cdot \hat{\Gamma}(s) \xi \leq c |\xi|^2 \text{ for all } \xi \in \mathbb{R}^N, s \in S^1.$$  

The extension to the case of several planes will be discussed in Section 5 below.

3. Small-$\varepsilon$ limit: straight dislocations

We consider a straight dislocation with Burgers vector $b \in B$ and orientation $t \in S^1$, so that the dislocation line $\gamma$ is a straight line through the origin parallel to $t$, $\gamma = t\mathbb{R} \subset \mathbb{R}^2$. We set, for $x \in \mathbb{R}^2$,

$$v_\varepsilon(x) = \begin{cases} 0 & \text{if } x \cdot t^\perp < 0, \\ bx \cdot t^\perp & \text{if } 0 \leq x \cdot t^\perp \leq \varepsilon, \\ b\varepsilon & \text{if } x \cdot t^\perp > \varepsilon, \end{cases}$$

where $t^\perp \in \mathbb{R}^2$ is the vector obtained rotating $t$ counterclockwise by 90 degrees. To compute the energy per unit length of the dislocation we focus on the part
contained in the ball of diameter one, \( B_{1/2} = \{ x \in \mathbb{R}^2 : |x| < 1/2 \} \). The energy \( F_\varepsilon[v_\varepsilon, B_{1/2}] \) of this segment of dislocation, which has unit length, is proportional to \( \varepsilon^2 \ln(1/\varepsilon) \) for \( \varepsilon \to 0 \), as explained in the introduction. We consequently define

\[
\varphi_0(b, t) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2 \ln \frac{1}{\varepsilon}} F_\varepsilon[v_\varepsilon, B_{1/2}].
\]  

(10)

The structure of \( \Gamma \) given in (7) permits a simpler representation for this limit (see, e.g., [11, Lemma 5.1]),

\[
\varphi_0(b, t) = 2 \int_\mathbb{R} b_i \Gamma_{ij}(t^+ + ts) b_j \, ds,
\]

(11)

where \( t^+ \) denotes a unit vector orthogonal to \( t \). Physically, the function \( \varphi_0 \) is the energy of a straight dislocation, which is not allowed to build oscillations. It can be shown that it is the same as obtained in classical theories by solving the equilibrium equations in \( \mathbb{R}^3 \) and computing the limit of \( E_{3D}[u, C_\varepsilon]/(\varepsilon^2 \ln(1/\varepsilon)) \) where \( C_\varepsilon \) is a cylinder with axis along \( t \) and unit height, whose cross-section is a circular corona obtained taking away a core region of radius \( \varepsilon \) from a circle of radius 1, see for example [1, 13].

4. Curved dislocations, relaxation

A dislocation network in a reference configuration \( \Omega \subset \mathbb{R}^3 \) is a \( \mathbb{R}^{N \times 3} \)-valued measure \( \mu \in \mathcal{M}(\Omega; \mathbb{R}^{N \times 3}) \) of the form

\[
\mu = \sum_i b^i \otimes t^i d\gamma^i,
\]

(12)

where \( \gamma^i \) are oriented Lipschitz curves in \( \Omega \) with tangent \( t^i \) and Burgers vector \( b^i \in \mathbb{Z}^N \). These measures are necessarily divergence-free, in the sense of distributions. We characterize the class of all dislocations in \( \Omega \) as

\[
\text{Disl}(\Omega) = \{ \mu = \sum_i b^i \otimes t^i d\gamma^i \in \mathcal{M}(\Omega; \mathbb{R}^{N \times 3}) \mid \text{div} \mu = 0 \}.
\]

(13)

