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Impact of lattice rotation on dislocation motion

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Abstract

We introduce a phenomenological theory of dislocation motion appropriate for two dimensional lattices. A coarse grained description is proposed that involves as primitive variables local lattice rotation and Burgers vector densities along distinguished slip systems of the lattice. We then use symmetry considerations to propose phenomenological equations for both defect energies and their dissipative motion. As a consequence, the model includes explicit dependences on the local state of lattice orientation, and allows for differential defect mobilities along distinguished directions. Defect densities and lattice rotation need to determined self consistently and we show specific results for both square and hexagonal lattices. Within linear response, dissipative equations of motion for the defect densities are derived which contain defect mobilities that depend nonlocally on defect distribution.

I. INTRODUCTION

A phenomenological model of dislocation motion in two dimensional lattices is introduced which is based on a coarse grained Burgers vector density. We extend existing treatments that are based on dissipative motion driven by plastic free energy minimization by introducing anisotropic mobilities along locally rotated slip systems. Local lattice rotation is self consistently determined with the evolving Burgers vector density distribution.

Coarse grained descriptions of defected crystalline lattices are often based on Nye's dislocation density tensor[1], and have been summarized in a number of excellent monographs[2–5]. The general starting point is the introduction of a coarse graining volume that contains a large number of defect lines threading it. The resulting dislocation density tensor α_{ik} depends on the distribution of geometrically necessary dislocations in the volume, while statistically stored dislocations (those portions of dislocation loops that do not contribute to the dislocation density tensor) are averaged out in the coarse-graining[6]. In three dimensions, the dislocation density tensor is $\alpha_{ik} = -\epsilon_{ilm}\partial_l \mathrm{w}_{mk}$ where ϵ_{ilm} is the anti symmetric Levi-Civita tensor, and $\mathrm{w}_{mk} = \partial_m u_k$ is the elastic distortion tensor. The dislocation density tensor can be represented by a vector in two dimensions which we refer to as the Burgers vector density $\mathbf{b}(\mathbf{r})$. In the $\mathbf{r} = (x, y)$ plane $b_k(\mathbf{r}) = \alpha_{3k}(\mathbf{r})$ and hence can be written as $b_k = \epsilon_{ml}\partial_l \mathrm{w}_{mk}$ where ϵ_{ml} is the two dimensional anti symmetric tensor.

Our approach follows closely the particular description employed in equilibrium theories of two dimensional melting[7–9]. In addition to the strain, the primary variables employed to describe this two dimensional defected medium include the Burgers vector density $\mathbf{b}(\mathbf{r})$ and the local (coarse grained) bond angle field $\theta(\mathbf{r})$ (also called lattice rotation). The system is assumed to be in elastic equilibrium at all times consistent with a given defect distribution, so that strain and bond orientation fluctuations are slaved to the instantaneous defect density distribution. Equilibrium fluctuations in $\theta(\mathbf{r})$ were computed within linear elasticity in Ref.[9], and shown not to destroy long range orientational bond order in a two dimensional crystalline lattice.

The same coarse grained description together with the methods of linear irreversible thermodynamics have been used to obtain the equations governing dissipative motion of the dislocation density tensor under the assumption that it is driven by free energy minimization[10–14]. We extend this research here by incorporating a defect mobility that

explicitly depends on variations in the local orientation of the slip lines in the defected medium.

Our study is motivated by recent developments that allow quantitative characterization of defect structures and motion at the nanoscale. For example, recent high resolution microscopy studies have enabled imaging of the displacement fields created by dislocations with sub Angstrom resolution[15]. At the same time, equilibrium configurations[16] and defect motion[17] have been investigated in a special realization of a two dimensional crystal: a colloidal lattice. This system affords convenient visualization of defect configurations and the concomitant strain fields. In particular, optical tweezers methods have recently allowed a very detailed analysis of the microscopic mechanisms of defect motion, including the emergence of dissipative motion as the extent of the defect increases[18]. The nanoscale structure of isolated defects has also been recently resolved in smectic liquid crystals with cryo-electron microscopy[19], with some surprising results concerning the structure and extent of edge dislocations. Additional interest in defect motion in two dimensional systems has been spurred by novel strain engineering methods that seek to control the electronic properties of graphene sheets[20–22].

Our study is also motivated by fully microscopic numerical investigations of a variety of defect mediated dynamics, including, for example, interactions among an ensemble of dislocations[23], plastic deformation or grain boundary motion[24]. Simple early models of plastic deformation in metals that are based on the existence of Frank-Read dislocation sources and their glide over lattice-specific slip planes have been greatly extended thanks to information obtained through massively parallel Molecular Dynamics studies. Such atomistic level simulations have enabled quantitative descriptions of complex situations in heavily deformed materials, e.g., dislocation nucleation at grain boundaries and their coupled motion[25]. Although atomistic in scale, the simulations methods are largely based on dissipative (or non-inertial) motion. This is accomplished by the introduction of suitable "thermostats" in the simulations, or by explicitly solving an elastic boundary value problem slaved to the instantaneous location of the defect lines[26]. The general assumption is that defect segment motion occurs in a time scale that is much slower than the characteristic time of elastic relaxation of the medium. This separation of time scales is also implicit in the model described in this paper. The model which we describe aims at a coarse grained description of these simulations while still retaining mesoscale information about the lattice slip planes

and their contribution to defect motion.

Bridging experiments at the nanoscale and related microscopic numerical studies with macroscopic descriptions based on continuum elasticity theory has proven difficult, but doing so is becoming a necessity in order to properly describe microstructural evolution in nanostructured materials[13,25,27–29]. We do not attempt here a derivation of dislocation mobilities from a microscopic model of a two-dimensional lattice. Rather we use symmetry arguments to propose phenomenological equations of defect motion that depend on the symmetry and local state of orientation of the lattice, and that allow for differential defect motion along distinguished directions. We consider two possible types of crystalline lattices in two dimensions: hexagonal and square. In the former case, the description is somewhat simpler in that, to linear order, defect energies are the same as in an isotropic material. However, the description of lattice effects near defect cores is complicated by the need to introduce geometrically unnecessary dislocations. On the square lattice, on the other hand, the anisotropic nature of the linear response is more complex. In both cases we obtain the orientation dependent mobilities under several approximations. We close by presenting an illustrative example involving the motion of two edge dislocations. We make a number of simplifications to make the calculation analytically tractable, and show how lattice rotation affects glide and climb motion, and how it can prevent dislocation annhilation thorough the local distortion of the slip planes.

II. MESOSCOPIC MODELS

We consider a two dimensional crystal that contains a large number of dislocations which are relatively close to each other, yet separated by distances much larger than the lattice spacing so that the distribution can be effectively coarse grained. A coarse graining cell is introduced with a net Burgers vector that is the sum of the many Burgers vectors of the underlying crystal dislocations within the cell. As is standard (see, e.g., Refs.[2,9]), the resulting Burgers vector density is approximated by a continuous vector field $\mathbf{b}(\mathbf{r})$ on this two dimensional space (with components $b_i(\mathbf{r}) = \alpha_{3i}(\mathbf{r}), i = x, y$ and 3 denoting the direction perpendicular to the plane). We first decompose the Burgers vector density into a

combination of a finite number of discrete slip systems[2,8,27,30]

$$\mathbf{b}(\mathbf{r}) = \sum_s b^{(s)}(\mathbf{r})\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) \tag{1}$$

where s runs over the possible slip systems with Burgers vector density $b^{(s)}$ locally oriented along the direction $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$. We assume that the unit vectors $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ can be expressed as $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) = (\cos(\theta(\mathbf{r}) + \pi s/2), \sin(\theta(\mathbf{r}) + \pi s/2))$, $s = 0, 1$, for a square lattice and $\hat{\boldsymbol{\theta}}^{s}(\mathbf{r}) = (\cos(\theta(\mathbf{r}) + 2\pi s/3), \sin(\theta(\mathbf{r}) + 2\pi s/3))$, $s = 0, 1, 2$, for a hexagonal lattice. The local rotation of the coarse graining cell is $\theta(\mathbf{r}) = (1/2)\epsilon_{ij}\mathrm{w}_{ij}(\mathbf{r})$ where ϵ_{ij} is the anti symmetric Levi-Civita tensor, and w_{ij} the elastic distortion tensor. The lines defined by the directions $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ do not cross if there are no unbound disclinations[31], which we assume throughout this paper.

In an unbounded medium, it is possible to express the elastic energy as a function of the Burgers vector density. For an isotropic system, this energy is given by[32,33]

$$H_{\mathrm{int}} = -\frac{K}{2}\int_{|\mathbf{r}-\mathbf{r}'|>a} d\mathbf{r}d\mathbf{r}' \left[\mathbf{b}(\mathbf{r})\cdot\mathbf{b}(\mathbf{r}')\ln\left(\frac{\rho}{a}\right) - \mathbf{b}(\mathbf{r})\cdot\hat{\boldsymbol{\rho}}\,\mathbf{b}(\mathbf{r}')\cdot\hat{\boldsymbol{\rho}}\right], \tag{2}$$

where a is a short distance cutoff on the order of the lattice spacing, K is the two dimensional Young's modulus and $\boldsymbol{\rho} = \mathbf{r} - \mathbf{r}'$, $\hat{\boldsymbol{\rho}}$ the corresponding unit vector, and $\rho = \|\boldsymbol{\rho}\|$. This expression does not include a nonlocal self-energy of the dislocation distribution due to their long ranged strain field because the total Burgers vector over the entire system is taken to be zero, so that dislocations are created and annihilated in opposing pairs. There is also, however, a local energy contribution associated with the nonlinear strain fields near the core of the dislocation. This energy is assumed to be approximately independent of the local strain field due to other sources[34], and is modeled by a quadratic term in the Burgers vector[32]

$$H_{\mathrm{loc}} = E_c\int d\mathbf{r}\;\mathbf{b}(\mathbf{r})\cdot\mathbf{b}(\mathbf{r}), \tag{3}$$

with E_c a constant core energy. Below we will propose a slightly different core energy to also include the energy of geometrically unnecessary dislocations (dislocation groups that do not contribute to the local Burgers vector density).

In an unbounded system, the solution of the equilibrium elasticity problem is equivalent to obtaining the Burgers vector density distribution. This is because the incompatibility of the plastic strain is completely balanced by an elastic strain that makes the total strain compatible[3]. This allows one to express the solution for the strain field as a function only of the Burgers vector density that acts as a source of strain[4,33].

Dislocations and other defects play a key role in determining the evolution, properties, and response of materials outside of thermodynamic equilibrium. While the systems under study here are assumed to be in elastic equilibrium relative to a given defect distribution, defects interact, and are free to move and annihilate to relieve stresses and reduce the overall energy of the system. Such an evolution can have reversible and irreversible contributions that correspond to different models of relaxation[18]. A number of theoretical studies in the literature have addressed dissipative motion of an ensemble of dislocations at the mesoscale[10–13,35–37]. A relaxational equation for the Burgers vector density is introduced under the assumption that the evolution of the density is driven by plastic energy minimization. The equation is of the general form,

$$\frac{\partial b_j}{\partial t} = -\epsilon_{lm} B_{mjsi} \epsilon_{sb} \partial_l \partial_b \frac{\delta H}{\delta b_i}, \tag{4}$$

where $H = H_{int} + H_{loc}$, and B_{mjst} is a constant mobility tensor. We propose in this paper a more accurate description of the kinetic motion of the defect distribution by considering anisotropic mobilities along slip lines of the lattice rather than along the orientations defined locally by the Burgers vector density as is the case in Eq. (4). Moreover, we show how to distinguish glide and climb in two dimensional lattices that are locally rotated, as they are in the presence of an ensemble of dislocations.

Within linear elasticity in an isotropic medium the local orientation of a two dimensional coarse graining cell is related to the Burgers vector density through a nonlocal relation[38],

$$\theta(\mathbf{r}) = -\frac{1}{2\pi} \int d\mathbf{r}' \, \frac{\mathbf{b}(\mathbf{r}') \cdot \hat{\boldsymbol{\rho}}}{\rho}. \tag{5}$$

On an infinite lattice in which the Burgers vector decays sufficiently fast at infinity we can take $\theta(\mathbf{r}) = 0$ at infinity[39]. The fact that the orientation is different at all points on the plane implies that the local slip lines $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ are also position dependent. Therefore if the dislocation mobility is anisotropic, Eq. (4) will not adequately describe defect motion along locally rotated slip systems.

We propose to extend Eq. (4) in two ways, both phenomenological and based on symmetry arguments. First, in the presence of an orientation field $\theta(\mathbf{r})$, or lattice torsion, there is no longer strict translational symmetry, but the composition of a translation and a rotation due to plastic deformation. In this way, the configurational energy depends explicitly on local orientation, as the lattice symmetries of reflection and rotation must be applied locally[9].

Second individual dislocations respond anisotropically to forcing so that the motion of an ensemble of dislocations depends on how the local Burgers vector density is decomposed among slip systems as shown in Eq. (1). We note that while we allow the slip system directions to be different from one coarse graining cell to another, we neglect changes to the relative angle between them due to deformation of the cell. Hence the local coordinate axis system defined by the slip systems $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ is, approximately, determined by a single angle $\theta(\mathbf{r})$ (as explicitly shown below Eq. (1)).

III. DISLOCATION MOTION ON A SQUARE LATTICE

The symmetry of the square lattice is generated by rotations about $\pi/2$ and reflections about the two bond axes forming the group D_4. This symmetry implies that a rank two tensor (a matrix) relating two vectors transforming under SO(2) has to be proportional to the identity matrix. This can be checked by assuming the most general 2×2 matrix and applying the transformation matrices, demanding equality of the initial and transformed matrices. A similar analysis for the compliance matrix, a rank four tensor relating the stress matrix to the strain matrix within linear elasticity (Hooke's Law) $u_{ij} = S_{ijkl}\sigma_{kl}$, shows that it can be written in general as,

$$S_{ijkl} = \alpha\delta_{ij}\delta_{kl} + \beta\delta_{i(k}\delta_{l)j} + \Delta\delta_{ijkl}, \tag{6}$$

where α, β, and Δ are constants related to the elastic constants of the lattice, and δ_{ijkl} is the fourth rank identity tensor. Here and below we will make use of the notation $A_{(bc)} = \frac{1}{2}(A_{bc} + A_{cb})$ and $A_{[bc]} = \frac{1}{2}(A_{bc} - A_{cb})$. There is an additional term allowed for a general fourth rank tensor which is not present here because the stress is symmetric $\sigma_{ij} = \sigma_{ji}$.

In the case of hexagonal symmetry addressed in Sec. IV, invariance under rotations of $\pi/3$ and reflections about the three independent bond orientations, and again within linear elasticity, leads to the same decomposition (6), but with $\Delta = 0$. Note that in this case, and within linear distortions, the compliance matrix has the same decomposition as in an isotropic system. In this latter case, the system is invariant under arbitrary rotations and reflections.

An approximate expression for the energy of a distorted and rotated lattice can be obtained by applying the tensorial decomposition above in the local coordinates of each rotated

coarse graining cell (it is still the case that the stress is symmetric on its indices in these coordinates). Introduce a local coordinate system with unit vectors $\hat{\mathbf{x}}'$ and $\hat{\mathbf{y}}'$ that are related to laboratory coordinates x and y by a rotation about $\theta(\mathbf{r})$: $\hat{\mathbf{x}}' = (\cos\theta, \sin\theta)^T$ and $\hat{\mathbf{y}}' = (-\sin\theta, \cos\theta)^T$. We use in what follows upper indices for tensors expressed in local coordinates and lower indices for tensors in the laboratory frame. Then, for example, $\sigma^{ab} = R^a_{.i}[\theta(\mathbf{r})]R^b_{.j}[\theta(\mathbf{r})]\sigma_{ij}$, where we have introduced the rotation matrix

$$R^a_{.i}[\theta] = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{7}$$

By reason of symmetry, we have

$$u^{ij} = \alpha\delta^{ij}\sigma^{kk} + \beta\sigma^{ij} + \Delta(\delta^{ix'}\delta^{jx'}\sigma^{x'x'} + \delta^{iy'}\delta^{jy'}\sigma^{y'y'}) \tag{8}$$

in local coordinates. Equation (8) transformed to the laboratory frame reads,

$$u_{ij} = \alpha\delta_{ij}\sigma_{kk} + \beta\sigma_{ij} + \Delta h_{ijkl}(\theta(\mathbf{r}))\sigma_{kl}. \tag{9}$$

with

$$\begin{aligned} &h_{xxxx} = h_{yyyy} = \cos^4\theta + \sin^4\theta, \qquad h_{xxyy} = \frac{1}{2}\sin^2 2\theta, \\ &h_{xxxy} = -h_{xyyy} = \frac{1}{4}\sin 4\theta, \end{aligned} \tag{10}$$

where the other components of the tensor function h_{klmn} come from that fact that it does not depend on the order of its indices (a general result for this symmetry). We also have used the notation $\sigma_{kk} = \mathrm{Tr}(\sigma_{ij})$.