The divergence-free constraint translates to the fact that the Burgers vector is constant on each curve and obeys a balance condition at the endpoints of the
curves $\gamma^i$: letting $I^-(z)$ be all indices of curves ending at $z$ and $I^+(z)$ all indices of curves starting at $z$, $\text{div} \, \mu = 0$ if and only if
\[
\sum_{i \in I^-(z)} b^i = \sum_{j \in I^+(z)} b^j
\] (14)
at all endpoints $z \in \Omega$. The set $\text{Disl}(\omega)$ correspondingly is the set of dislocations localized in a two-dimensional set $\omega$. We denote by $E^0_{LT}$ the line-tension energy defined as in (4) with the energy density $\varphi_0$ from (10), which can be seen as a functional on the space $\text{Disl}(\omega)$. If a dislocation is completely contained within the $(e_1, e_2)$ plane, the rotated measure $\mu^\perp = \sum_i b^i \otimes (t^i)^\perp \, d\gamma^i$ is curl-free and consequently the gradient of a slip field $v \in SBV(\omega; B)$. This identification and the $L^1$ convergence of the slip fields gives the natural convergence concept for dislocation networks.

Minimization of the functional $E^0_{LT}$ leads, for some boundary conditions, to the formation of fine-scale oscillations. This is due to the fact that the energy of certain dislocations can be reduced by decomposing them into several components. For example, since $E_{3D}$ is quadratic, one obtains from (10) or directly from (11) that $\varphi_0(2e_1, t) = 4\varphi_0(e_1, t)$. This implies that a dislocation with Burgers vector $2e_1$ will be unstable with respect to splitting into two parallel and very close dislocations with Burgers vector $e_1$ each (see sketch in Figure 1). For other Burgers vectors a more complex situation arises; for example in a cubic crystal the Burgers vector $e_1 + e_2$ is stable for some orientations, and unstable towards splitting into $e_1$ and $e_2$ for other orientations, see Figure 1 and Section 6 for details. Mathematically, one says that $E^0_{LT}$ is not lower semicontinuous.

The study of the relaxation of $E^0_{LT}$ permits understanding the macroscopic material behavior without resolving the details of these microstructures. Precisely, one considers a similar functional with a different energy density $\varphi^{\text{rel}}$. This is defined optimizing over all possible microstructures with given average,

\[
\varphi^{\text{rel}}(b, t) = \inf \{ E^0_{LT}[\mu, B_{1/2}] : \mu \in \text{Comp}(b, t) \} .
\] (15)

Here the set of competitors $\text{Comp}(b, t)$ is the set of dislocation networks $\mu \in \text{Disl}(\mathbb{R}^2)$ which coincides with the straight dislocation with Burgers vector $b$ and
Figure 1: A straight dislocation can locally (inside a small ball) be replaced by a microstructure consisting of several dislocations. This is not always energetically convenient. Left panel: a straight dislocation with Burgers vector \( e_1 \) is stable. Middle panel: A straight dislocation with Burgers vector \( 4e_1 \) will spontaneously decay into four parallel dislocations with Burgers vector \( e_1 \), since \( \varphi_0(4e_1,t) > 4\varphi_0(e_1,t) \). Right panel: A dislocation with Burgers vector \( e_1 + e_2 \) may decay into two parallel dislocations with Burgers vector \( e_1 \) and \( e_2 \); this is only energetically favorable for certain orientations \( t \).

The effective line-tension model will then be the functional \( E_{LT}^{\text{rel}} \), defined as in (4) but using the relaxed energy \( \varphi^{\text{rel}} \).

This means that \( E_{LT}^{\text{rel}}[\mu, \omega] \) gives the smallest possible asymptotic energy among all energies \( F_\varepsilon[v_\varepsilon, \omega] \) of slip fields \( v_\varepsilon \) which approximate the dislocation distribution \( \mu \), in the sense that \( \varepsilon^{-1} Dv_\varepsilon \) converges weakly to \( \mu^\perp \). For example, if \( \mu \) is the straight dislocation discussed above, \( v_\varepsilon \) may take the form (9) but can also make use of any possible microstructure. Examples are discussed in Section 6 below. Mathematically the statement is phrased in terms of \( \Gamma \)-convergence [17, 18, 11],

\[
\Gamma\text{-lim}_{\varepsilon \to 0} \frac{1}{\varepsilon^2 \ln \frac{1}{\varepsilon}} F_\varepsilon = E_{LT}^{\text{rel}}.
\] (16)