The elastic energy can now be calculated as follows: Since $\partial_j\sigma_{ij} = 0$ and $\sigma_{ij} = \sigma_{ji}$ an Airy stress function $\chi(\mathbf{r})$ is introduced such that

$$\sigma_{ij} = \epsilon_{ik}\epsilon_{jl}\partial_k\partial_l\chi. \tag{11}$$

When there are no free disclinations, it is possible to express the Airy stress function in terms of Burgers vector density[33]. Apply $\epsilon_{ik}\epsilon_{jl}\partial_k\partial_l$ to Eq. (9) and substitute the definition (11) to find,

$$\epsilon_{ik}\epsilon_{jl}\partial_k\partial_l u_{ij} = \alpha'\nabla^4\chi + \Delta\epsilon_{ik}\epsilon_{jl}\partial_k\partial_l\hat{\mathcal{D}}_{ij}\chi, \tag{12}$$

where we have introduced $\alpha' = \alpha + \beta$, and the differential operator

$$\hat{\mathcal{D}}_{ij}[\theta] = h_{ijkl}(\theta)\epsilon_{km}\epsilon_{ln}\partial_m\partial_n. \tag{13}$$

The left hand side of Eq. (12) is, by definition, $\epsilon_{ik}\epsilon_{jl}\partial_k\partial_l u_{ij} = \epsilon_{ij}\partial_i b_j$. This definition, together with Eqs. (12) and (13), is the solution of the equilibrium elastic problem that gives $\chi(\mathbf{r})$ as a function distribution of the Burgers vector density $\mathbf{b}(\mathbf{r})$ and rotation $\theta(\mathbf{r})$ that still remains to be determined.

Once the solution $\chi(\mathbf{r})$ is determined, the energy of the configuration $H_{\rm int} = \frac{1}{2}\int d^2r u_{ij}\sigma_{ij}$ can be found by substituting Eq. (9) for the strain, and the definition of the Airy function, Eq. (11), for the stress. We find,

$$H_{\rm int} = \frac{1}{2}\int d^2r \chi(r)\left[\alpha'\nabla^4 + \Delta\epsilon_{ik}\epsilon_{jl}\partial_k\partial_l\hat{\mathcal{D}}_{ij}\right]\chi(r), \tag{14}$$

Equation (12) cannot be solved explicitly for the Airy function, and hence we cannot express the energy (14) explicitly as a function of the Burgers vector density, unlike the isotropic case of $\Delta = 0$ (in this latter case, the differential equation (12) is solved by using a Green's function method, see Nelson in his seminal paper[32], leading to Eq. (2) for the energy of interaction). Furthermore, the energy depends on the rotation θ through the dependence of the differential operator $\hat{\mathcal{D}}_{ij}$, Eq. (13). Obtaining such a relation is the subject of the next subsection.

Before proceeding, we note that it is possible to find a closed form of the energy if rotation is neglected, and one starts from the general form of Hooke's law for a square lattice, Eq. (8), written in laboratory frame coordinates (the linear elasticity regime, see, e.g.,[40]). Since

$$\hat{\mathcal{D}}_{ij}(\theta = 0) = \left[\delta_{ix}\delta_{jx}\epsilon_{xl}\epsilon_{xk} + \delta_{iy}\delta_{jy}\epsilon_{yl}\epsilon_{yk}\right]\partial_l\partial_k\chi = \left[\delta_{ix}\delta_{jx}\partial_y^2 + \delta_{iy}\delta_{jy}\partial_x^2\right]\chi, \tag{15}$$

Eq. (14) reduces to

$$H_{\rm int} = \frac{1}{2}\int d^2r \chi(r)\left[(\alpha' + \Delta)\nabla^4 - 2\Delta\partial_x^2\partial_y^2\right]\chi(r). \tag{16}$$

After Fourier transformation, substitution of Eq. (12) into Eq. (16) leads to an explicitly form of the energy in terms of the Burgers vector density

$$H_{\rm int} = \frac{1}{2}\int \frac{d^2q}{(2\pi)^2}\frac{|i\epsilon_{ij}q_i b_j|^2}{(\alpha' + \Delta)q^4 - 2\Delta q_x^2 q_y^2} = \frac{1}{2}\int \frac{d^2q}{(2\pi)^2}\frac{(q^2\delta_{ij} - q_i q_j)}{(\alpha' + \Delta)q^4 - 2\Delta q_x^2 q_y^2} b_i(q)b_j(-q). \tag{17}$$

This extends the isotropic result of $\Delta = 0$ to the square lattice.

A. Lattice rotation field

We next determine the nonlocal relationship between the local rotation of a coarse graining cell and the Burgers vector distribution to generalize Eq. (5) to a square lattice. The

local rotation $\theta(\mathbf{r})$, relative to an undistorted reference lattice with $\theta = 0$, is related the distortion tensor w_{ij}. The symmetric and anti symmetric parts of the distortion tensor are identified as the strain and orientation tensors respectively[3]

$$\mathrm{w}_{ij} = u_{ij} + \theta(\mathbf{r})\epsilon_{ij}. \tag{18}$$

By recalling the definition of the Burgers vector density in terms of the distortion tensor $b_k = \epsilon_{ij}\partial_j \mathrm{w}_{ik}$, and substituting the decomposition of the distortion tensor, Eq. (18), one has

$$b_k = \epsilon_{ij}\partial_j \left(\theta\epsilon_{ik} + u_{ik}\right) = \partial_k\theta + \epsilon_{ij}\partial_j u_{ik}. \tag{19}$$

Thus up to a constant, θ is specified by $\partial_k\theta = b_k - \epsilon_{ij}\partial_j u_{ik}$.

The divergence of second term in the r.h.s. of Eq. (19) can be calculated with the help of Eqs. (11) and (13),

$$\partial_k\epsilon_{ij}\partial_j u_{ik} = \alpha\left(\epsilon_{ij}\partial_j\partial_i\right)\sigma_{ll} + \beta\epsilon_{ij}\partial_j\left(\partial_k\sigma_{ik}\right) + \Delta\epsilon_{ij}\partial_k\partial_j\hat{\mathcal{D}}_{ik}\chi = \Delta\epsilon_{ij}\partial_k\partial_j\hat{\mathcal{D}}_{ik}\chi, \tag{20}$$

where we have used the anti symmetry of ϵ_{ij} and the condition of elastic equilibrium $\partial_k\sigma_{ik} = 0$. Thus the divergence of Eq. (19) is given by,

$$\nabla^2\theta = \partial_k b_k + \Delta\epsilon_{ij}\partial_k\partial_j\hat{\mathcal{D}}_{ik}\chi.$$

To solve for θ we introduce the Green's function of the two dimensional Laplacian operator and find,

$$\theta(\mathbf{r}) = \frac{1}{2\pi}\int_{|\mathbf{r}-\mathbf{r}'|>a} d\boldsymbol{r}' \ln\left(\frac{|\mathbf{r}-\mathbf{r}'|}{a}\right)\partial'_k\mathcal{B}_k(\theta,\mathbf{r}') = -\frac{1}{2\pi}\int_{|\mathbf{r}-\mathbf{r}'|>a} d\boldsymbol{r}'\frac{r_k - r'_k}{|\mathbf{r}-\mathbf{r}'|^2}\mathcal{B}_k[\theta,\mathbf{r}'], \tag{21}$$

where

$$\mathcal{B}_k[\theta,\mathbf{r}'] = b_k(\mathbf{r}') + \Delta\epsilon_{ij}\partial'_j\hat{\mathcal{D}}_{ik}(\theta(\mathbf{r}'))\chi(\mathbf{r}'), \tag{22}$$

which reduces to the Burgers vector density of an isotropic system when $\Delta = 0$.

Equations (12), (21), and (22), now constitute a closed set of equations for the elastostatics of a square lattice in terms of θ and $\mathbf{b}$. Equation (21), however, is only an implicit equation for $\theta(\mathbf{r})$. As pointed out by Kröner[3], to obtain a relation between $\mathbf{b}$ and θ one must solve the problem of elastic equilibrium everywhere in order to relate the stress σ_{ij} to the Burger's vector density $\mathbf{b}$.