5. Multiple planes

In this section we extend the model to the case of multiple parallel planes. We denote by \( M \) the number of planes, by \( h \) the distance between two adjacent planes, and by \( \mathbf{v} = \{v_1, \ldots, v_M\} \in \mathbb{R}^{M \times N} \) the global slip, with \( v_j \in \mathbb{R}^N \) the slip in plane \( j \), corresponding to the set \( \omega_j = \omega \times \{jh\} \), and we assume \( \Omega = \omega \times (-H,H) \) with \( H > Mh \). The corresponding multiplane Burgers vector \( b \)
The elastic displacement \( u : \Omega \to \mathbb{R}^3 \) has jump \( v_j \) on \( \omega_j \),

\[
    u^+(x, y, jh) - u^-(x, y, jh) = v_j(x, y).
\]  

(17)

The generalization of the energy (5) is

\[
    \frac{1}{\varepsilon} \sum_j \int_{\omega_j} \text{dist}^2(v_j, \varepsilon B)dx + \min_u \{ E_{3D}[u, \Omega] : u^+ - u^- = v_j \text{ on } \omega_j \}.
\]  

(18)

The elastic problem is, as in the previous case, linear; the minimizer \( u \) thus depends linearly on \( v = (v_1, \ldots, v_M) \). Neglecting boundary terms the elastic energy can be characterized as

\[
    F_{\varepsilon, h}[v, \omega] = \frac{1}{\varepsilon} \sum_j \int_{\omega_j} \text{dist}^2(v_j, \varepsilon B)dx + \int_\omega \int_\omega (v(x) - v(y)) \cdot \nabla \Gamma_h(x-y)(v(x) - v(y))dxdy.
\]  

(19)

A detailed analysis of the kernel \( \Gamma_h : \mathbb{R}^2 \to \mathbb{R}^{NM \times NM} \) shows that it has singular diagonal terms \( \Gamma(x-y) \), corresponding to intra-plane interactions, and regular off-diagonal terms \( K_h(x-y) \), corresponding to inter-plane interactions. In fact, for \( |x-y| \ll h \), the off-diagonal terms are negligible in comparison to \( \Gamma(x-y) \), and for \( |x-y| \gg h \) we have \( K_h(x-y) \approx \Gamma(x-y) \). Here \( \Gamma \) is the single-plane kernel entering (6). The multiplane kernel \( \Gamma_h \) is therefore characterized as follows:

\[
    \Gamma_h(x-y) \approx \begin{cases}
        \begin{pmatrix}
            \Gamma(x-y) & 0 \\
            \vdots & \ddots \\
            0 & \Gamma(x-y)
        \end{pmatrix} & \text{for } |x-y| \ll h, \\
        \begin{pmatrix}
            \Gamma(x-y) & \cdots & \Gamma(x-y) \\
            \vdots & \ddots & \vdots \\
            \Gamma(x-y) & \cdots & \Gamma(x-y)
        \end{pmatrix} & \text{for } |x-y| \gg h,
    \end{cases}
\]  

(20)

see [19] for details.

As in the single-plane case we start from the pointwise limit, in which \( \varepsilon \) is made small keeping the dislocation straight and fixed. Precisely, we fix a
multiplane Burgers vector $b \in B^M$, an orientation $t \in S^1$, and define as in \([10]\) 

$$\varphi_M(b, t) = \lim_{\varepsilon \to 0, h \to 0} \frac{1}{\varepsilon^2 \ln \frac{1}{\varepsilon}} F_{\varepsilon, h}[v_\varepsilon, B_{1/2}]$$ \hspace{1cm} (21)$$

where $v_\varepsilon$ is defined as in \([9]\). The corresponding line-tension energy is denoted as before by $E_{LT}^n[\mu, \omega] = \int_\omega \varphi_M(b, t) d\gamma$. The limit in \([21]\) depends on the relation between the plane separation $h$ and the lattice spacing $\varepsilon$. Three regimes can be identified:

i) If $\varepsilon$ is much smaller than $h(\varepsilon)$, in the sense that for all $\beta \in (0, 1)$ one has $h(\varepsilon) \gg \varepsilon^\beta$, then the planes do not interact and $\varphi_M = \varphi_S$, where

$$\varphi_S(b, t) = \sum_{j=1}^M \varphi_0(b_j, t).$$ \hspace{1cm} (22)$$

In particular, this includes the cases where $h$ is fixed or $h(\varepsilon) = 1 / \ln(1/\varepsilon)$.

In this case we only see the short-range kernel in \([20]\), since the planes are widely separated.

ii) If $h(\varepsilon) = O(\varepsilon)$, then $\varphi_M = \varphi_L$, where

$$\varphi_L(b, t) = \varphi_0(\sum_{j=1}^M b_j, t).$$ \hspace{1cm} (23)$$

In particular, this includes the case where $h(\varepsilon) = \varepsilon$. In this case we only see the long-range kernel, and the limit only depends on the total Burgers vector $\sum_j b_j$. The planes are so close to each other that the $M$ dislocations are not distinguished from a single one.

iii) If $h(\varepsilon) = \varepsilon^\beta$ for some $\beta \in (0, 1)$, then we see a mixture of the short-range energy from \([22]\) and the long-range one from \([23]\),

$$\varphi_M(b, t) = (1 - \beta)\varphi_S(b, t) + \beta \varphi_L(b, t).$$ \hspace{1cm} (24)$$

Of the relevant length scales $\varepsilon^\alpha$, $\alpha \in (0, 1)$, $1 - \beta$ many see the short-range kernel, the remaining $\beta$ many see the long-range kernel.
Figure 2: Dislocations in different planes interact only if they run in parallel for an extended length. The interaction increases the energy for equal Burgers vectors and decreases it for opposite ones, causing minimizing dislocations in different planes to repel or attract each other respectively.

When only one dislocation (in one plane) is present, as for example in the case $b = (b, 0, \ldots, 0)$ for some $b \in B$, then $\varphi_S(b, t) = \varphi_L(b, t) = \varphi_0(b, t)$ and all limit energies coincide. If dislocations in different planes have different orientation, then they only cross at isolated points (after projecting to one plane).

Then to leading order there is no interaction in this case. The most interesting cases, which arise if dislocations are present in different planes which overlap over a finite length (and therefore have the same orientation over the overlapping segment) is discussed in detail below. See also Figure 2.

We now turn to the $\Gamma$-limit, which corresponds to the study of the asymptotic behavior along an “optimal” sequence. Optimal here means that it is the sequence which asymptotically has the smallest energy, among all those which converge to the same dislocation distribution. Our main result is

$$\Gamma\text{-lim}_{\varepsilon \to 0, h \to 0} \frac{1}{\varepsilon^2 \ln \frac{1}{\varepsilon}} F_{\varepsilon, h} = E_{LT}^{M,*}$$

(25)

where

$$E_{LT}^{M,*}[\mu, \omega] = \int_{\omega} \varphi_M^*(b, t) \, d\gamma,$$

(26)

see [19] for details. Using the $\Gamma$-limit result in [11] we see, in case (i), that the planes are well separated and in the relaxation procedure different microstructures can be used in the different planes, leading to an independent relaxation of the energy in each plane,

$$\varphi_M^*(b, t) = \varphi_S^* (b, t) = \sum_{j=1}^{M} \varphi_0^* (b_j, t),$$

(27)
where $\varphi_{rel}^0$ is the single-plane relaxed energy defined in (15). In case (ii) instead the planes are very close and interact strongly, so that one can only use a single microstructure, which affects all planes at the same time, leading to

$$\varphi_M^*(b, t) = \varphi_{rel}^L(b, t) = \varphi_{rel}^0(M \sum_{j=1}^M b_j, t),$$  

(28)

where $\varphi_{rel}^L$ is obtained from $\varphi_L$ with the same procedure as in (15).