A simpler form follows if θ is everywhere small so that it can be approximated by a constant in the right-hand side of Eq. (21). Then

$$\theta(\mathbf{r}) = -\frac{1}{2\pi}\int_{|\mathbf{r}-\mathbf{r}'|>a} \frac{d\boldsymbol{r}'}{|\mathbf{r}-\mathbf{r}'|^2}\left[(r_k - r'_k)b_k(\mathbf{r}') + \Delta(x-x')(y-y')\left(\sigma_{xx}(\mathbf{r}') - \sigma_{yy}(\mathbf{r}')\right)\right], \quad (23)$$

where a is a short distance cutoff on the order of the lattice spacing and we have dropped some boundary terms. This reduces to Eq. (5) in the isotropic limit $\Delta = 0$.

B. Dynamics

We extend next the kinetic equation (4). We decompose the Burgers vector density into a finite number of slip systems $\mathbf{b}(\mathbf{r}) = \sum_s b^{(s)}(\mathbf{r})\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$, each defined by its own density $b^{(s)}$ oriented along the direction $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$. On the square lattice we simply have $b^{(s)} = b^s$ and $\hat{\boldsymbol{\theta}}^{(s)} = \hat{\boldsymbol{\theta}}^s$, the variables along the locally rotated coordinate system.

Since the Burger's vector is a pseudo-vector (it is even under a parity transformation, whereas a vector is odd under parity) the natural Burgers vector flux is a pseudo-tensor Φ^i_k, which represents the flux along the k-direction of dislocations along the i-direction. For simplicity, we limit our analysis here to the case in which the Burgers vector densities are separately conserved[36]

$$\frac{\partial b^i(\mathbf{r})}{\partial t} = -\partial_k \Phi^i_k. \quad (24)$$

Explicitly, the assumption is that dislocations can only be created or destroyed by pair annihilation and creation on each slip system. This requirement also guarantees that the energy integral is finite for an infinite system. As stated earlier, we require that the bond directions are well defined, which implies the absence of free disclinations[31].

Thermodynamic forces leading to defect motion arise from $\frac{\delta H}{\delta b^i(\mathbf{r})}$, the change in energy for a dislocation along slip plane direction i to be placed at $\mathbf{r}$. Therefore its partial derivative $\partial_k \frac{\delta H}{\delta b^i(\mathbf{r})}$ represents the local difference in energy for dislocation placement, and is thus the thermodynamic force. The total energy H is quadratic in b^i so that the resulting thermodynamic force will be linear in b^i, although nonlocal. Since b^i is pseudo-scalar, we find that the thermodynamic force is a pseudo-scalar. In linear response, forces and fluxes are linearly related as,

$$\Phi^i_k(\mathbf{r}) = -D^i_{kj}(\mathbf{r}) \;\; \partial_j \frac{\delta H}{\delta b^i(\mathbf{r})}. \quad (25)$$

This expression is nonlocal because the thermodynamic force is a nonlocal functional of the dislocation densities. Of course, this is only the case in the slow temporal scale of dislocation segment motion, and is a consequence of the assumption that the system is at all times in elastic equilibrium. We now distinguish glide and climb motion and decompose D^i_{kj} along the direction $\hat{\boldsymbol{\theta}}^i(\mathbf{r})$ and transverse to it

$$D^i_{kj} = D_g \theta^i_k \theta^i_j + D_c \left(\delta_{kj} - \theta^i_k \theta^i_j\right), \tag{26}$$

where D_g is identified as the mobility for glide motion, and D_c for climb. For a square lattice, we write

$$\hat{\boldsymbol{\theta}}^l(\mathbf{r}) = \begin{pmatrix} \cos[\theta(\mathbf{r}) + l\frac{\pi}{2}] \\ \sin[\theta(\mathbf{r}) + l\frac{\pi}{2}] \end{pmatrix}, \tag{27}$$

where $l = 0$ defines x' and $l = 1$, y'. A similar decomposition of the dislocation mobility into climb and glide components was given in the study of elastic instabilities of thin films[36], and for the motion of isolated dislocations[8,41].

By combining Eqs. (24), (25), and (26) we obtain the phenomenological equation of motion for the Burgers vector densities,

$$\frac{\partial b^i(\mathbf{r})}{\partial t} = \left[\partial_k (D_g - D_c)\theta^i_k \theta^i_j \partial_j + D_c \nabla^2\right] \frac{\delta H}{\delta b^i(\mathbf{r})}. \tag{28}$$

This dynamical equation along with Eqs. (12), (14), (21), and (22) completely specify our anisotropic model on the square lattice. This, and the corresponding expression for a hexagonal lattice to be given below, are the central results of this paper.

Prior work has not considered lattice rotation effects on dislocation motion. We briefly show that Eq. (28) reduces to simpler expressions, already in the literature, when rotation is uniform. This simpler description allows for a more direct comparison with isotropic theories in which the laboratory coordinate system is the natural choice. We begin by writing

$$\partial_t b_k = \partial_t \sum_i \hat{\theta}^i_k b^i = \sum_i \hat{\theta}^i_k \partial_t b^i, \tag{29}$$

Then inserting Eq. (28), we find

$$\partial_t b_k = \sum_i \hat{\theta}^i_k \partial_n D^i_{nm} \partial_m \frac{\delta H}{\delta b^i}. \tag{30}$$

We also have the relation $\frac{\delta H}{\delta b^i} = \hat{\theta}^i_l \frac{\delta H}{\delta b_l}$, which follows from the chain rule. Then we can write the response explicitly in terms of the Burgers vector density alone,

$$\partial_t b_k = \sum_i \hat{\theta}^i_k D^i_{nm} \hat{\theta}^i_l \left\{ \partial_n \partial_m \frac{\delta H}{\delta b_l} \right\}, \tag{31}$$

which explicitly separates the current originating from the excess energy associated with dislocations and a mobility coefficient that depends on local orientation. Substitute Eq. (26) into Eq. (31) and evaluate the sums over the orientation directions

$$\sum_i \theta^i_k \theta^i_l = \delta_{kl}, \qquad \sum_i \theta^i_k \theta^i_l \theta^i_m \theta^i_n = h_{klmn}(\theta), \tag{32}$$

where the rank four tensor h is defined in Eq. (10), so that Eq. (31) reduces to

$$\partial_t b_k = K \left[(D_g - D_c) h_{kmnl} + D_c \delta_{mn} \delta_{kl} \right] \partial_n \partial_m \frac{\delta H}{\delta b_l}. \tag{33}$$

Just taking the rotation angle to be zero, the equations of motion reduce to[40]

$$\begin{aligned} \partial_t b_x(\mathbf{q}, t) &= - \left[D_g q_x^2 + D_c q_y^2 \right] \frac{q_y \left[q_y b_x(\mathbf{q}) - q_x b_y(\mathbf{q}) \right]}{(\alpha' + \Delta) q^4 - 2\Delta q_x^2 q_y^2} \\ \partial_t b_y(\mathbf{q}, t) &= - \left[D_g q_y^2 + D_c q_x^2 \right] \frac{-q_x \left[q_y b_x(\mathbf{q}) - q_x b_y(\mathbf{q}) \right]}{(\alpha' + \Delta) q^4 - 2\Delta q_x^2 q_y^2}. \end{aligned}$$

IV. DISLOCATION MOTION ON A HEXAGONAL LATTICE

The fact that the linear elastic response of a hexagonal lattice is isotropic makes the evaluation of the elastic energy in Eq. (14) much simpler because any dependence on lattice orientation vanishes at this order in the strain. On the other hand, on a two dimensional hexagonal lattice there are three independent slip planes along which individual Burgers vectors can be oriented. As was the case for the square lattice, the Burgers vector distribution can be written as $\mathbf{b}(\mathbf{r}) = \sum_s b^{(s)}(\mathbf{r}) \hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ with[8]

$$\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) = \begin{pmatrix} \cos[\frac{2\pi s}{3} + \theta(\mathbf{r})] \\ \sin[\frac{2\pi s}{3} + \theta(\mathbf{r})] \end{pmatrix} \qquad s = 0, 1, 2. \tag{34}$$

Unlike the case of a square lattice, a two dimensional hexagonal lattice has three separate slip systems, and hence three separate Burgers vector densities. This implies that the two dimensional Burgers vector density has to be decomposed along three independent projections, not two. To solve this difficulty, we propose to introduce a new coarse grained field