In case (iii), using a separate microstructure in each plane, at a scale larger than $h(\varepsilon)$, leads to the upper bound

$$\varphi_M^* \leq [(1 - \beta)\varphi_S^* + \beta\varphi_L^*]_{rel}.$$  

(29)

However, the actual $\Gamma$-limit is smaller and characterized by the integrand

$$\varphi_M^* = [(1 - \beta)\varphi_S^{rel} + \beta\varphi_L^{rel}].$$  

(30)

This iterated relaxation is achieved by dislocation networks realizing the exterior relaxation which are then perturbed at scale $h(\varepsilon)$ by microstructures realizing the interior relaxation. This corresponds to a combination of fine-scale microstructures, which are independent in each plane and have a length scale smaller than the separation between the planes, with a single large-scale microstructure, which is the same for all planes and has a length scale larger than the separation between the planes. See Figure 3 for an example of such a two-scale microstructure.

The lower bound

$$(1 - \beta)\varphi_S^{rel} + \beta\varphi_L^{rel} \leq \varphi_M^*,$$  

(31)

which corresponds to a separate relaxation of the short-range and long-range terms, is generally unattainable because the short-range microstructure complies with the exterior one at intermediate scales. We show in the next section that the inequalities (31) and (29) can be strict, meaning the two-scale microstructure produces a lower energy than any single-scale structure in some cases.

In order to explain the meaning of the iterated relaxation in (30) we explain how a possible microstructure for a straight dislocation with Burgers vector $b \in B^M$ in direction $t \in S^1$ is constructed.
Figure 3: A dislocation network in two planes with global Burgers vector $b = (1, 1, 1, -1)$ and orientation $t = e_1$. Macroscopically, the lower dislocation line splits in two while the upper line follows one of the branches. The upper dislocation develops microstructure at scale $h(\varepsilon)$. See Section 6 for details.

- One constructs an admissible exterior microstructure $\mu_{\text{ext}} \in \text{Comp}(b, t)$ such that (with a slight abuse of notation)

$$
\left[ (1 - \beta)\varphi_S^{\text{rel}} + \beta \varphi_L \right] (\mu_{\text{ext}}) = \left[ (1 - \beta)\varphi_S^{\text{rel}} + \beta \varphi_L \right]^{\text{rel}} (b, t). \tag{32}
$$

One then shows that $\mu_{\text{ext}}$ can be chosen to be polygonal, in the sense that all curves $\gamma_i$ are segments.

- For every jump $b^i \in B^M$ of $\mu_{\text{ext}}$ in direction $t^i \in S^1$, one finds an admissible microstructure $\mu_{\text{int}}^i \in \text{Comp}(b^i, t^i)$ with

$$\varphi_S(\mu_{\text{int}}^i) = \varphi_S^{\text{rel}}(b^i, t^i). \tag{33}$$

Note that the interior structure can be chosen componentwise. We denote by $b^i$ the Burgers vector along a segment of the dislocation network described by $\mu_{\text{ext}}$ and by $t^i$ its orientation, $\mu_{\text{ext}} = \sum_i b^i \otimes t^i d\gamma^i$.

- Given $\varepsilon > 0$ and $h(\varepsilon) \approx \varepsilon^\beta$, one rescales $\mu_{\text{ext}}$ to a fixed $l < 1$ and tiles along $t\mathbb{R}$. Then for every line segment $\gamma^i$ of $\mu_{\text{ext}}$ with jump $(b^i, t^i)$ one rescales $\mu_{\text{int}}^i$ to $h(\varepsilon)$ and tiles along $\gamma^i$. The resulting measure is called $\mu_{\text{int}}$.

The corresponding slip $v_{\varepsilon, \beta, l} : \omega \rightarrow \mathbb{R}^{NM}$ is then obtained by applying
construction (9) to all curves making up $\mu_{\text{int}}$. Then

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2 \ln \frac{1}{\varepsilon}} F_{\varepsilon, h(\varepsilon)}[u_{\varepsilon}, \beta, t, B_{1/2}] = (1 - \beta) \sum_i |\gamma^i| \varphi_S(\mu^i_{\text{int}}) + \beta \varphi_L(\mu_{\text{ext}})$$

$$= \left[(1 - \beta)\varphi^\text{rel}_S + \beta\varphi_L\right]^{\text{rel}}(b, t).$$

Letting $l(\varepsilon) \to 0$, the normalized slip fields $\varepsilon^{-1} u_{\varepsilon, \beta, t(\varepsilon)}$ converge in $L^1$ to the slip associated with the straight dislocation with Burgers vector $b$ in direction $t$.