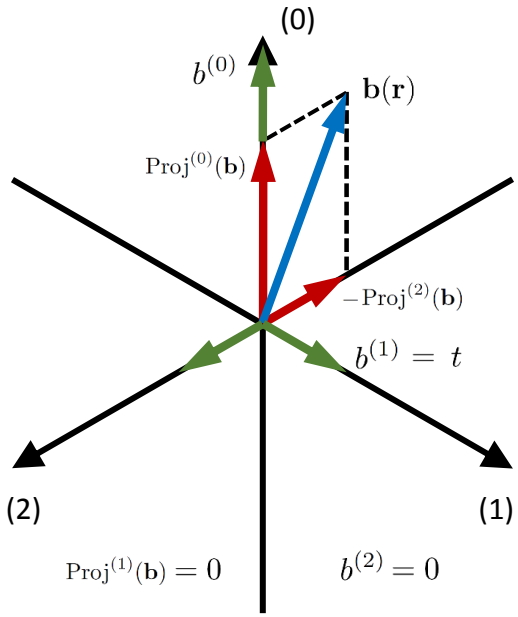

FIG. 1. An illustration of the two decompositions used (color online). The Burger's vector is shown in blue and its projections onto the nearest glide planes are in red. The green vectors represent the triplet density. The dislocation densities are the sum of the corresponding projection (red) and the triplet density (green). The case shown is when the dislocation density $b^{(2)}$ vanishes and $b^{(1)}$ does not receive a projection. $\hat{\theta}^{(0)}$ is shown vertical for convenience, but its orientation with respect to $\hat{x}$ is given by θ.

that captures dislocation configurations not describable by the Burgers vector density. For instance, a dislocation triplet within a single coarse graining cell, one in each of the positive $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ directions, has zero Burgers vector. These dislocations are considered geometrically unnecessary since they do not contribute to the elastic energy, but they can be considered to contribute to the local anisotropic response. We therefore define the triplet density field $t(\mathbf{r})$ as

$$b^{(s)} = t + \mathrm{Proj}^{(s)}(\mathbf{b}), \tag{35}$$

with

$$\mathrm{Proj}^{(s)}(\mathbf{b}) = \left| \hat{\theta}_i^{(s)} \left(\delta_{ij} - \frac{1}{\sqrt{3}} \epsilon_{ij} \right) b_j \right| \times \mathrm{sgn} \left(\hat{\boldsymbol{\theta}}^{(s)} \cdot \mathbf{b} \right) \Theta \left[\| \hat{\boldsymbol{\theta}}^{(s)} \cdot \mathbf{b} \| - \frac{1}{2} \right], \tag{36}$$

being the local projection of the Burgers vector density onto the *nearest* two directions $\hat{\boldsymbol{\theta}}^{(s)}$. This term can almost be written as a tensor; the sign function arises from the fact that our

choice of non orthogonal axes depends on the angle of $\mathbf{b}$, and the step function Θ ensures that one axis does not receive a projection from $\mathbf{b}$. This can also be written directly in terms of the absolute angle $\omega^{(\alpha)}$ between $\hat{\boldsymbol{\theta}}^{(s)}$ and $\mathbf{b}$,

$$\mathrm{Proj}^{(s)}(\mathbf{b}) = \|\mathbf{b}\| \left| \frac{2}{\sqrt{3}} \cos\left(\omega^{(s)} - \frac{\pi}{6}\right) \right| \times \mathrm{sgn}(\cos\omega^{(s)}) \Theta \left[|\cos(\omega^{(s)})| - \frac{1}{2} \right]. \tag{37}$$

A positive triplet has an equal Burgers vector in each of the positive $\hat{\theta}^{(s)}$ directions. Note that t is odd under rotations about $\pi/3$, and hence also under reflections.

While it is simple to write down the Burgers vector density given the Burgers density components along the slip systems, the inverse problem requires the determination of the geometrically unnecessary density t. For simplicity, our assumption here is that all of the geometrically unnecessary dislocation content is in t. Therefore, the decomposition of the coarse-grained $\mathbf{b}$ onto the two nearest lattice directions $\hat{\boldsymbol{\theta}}^{(s)}$ is minimal in the following sense: If $\mathbf{b}$ is parallel or anti parallel to one of the slip planes $\hat{\boldsymbol{\theta}}^{(s)}$, the lowest energy configuration is assumed to be the one that only has dislocations pointing along this axis: $b^{(s)} = \|\mathbf{b}\|$ with $b^{(r\neq s)} = 0$. Otherwise, we project $\mathbf{b}$ onto the two (of six) closest non-orthogonal directions along which a Burgers vector can point. Then the remaining dislocation densities must form a zero-vector configuration. This choice of decomposition is motivated because it is the one that minimizes a local defect energy associated with a core energy that depends on the number of dislocations rather than the magnitude of the Burgers vector.

We consider only three separate signed densities, and opposite pairs within the same coarse graining cell are assumed to annihilate; the only remaining coarse-grained configurations of geometrically unnecessary defects are dislocation triplets. We could, on the other hand, consider six separate dislocation densities on the three slip systems. This may be a more accurate description for large coarse graining cells. Here we may consider smaller coarse graining cells so that opposite dislocations in the same cell would be unstable to annihilation energetically. However, this ignores the fact that opposite dislocations on different glide planes can form a stable dislocation pattern that has no vector component and corresponds to a vacancy defect. We do not consider this complication here and only add more variables as are necessary to introduce a dependence of the response on the local bond orientation.

In summary, we choose the three densities $b^{(s)}(\mathbf{r})$ to be our primitive variables. The lattice orientation field $\theta(\mathbf{r})$ and the Burgers vector density $\mathbf{b}(\mathbf{r})$ can be obtained by simultaneously

solving Eqs. (1), (5), and (34). From them the triplet density $t(\mathbf{r})$ can be obtained. We note that the three Burgers vector densities and the triplet dislocation density at every point in space contain all of the information of the defected lattice configuration that we are considering.

The equilibrium linear elasticity of the hexagonal system is simple: decompositions of rank two and rank four tensors are the same as for isotropic systems. We can therefore use known results for isotropic systems: Given the two dimensional Young modulus K, the elastic energy of a configuration of defects is well described by the long ranged transverse interaction of Eq. (2)[33]. The energy depends only on the Burgers vector density $\mathbf{r}$, and not on the make-up of that defect density in terms of dislocations densities $b^{(s)}(\mathbf{r})$ in the three different slip directions.

In terms of the core energy, we proceed by analogy with Eq. (3), and introduce a local contribution to the energy from defect cores of the form

$$H_{loc} = \frac{E_c}{2} \int d\mathbf{r} \sum_s b^{(s)}(\mathbf{r}) b^{(s)}(\mathbf{r}). \tag{38}$$

The energy E_c is the approximate local energy cost due to lattice distortion to have a dislocation pair along a given direction. Note that this expression allows both geometrically necessary and unnecessary dislocations. The above form is different than Eq. (3), although the two definitions coincide on the square lattice. Equation (38) predicts that the core energy of a dislocation triplet is $\frac{3}{2}E_c$. The ratio of 3/2 between triplets and pairs is in good agreement with experiments on two-dimensional colloids[16] where the energies of dislocation pairs and triplets were measured for various configurations, each of which create a vacancy defect.

It is our expectation, however, that as the coarse graining cell size increases, the core energy Eq. (38) would simply reduce to the core energy in Eq. (3). In fact, the local driving force arising from the core energy satisfies the relation

$$\sum_s \hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) \frac{\delta H_{loc}}{\delta b^{(s)}(\mathbf{r})} \propto \mathbf{b}(\mathbf{r}), \tag{39}$$

in agreement with the result that follows from the standard form of the core energy in Eq. (2). Hence the degree of anisotropy in the core energy of a hexagonal lattice is expected be a function of the coarse graining size, with the limiting behavior being that of an isotropic system.

A. Dynamics

The equation of conservation of Burgers vector is still Eq. (24), but the linear response assumption relating forces and fluxes is given by

$$\Phi_k^{(s)}(\mathbf{r}) = -\frac{2}{3} D_{kj}^{(s)}(\mathbf{r}) \;\; \partial_j \frac{\delta H}{\delta b^{(s)}(\mathbf{r})}. \tag{40}$$

The constant factor of 2/3 corrects for the fact that the sum of the projections onto three linearly dependent axes over represents a vector by the factor γ in $\sum_s \theta_k^{(s)} \theta_l^{(s)} = \gamma \delta_{kl}$, which is 3/2 for the hexagonal lattice (Eq. (45)).