6. Applications and examples

We start from the case of a single plane. In the case of a simple cubic lattice the Burgers vectors in the $(x_1, x_2)$-plane are $e_1$ and $e_2$, so that $\mathcal{B} = \mathbb{Z}^2$. Assuming isotropic elasticity (and after rescaling) the limit $\varphi_0$ takes the form

$$\varphi_0(b, t) = \lambda(|b|^2 + \eta(b \cdot t)^2),$$

where $\lambda$ is the shear modulus divided by $2\pi$ and $\eta = \nu/(1 - \nu) \in [0, 1]$, with $\nu$ the Poisson ratio, see [7]. Since in the single-plane case this line-tension energy was already studied in [7, 10, 12] we only briefly sketch the key properties.

The function $\varphi_0$ is convex in $t$, thus it generally prefers straight dislocations over curved ones. Further, since it is quadratic in $b$ one can show that optimal microstructures contain only jumps $b \in \mathbb{Z}^2$ with $\max\{|b_1|, |b_2|\} \leq 1$ (see [12 Sect. 4]). From here one can establish that the only minimizing compatible microstructure for $(e_1, t)$ is the single straight line with tangent $t$. In other words, straight dislocations with Burgers vector $e_1$ are stable and

$$\varphi^\text{rel}_0(e_i, t) = \varphi_0(e_i, t) \text{ for } i = 1, 2 \text{ and } t \in S^1.$$ (36)

For multiples $ke_i$, $k \in \mathbb{N}$, one can show that the only minimizing compatible microstructure consists of $k$ parallel straight lines with tangent $t$ and jumps $e_i$, see Figure 1 and [12] for details.

For $b = (1, 1)$ however, the situation is different. Indeed, the numerical simulations in [7 Fig. 1] show that dislocations with orientation $t = (e_1 + e_2)/\sqrt{2}$
and \( t = (e_1 - e_2)/\sqrt{2} \) give a different pattern; in one case the two dislocations are superimposed, in the other they are not. This fact can be used to show that the straight dislocation with \( b = (1, 1) \) and \( t \) close to \( e_1 \) is not stable, see [10][12]. Precisely, for any \( t_\theta = (\cos \theta, \sin \theta) \), two competitors in \( \text{Comp}(b, t_\theta) \) are a pattern with a single straight dislocation and \( b = (1, 1) \) and a pattern with two very close parallel dislocations with Burgers vector \((1, 0)\) and \((0, 1)\) (as in the right panel of Figure 1). The associated energies are

\[
\begin{align*}
\varphi_0(e_1 + e_2, t_\theta) &= \lambda(2 + \eta(1 + \sin(2\theta))) \\
\varphi_0(e_1 - e_2, t_\theta) &= \lambda(2 + \eta + \eta(1 + \sin(2\theta)))
\end{align*}
\] (37)

and

\[
\begin{align*}
\tilde{\varphi}_0(e_1, t_\theta) + \varphi_0(e_2, t_\theta) &= \lambda(2 + \eta).
\end{align*}
\] (38)

For \( t = e_1 \), i.e. \( \theta = 0 \), the two energies are equal. One can however construct a more complex competitor, which is sketched in Figure 4 which achieves a smaller energy. We first replace the straight dislocation with orientation \( e_1 \) with a zig-zag which alternates between the orientations \( t_\theta \) and \( t_{-\theta} \), for some angle \( \theta \), and then separate the two dislocations in the second segment, see sketch in Figure 4. The dislocation becomes longer by a factor of \( 1/\cos \theta \) and has the energy

\[
g(\theta) = \frac{\varphi_0(e_1 + e_2, t_\theta) + \varphi_0(e_1 - e_2, t_\theta)}{2 \cos \theta} = \frac{\lambda}{\cos \theta} \left(2 + \eta + \frac{\eta}{2} \sin(2\theta)\right).
\] (39)
A simple computation shows that for \( \theta \) small and negative this is smaller than both \( f(0) \) and \( \hat{f}(0) \), see Figure 4. In fact, a similar procedure gives the minimizer and the exact value of \( \varphi_0^{\text{rel}} \); see [12, Lemma 4.6].

We now turn to the case of two planes, which is representative of the general situation of multiple planes. We show in an example that both of the inequalities (29) and (31) can be strict. For simplicity we focus here on the case \( \beta = 1/2 \). Then for \( \mathbf{b} = (b_1, b_2) \in \mathbb{Z}^4 \) we have from (24)

\[
\varphi_M(\mathbf{b}, t) = \frac{1}{2} \varphi_S(\mathbf{b}, t) + \frac{1}{2} \varphi_L(\mathbf{b}, t) = \frac{1}{2} \varphi_0(b_1, t) + \frac{1}{2} \varphi_0(b_2, t) + \frac{1}{2} \varphi_0(b_1 + b_2, t) .
\]

(40)

Our first example, which will show that (29) is strict, is the case \( \mathbf{b} = (1, 1, 0, -1) \), \( t = e_1 \). Namely, we show that in this case

\[
\varphi^*_M(\mathbf{b}, t) = \frac{[\varphi_{S}^{\text{rel}} + \varphi_{L}^{\text{rel}}]^{\text{rel}}(\mathbf{b}, t)}{2} < \frac{[\varphi_{S}^{\text{rel}} + \varphi_{L}^{\text{rel}}](\mathbf{b}, t)}{2} .
\]

(41)

Then using the fact that the relaxation reduces the energy, we estimate

\[
\varphi^*_M(\mathbf{b}, t) = \frac{[\varphi_{S}^{\text{rel}} + \varphi_{L}^{\text{rel}}]^{\text{rel}}(\mathbf{b}, t)}{2} \leq \frac{\varphi_{S}^{\text{rel}} + \varphi_{L}^{\text{rel}}(\mathbf{b}, t)}{2} .
\]

(42)

Using (27) for \( \varphi_{S}^{\text{rel}} \) and (23) for \( \varphi_L \) gives

\[
\varphi^*_M(\mathbf{b}, t) \leq \frac{\varphi_0^{\text{rel}}(b_1, t) + \varphi_0^{\text{rel}}(b_2, t) + \varphi_0(b_1 + b_2, t)}{2} .
\]

(43)

Inserting \( b_1 = e_1 + e_2, b_2 = -e_2, b_1 + b_2 = e_1 \), and using (36) one then obtains

\[
\varphi^*_M(\mathbf{b}, t) \leq \frac{\varphi_0^{\text{rel}}(e_1 + e_2, t) + \varphi_0(-e_2, t) + \varphi_0(e_1, t)}{2} .
\]

(44)

see Figure 5. If (29) were an equality, there would be some admissible microstructure \( \mathbf{\mu} = (\mu_1, \mu_2) \in \text{Comp}(\mathbf{b}, t) \) with

\[
E_{1/2}^0[\mathbf{\mu}, B_{1/2}] = \varphi^*_M(\mathbf{b}, t) \leq \frac{\varphi_0^{\text{rel}}(e_1 + e_2, t) + \varphi_0(-e_2, t) + \varphi_0(e_1, t)}{2}
\]

(45)

(although \( E_{1/2}^0 \) does not, in general, have a minimizer in Comp, existence can be obtained in the finite-dimensional minimization problem discussed in [12 Sect. 4], for simplicity of notation we do not distinguish the two problems here). If that were the case, then \( \mu_1 \in \text{Comp}(e_1 + e_2, t), \mu_2 \in \text{Comp}(-e_2, t), \)

16
and $\mu_1 + \mu_2 \in \text{Comp}(e_1, t)$, therefore using (40) and the definition of $\varphi_0^{\text{rel}}$ we obtain

$$\frac{\varphi_0^{\text{rel}}(e_1 + e_2, t) + \varphi_0^{\text{rel}}(-e_2, t) + \varphi_0^{\text{rel}}(e_1, t)}{2} \leq E_{\text{LT}}^0[\mu, B_{1/2}].$$

(46)

Recalling (36) we see that equality holds throughout. But $E_{\text{LT}}^0[\mu_2, B_{1/2}] = \varphi_0(-e_2, t)$ implies that $\mu_2$ is a single straight line, and the same for $\mu_1 + \mu_2$.