The energy in terms of the Burgers vector densities is the same as in an isotropic system. Inserting Eq. (1) into Eq. (2), we have

$$H_{\rm int} = -\frac{K}{2} \int d\mathbf{r} d\mathbf{r}' \sum_{s,r} \left[\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) \cdot \hat{\boldsymbol{\theta}}^{(r)}(\mathbf{r}') \ln\left(\frac{\rho}{a}\right) - \left(\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) \cdot \hat{\boldsymbol{\rho}}\right) \left(\hat{\boldsymbol{\theta}}^{(r)}(\mathbf{r}') \cdot \hat{\boldsymbol{\rho}}\right) \right] b^{(s)}(\mathbf{r}) b^{(r)}(\mathbf{r}'), \tag{41}$$

so that the functional derivatives are

$$\frac{\delta H_{\rm int}}{\delta b^{(s)}(\mathbf{r})} = -K \int d\mathbf{r}' \sum_{r} \left[\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) \cdot \hat{\boldsymbol{\theta}}^{(r)}(\mathbf{r}') \ln\left(\frac{\rho}{a}\right) - \left(\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r}) \cdot \hat{\boldsymbol{\rho}}\right) \left(\hat{\boldsymbol{\theta}}^{(r)}(\mathbf{r}') \cdot \hat{\boldsymbol{\rho}}\right) \right] b^{(r)}(\mathbf{r}') \tag{42}$$

or,

$$\frac{\delta H_{\rm int}}{\delta b^{(s)}(\mathbf{r})} = -K \int d\mathbf{r}' \;\; \left[\theta_k^{(s)}(\mathbf{r}) \ln\left(\frac{\rho}{a}\right) - \left(\hat{\boldsymbol{\theta}}^{(\boldsymbol{s})}(\mathbf{r}) \cdot \hat{\boldsymbol{\rho}}\right) \rho_k \right] b_k(\mathbf{r}'). \tag{43}$$

We now assume that the mobility in Eq. (40) can be decomposed along the local slip planes into glide and climb components as in Eq. (26). The resulting equation of motion for a hexagonal lattice is also

$$\frac{\partial b^{(s)}(\mathbf{r})}{\partial t} = \frac{2}{3} \left[(D_g - D_c) \partial_k \left(\theta_k^{(s)}(\mathbf{r}) \theta_l^{(s)}(\mathbf{r}) \right) \partial_l + D_c \nabla^2 \right] \frac{\delta H_{\rm int}}{\delta b^{(s)}(\mathbf{r})}. \tag{44}$$

The orientations $\hat{\boldsymbol{\theta}}^{(\boldsymbol{s})}$ follow from Eq. (5) and (34).

If we consider again the limiting case in which the orientation is taken to be uniform, $H_{\rm int}$ and the kinetic equation only depend on the Burgers vector density not on the separate components along the slip systems. This can be shown by multiplying Eq. (44) by $\theta_k^{(s)}$ and summing over s. For rank two and four tensors the corresponding sums are isotropic tensors due to the hexagonal lattice symmetry,

$$\begin{aligned} \sum_s \theta_k^{(s)} \theta_l^{(s)} \theta_m^{(s)} \theta_n^{(s)} &= \frac{3}{8} \left[\delta_{kl} \delta_{mn} + \delta_{kn} \delta_{lm} + \delta_{km} \delta_{ln} \right] \\ \sum_s \theta_k^{(s)} \theta_l^{(s)} &= \frac{3}{2} \delta_{kl}. \end{aligned} \tag{45}$$

We find,

$$\frac{\partial b_k(\mathbf{r})}{\partial t} = D_{klmn}\partial_l\partial_m \frac{\delta H_{\rm int}}{\delta b_n(\mathbf{r})}, \tag{46}$$

with

$$D_{klmn} = \frac{1}{4}\left[(D_g + 3D_c)\delta_{lm}\delta_{kn} + (D_g - D_c)2\delta_{k(l}\delta_{m)n}\right]. \tag{47}$$

This expression reduces to the expected isotropic limit of $D_g = D_c$.

Before addressing the contribution to dislocation motion in a hexagonal lattice that arises from H_{loc} , we compare our results, Eqs. (46) and (47), with prior coarse grained treatments of the form (4),[11,13,37]. Comparison of Eqs. (4) and (46) leads to the identification,

$$B_{jksn} = \epsilon_{jl}\epsilon_{sm}D_{klmn} \tag{48}$$

where we have made repeated use of the identity $\epsilon_{ij}\epsilon_{jn} = -\delta_{in}$ in two dimensions. Explicit substitution of Eq. (47) leads to,

$$\begin{aligned} B_{jksn} &= \frac{1}{4}\left[(3D_g + D_c)\delta_{js}\delta_{kn} + (D_c - D_g)2\delta_{k(s}\delta_{j)n}\right] \\ &= \frac{1}{2}(D_g + D_c)\left(\delta_{j(s}\delta_{n)k} - \frac{1}{2}\delta_{jk}\delta_{sn}\right) + D_g\delta_{j[s}\delta_{n]k} + D_c\frac{1}{2}\delta_{jk}\delta_{sn}. \end{aligned} \tag{49}$$

where we have separated the tensor B into a symmetric but traceless part, an anti symmetric part, and the trace part with respect to the first two indices (equivalently the last two). This allows us to make a connection with the properties of the dislocation density current $J_{jk} \propto B_{jksn}$[11] as already argued by Limkumnerd based on volume change arguments[37]: the trace of the current is proportional to D_c so that the dislocation current is indeed traceless if there is no climb.

Equation (49) is symmetric under the exchange of first and second pairs of indices ($(j,k) \leftrightarrow (s,n)$) which is consistent with Onsager's reciprocity relation because the rate of free energy change is

$$\frac{dF}{dt} = -\int d^3r \frac{\delta H}{\delta b_j} B_{mjst}\epsilon_{lm}\epsilon_{sb}\partial_l\partial_b\frac{\delta H}{\delta b_t}.$$

However, we obtain two additional allowed terms in B_{mjst} compared to Ref.[11]. The latter only give the traceless symmetric contribution in Eq. (49). In addition, and unlike prior work, our expression for the mobility does explicitly distinguish between climb and glide motion.

We turn next to the calculation of the contribution to the motion of the Burgers vector density arising from the local part of the energy. Replace $H_{\rm int}$ by H_{loc} given in Eq. (38)

in Eq. (44). The isotropic term in Eq. (44), proportional to D_c, leads to diffusion of $\mathbf{b}(\mathbf{r})$ when the equation is multiplied by $\hat{\boldsymbol{\theta}}^{(\alpha)}$ and summed over α. However, the term involving the longitudinal derivative is quite nontrivial because it involves products of three bond unit vectors. When such a product is summed over bonds α the resulting rank three tensor is not independent of the bond orientation $\theta(\mathbf{r})$ although it does have hexagonal symmetry with respect to the bond angle. Neglecting terms involving time derivatives of the slip line orientations, we find the core contribution to the evolution equation to be,

$$\left(\frac{\partial b_k(\mathbf{r})}{\partial t}\right)_c \approx \frac{2}{3}(D_g - D_c)\sum_\alpha \theta_k^{(\alpha)}\theta_l^{(\alpha)}\theta_m^{(\alpha)}\partial_l\partial_m\frac{\delta H_c}{\delta b^{(\alpha)}(\mathbf{r})} + \frac{2}{3}D_c\nabla^2 b_k. \tag{50}$$

Given Eqs. (38) and (35) we find

$$\frac{\delta H_c}{\delta b^{(\alpha)}(\mathbf{r})} = E_c b^{(\alpha)}(\mathbf{r}) = E_c\left(t + \mathrm{Proj}^{(\alpha)}(\mathbf{b})\right). \tag{51}$$

We define the third rank tensor

$$g_{klm}(\theta) = \frac{4}{3}\sum_\alpha \theta_k^{(\alpha)}\theta_l^{(\alpha)}\theta_m^{(\alpha)}, \tag{52}$$

so that

$$\begin{aligned} g_{xxx} &= \cos 3\theta \qquad & g_{xxy} &= \sin 3\theta \\ g_{yyy} &= -\sin 3\theta \qquad & g_{yyx} &= -\cos 3\theta. \end{aligned} \tag{53}$$

Here again the tensor does not depend on the order of its indices since it comes from a tensor product over a single vector. Then Eq. (50) reduces to,

$$\left(\frac{\partial b_k(\mathbf{r})}{\partial t}\right)_c = \frac{2}{3}D_c\nabla^2 b_k + \frac{1}{2}E_c(D_g - D_c)g_{klm}(\theta)\partial_l\partial_m t(\mathbf{r}) + \ldots \tag{54}$$

We have not explicitly written here the term involving projections of $\mathbf{b}$ since we just want to point out that there exists a dependence of the motion of the Burgers vector density on geometrically unnecessary defects through the triplet density t. Although expression (54) is largely formal, it does show a kinetic equation that explicitly depends on the rotation field θ through a term that includes the density of unnecessary dislocations.