This implies that $\mu_1$ is either one or two straight lines, but then $E_{\text{LT}}^0[\mu_1, B_{1/2}]$ cannot equal $\varphi_0^{\text{rel}}(e_1 + e_2, t)$, which is achieved only by a zig-zag pattern, a contradiction.

We shall show in a similar fashion that (31) can be strict. We take $b = (1, 0, 0, 1)$ and $t = e_1$ and show that for these values

$$\frac{\varphi_S^{\text{rel}} + \varphi_L^{\text{rel}}}{2}(b, t) < \frac{[\varphi_S^{\text{rel}} + \varphi_L^{\text{rel}}]}{2}(b, t) = \varphi_M^*(b, t).$$

(47)

The left-hand side then obeys

$$\frac{[\varphi_S^{\text{rel}} + \varphi_L^{\text{rel}}]}{2}(b, t) \leq \varphi_0^{\text{rel}}(e_1, t) + \varphi_0^{\text{rel}}(e_2, t) + \varphi_0^{\text{rel}}(e_1 + e_2, t) \quad (48)$$

where we used (27) for $\varphi_S^{\text{rel}}$ and (28) for $\varphi_L^{\text{rel}}$ and inserted $b_1 = e_1$, $b_2 = e_2$, $b_1 + b_2 = e_1 + e_2$. Recalling (36) one then obtains

$$\frac{[\varphi_S^{\text{rel}} + \varphi_L^{\text{rel}}]}{2}(b, t) \leq \varphi_0(e_1, t) + \varphi_0(e_2, t) + \varphi_0^{\text{rel}}(e_1 + e_2, t).$$

(49)

Assume that a microstructure $\mu = (\mu_1, \mu_2) \in \text{Comp}(b, t)$ exists with

$$E_{\text{LT}}^0[\mu, B_{1/2}] \leq \frac{\varphi_0(e_1, t) + \varphi_0(e_2, t) + \varphi_0^{\text{rel}}(e_1 + e_2, t)}{2}.$$ (50)

Then, as before, the components $\mu_1, \mu_2, \mu_1 + \mu_2$ are admissible competitors in the definition of $\varphi_0^{\text{rel}}$, therefore equality must hold throughout, $E_{\text{LT}}^0[\mu_1, B_{1/2}] = \varphi_0(e_1, t)$, $E_{\text{LT}}^0[\mu_2, B_{1/2}] = \varphi_0(e_2, t)$ and $E_{\text{LT}}^0[\mu_1 + \mu_2, B_{1/2}] = \varphi_0^{\text{rel}}(e_1 + e_2, t)$. The first two equalities imply that both $\mu_1$ and $\mu_2$ must be single straight lines. Then, however, $\mu_1 + \mu_2$ must be either one or two straight lines, which contradicts the third equality.
We have presented a Peierls-Nabarro model for dislocations localized to several parallel planes and discussed its asymptotic behavior in the limit of small lattice spacing. To leading order we obtain a line-tension model, with a line-tension energy which depends on the dislocation’s Burgers vector and orientation, and the elastic constants of the crystal. The resulting line-tension model predicts that straight dislocations with certain orientations are unstable and are expected to spontaneously form zig-zag microstructures. In the case of several planes, complex microstructures are expected, which have a different structure at scale smaller and larger than the separation between the planes. We made specific predictions for the Burgers vectors and the orientations for which these microstructures can be observed in cubic crystals. Examples for fcc and bcc geometries remain to be investigated.

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