We reiterate that the exact projections of the Burgers vector along slip systems, and the concomitant triplet density, will depend on the size of the coarse graining cell. As its size becomes larger, the triplet density will decrease as the geometrically unnecessary dislocations are averaged out. As a consequence, the contribution from Eq. (54) to the motion of the

Burgers vector will become smaller as the coarse graining cell becomes larger. Eventually, at sufficiently long spatial scales, the evolution on the hexagonal lattice should become the same as in an isotropic system.

In summary, although we cannot provide complete explicit equations for the model that we have introduced except within the approximations given, the implicit relations between magnitudes can be obtained via a numerical implementation. In it, given the Burgers vector density distribution as initial condition, Eq. (44) needs to be iterated in time, together with Eq. (54) and the related equation that results from the local projection of $\mathbf{b}$. Equations (5) and (34) allow the determination of the orientations $\hat{\boldsymbol{\theta}}^{(s)}(\mathbf{r})$ from the densities. From the densities and the orientations the Burgers vector follows. The interaction energy $H_{\rm int}$ can now be evaluated. Equation (35) is then used to determine the triplet density, and the system of equations evolved in time.

V. TWO EDGE DISLOCATIONS

The coarse grained theory presented has a simpler representation when the defects are assumed to be discrete and isolated, although the assumptions of the theory fail in this limit. For the sake of illustration only, we consider in this section the motion of two point edge dislocations and also assume that both defect interaction energies and lattice rotation can be approximated by the results for an isotropic solid.

Consider as initial condition two edge dislocations at $\mathbf{r} = \mathbf{r}_1$ and $\mathbf{r} = \mathbf{r}_2$ of Burgers vectors $b\ \hat{\boldsymbol{x}}$ and $-b\ \hat{\boldsymbol{x}}$ respectively on an undistorted, infinite, two dimensional space. In order to avoid the complication of unnecessary dislocations, we consider the case of only two slip planes as would be appropriate for a square lattice. As was the case in Sec. III, superindices correspond to magnitudes expressed in the rotated lattice.

Insertion of these two dislocations in the otherwise undistorted lattice leads to rotation. For the purposes of the present example, we estimate the lattice rotation by assuming that the medium is isotropic instead, Eq. (5)[38],

$$\theta(\mathbf{r}) = -\frac{1}{2\pi}\left[\frac{b(\mathbf{r}-\mathbf{r}_1)\hat{\boldsymbol{\theta}}^0(\mathbf{r}_1)}{|\mathbf{r}-\mathbf{r}_1|^2} - \frac{b(\mathbf{r}-\mathbf{r}_2)\hat{\boldsymbol{\theta}}^0(\mathbf{r}_2)}{|\mathbf{r}-\mathbf{r}_2|^2}\right]. \tag{55}$$

The initial condition (55) assumes that the Burgers vectors are directed along one slip plane at the location of the defects. As shown following Eq. (1), the directions of the slip planes

of this notional square lattice are

$$\hat{\boldsymbol{\theta}}^0(\mathbf{r}) = (\cos\theta(\mathbf{r}), \sin\theta(\mathbf{r})) \qquad \hat{\boldsymbol{\theta}}^1(\mathbf{r}) = (\cos\theta(\mathbf{r}+\pi/2), \sin\theta(\mathbf{r}+\pi/2)) \tag{56}$$

The rotation field (55) becomes singular at the defect location. This singularity can be eliminated, for example, by noting that near the defect the smallest possible distance is on the order of the lattice spacing, itself on the order of the Burgers vector. Other models of defect structures[42] lead to zero rotation near the defect core. We adopt the latter and by combining Eqs. (55) and (56), we find the following implicit relations for the lattice rotation,

$$\begin{aligned}\theta(\mathbf{r}_1) &= \frac{b}{2\pi}\frac{(\mathbf{r}_1-\mathbf{r}_2)\cdot(\cos\theta(\mathbf{r}_2), \sin\theta(\mathbf{r}_2))}{|\mathbf{r}_1-\mathbf{r}_2|^2} \\ \theta(\mathbf{r}_2) &= \frac{b}{2\pi}\frac{(\mathbf{r}_1-\mathbf{r}_2)\cdot(\cos\theta(\mathbf{r}_1), \sin\theta(\mathbf{r}_1))}{|\mathbf{r}_1-\mathbf{r}_2|^2}\end{aligned} \tag{57}$$

The location of the defects and the two rotations of Eq. (57) constitute the initial conditions of the problem.

A. Dynamics

Defect motion on a square lattice is governed by Eq. (28). The initial discrete Burgers vector distribution can be written as

$$\mathbf{b} = b\,\delta(\mathbf{r}-\mathbf{r}_1(t))\,\hat{\boldsymbol{\theta}}^0(\mathbf{r}_1) - b\,\delta(\mathbf{r}-\mathbf{r}_2(t))\,\hat{\boldsymbol{\theta}}^0(\mathbf{r}_2), \tag{58}$$

where $\delta(\mathbf{r})$ is the two dimensional Dirac delta distribution. The initial Burgers vector of both dislocations is taken along $\hat{\boldsymbol{\theta}}^0$, and given the assumed separate conservation of Burgers vector components along each slip plane, $\mathbf{b}$ will remain along $\hat{\boldsymbol{\theta}}^0$ for all times.

Given the relation $\partial_t\delta(\mathbf{r}-\mathbf{r}(t)) = -\partial_j\left(\delta(\mathbf{r}-\mathbf{r}(t))\frac{dr_j}{dt}\right)$, the conservation law of Burgers vector, Eq. (24) can be written as,

$$b\left[\delta(\mathbf{r}-\mathbf{r}_1(t))\frac{d(\mathbf{r}_1)_k}{dt} - \delta(\mathbf{r}-\mathbf{r}_2(t))\frac{d(\mathbf{r}_2)_k}{dt}\right] = -\left(D_g\theta^0_k\theta^0_j + D_c(\delta_{kj}-\theta^0_k\theta^0_j)\right)\partial_j\frac{\delta H}{\delta b^1(\mathbf{r})}, \tag{59}$$

where we have also used the linear constitutive assumption of Eq. (25), and the relation for the anisotropic diffusivity of Eq. (26).

In order to compute the thermodynamic driving force in the right hand side of Eq. (59) we write Eq. (41) as

$$H = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}' V_{st}(\mathbf{r},\mathbf{r}')b^s(\mathbf{r})b^t(\mathbf{r}'). \tag{60}$$

Then, given the discrete Burgers vector distribution of Eq. (58), we find

$$\partial_j \frac{\delta H}{\delta b^1(\mathbf{r})} = -b\left[\partial_j V(\mathbf{r},\mathbf{r}_1(t)) - \partial_j V(\mathbf{r},\mathbf{r}_2(t))\right], \tag{61}$$

also having defined $V = V_{11}$. Finally, the kinetic equation for the location of dislocation one is

$$\frac{d(\mathbf{r}_1)_k}{dt} = \left(D_g \theta^0_k(\mathbf{r}_1)\theta^0_j(\mathbf{r}_1) + D_c(\delta_{kj} - \theta^0_k(\mathbf{r}_1)\theta^0_j(\mathbf{r}_1))\right)\left(-\partial_j V(\mathbf{r},\mathbf{r}_2)\right)_{\mathbf{r}=\mathbf{r}_1}, \tag{62}$$

and the analogous equation for the second dislocation. This equation has the form $\frac{d(\mathbf{r}_1)_k}{dt} = L_{kj}F_j$ according to which the defect velocity equals a mobility times a thermodynamic force. The mobility in this example depends explicitly on lattice variables: the orientation of the slip systems at the defect location.

The thermodynamic force can now be evaluated explicitly from the interaction energy (41) if we also approximate it by that of an isotropic medium. In Fourier space, it is given by

$$H = \frac{K}{2}\int \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{1}{q^2}\left(\delta_{ij} - \hat{q}_i\hat{q}_j\right) b_i(\mathbf{q})b_j(-\mathbf{q}). \tag{63}$$

For example, for a single edge dislocation at the origin, $b_j(\mathbf{r}) = b\delta(x_1)\delta(x_2)\delta_{j1}$, the energy of the configuration V_1 is

$$V_1 = \frac{Kb^2}{2}\int \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{q_2^2}{q^4}. \tag{64}$$

If we now consider instead two edge dislocations as in Eq. (58) with $\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2$, their interaction energy (excluding self energies) is

$$V(\boldsymbol{\rho}) = -Kb^2\int \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{q_2^2 e^{i\mathbf{q}\cdot\boldsymbol{\rho}}}{q^4}. \tag{65}$$

This integral can be evaluated explicitly. Let

$$J(\boldsymbol{\rho}) = \int d\mathbf{q}\frac{e^{i\mathbf{q}\cdot\boldsymbol{\rho}}}{q^4}, \tag{66}$$

then $V(\boldsymbol{\rho}) = (Kb^2/(2\pi)^2)(\partial^2 J(\boldsymbol{\rho})/\partial\rho_2^2)$. The two dimensional Green's function of the bi-harmonic operator $\nabla^4 G(\mathbf{r}-\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}')$ is $G(\mathbf{r}-\mathbf{r}') = -\frac{|\mathbf{r}-\mathbf{r}'|}{8\pi}\left(\ln|\mathbf{r}-\mathbf{r}'| - 1\right)$. Then $J(\boldsymbol{\rho}) = (\pi/4)|\boldsymbol{\rho}|^2\left(\ln|\boldsymbol{\rho}|^2 - 2\right)$ and,

$$V(\boldsymbol{\rho}) = -\frac{Kb^2}{(2\pi)^2}\frac{\pi}{2}\left[1 - \frac{2\rho_2^2}{\rho^2} - \ln\rho^2\right]. \tag{67}$$

This leads to the thermodynamic forces,

$$-\frac{\partial V}{\partial\rho_1} = -\frac{Kb^2}{(2\pi)^2}\frac{1}{\rho}\cos\phi\cos 2\phi, \quad -\frac{\partial V}{\partial\rho_2} = -\frac{Kb^2}{(2\pi)^2}\frac{1}{\rho}\sin\phi(1+2\cos^2\phi), \tag{68}$$

where ϕ is the angle between the line joining the two dislocations and the x axis. The functional dependence in Eq. (68) agrees with the classical result for the interaction force between two straight edge dislocations in an isotropic medium (noting, e.g., that $\sin\phi(1 + 2\cos^2\phi) = y(3x^2 + y^2)/(x^2 + y^2)^{3/2}$)[43]. The coefficients differ in the planar strain considered there because the stress in the direction along the dislocation line in three dimensions is not zero, but rather $\sigma_{33} = \nu(\sigma_{11} + \sigma_{22})$, with ν the Poisson ratio. This component of the stress tensor does not appear in the purely two dimensional calculation addressed here.

Given an initial configuration comprising two edge dislocations, Eqs. (68) would give the force acting on each one that is required in the right hand side of Eq. (62). The anisotropic mobility depends of lattice rotation at the location of each defect, which is given by Eqs. (57). Equation (62) then gives the defect velocities.

We next evaluate the system of equations numerically. Consider that the two opposite edge dislocations lie along the line $y = 0$ separated by a distance $10b$. For convenience, we work in reduced units such that distances are expressed in units of b and speed in units of $D_g K b$. In a first scenario, we suppose that only glide is possible (i.e., $D_c/D_g = 0$) and examine the impact of lattice rotation on the motion of the dislocations. Figure 2a shows the dependence of dislocation position on the $y = 0$ line, $x(t)$, on time, t, for each dislocation. As is evident from the figure, in the absence of lattice rotations, the dislocations move with increasing speed until annihilation. Figure 2b shows the dislocation position normal to this plane, $y(t)$. In the absence of lattice rotations, there is no motion perpendicular to the plane, as expected.

If lattice rotations are incorporated in the model, qualitatively new behavior is observed. Figures 2a and 2b also show that the motion of two dislocations is similar to the case of no rotation for large separations, but the two defects come to rest at a fixed separation. The local rotation of the lattice has evidently resulted in motion in the y-direction leading to the formation of a stable, dipolar configuration oriented at somewhat less than 45° from the x-axis. (One would expect a 45°-dipole for two opposite edge dislocations moving on parallel slip planes in the absence of lattice rotations.)

In the second scenario, we assess the effect of defect climb on the trajectory of the dislocations. Figures 3 show the positions, $x(t)$, and $y(t)$, respectively, for $D_c/D_g = 0.02$ with lattice rotations for the two dislocations. The inclusion of climb is seen to lead to an instability in the dipolar configuration resulting in annihilation, as might be expected from

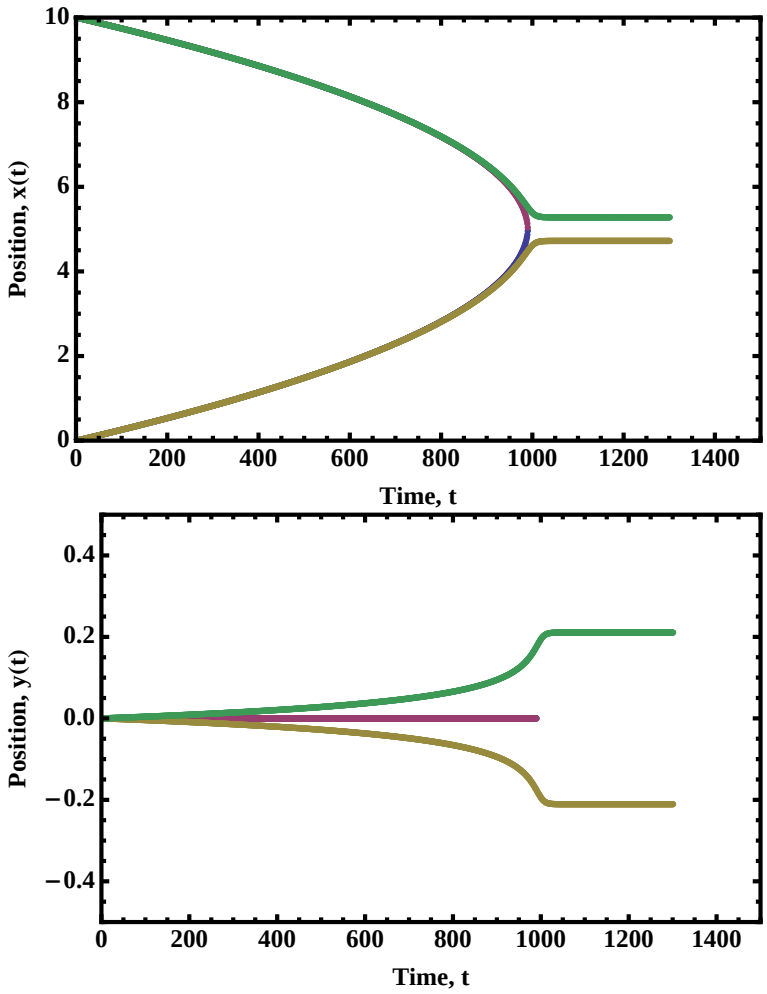

FIG. 2. a.) The dislocation position on the $y = 0$ line, $x(t)$, as a function of time, t, for two opposite edge dislocations that are initially separated by a distance of 10, in units of b. For each case there is no climb mobility. The blue and red curves are the positions in the absence of lattice rotations, while the gold and green curves pertain to a system with lattice rotations. Note that, in the latter case, motion is arrested after some time. b.) The corresponding dislocation position, $y(t)$, as a function of time, t, for the two dislocations.

the functional form of the force in the y-direction given in Eqs. (68).

This illustrative example, while highlighting the main elements and dependencies of the model described in Sections III and IV, has several shortcomings. First and foremost, the theory as presented is expected to apply to a coarse grained defect distribution but not to isolated defects. Thus the overdamped nature of Eq. (25) can only be assumed at the mesoscale, not at the scale of individual dislocations. Second, and for the purpose of the

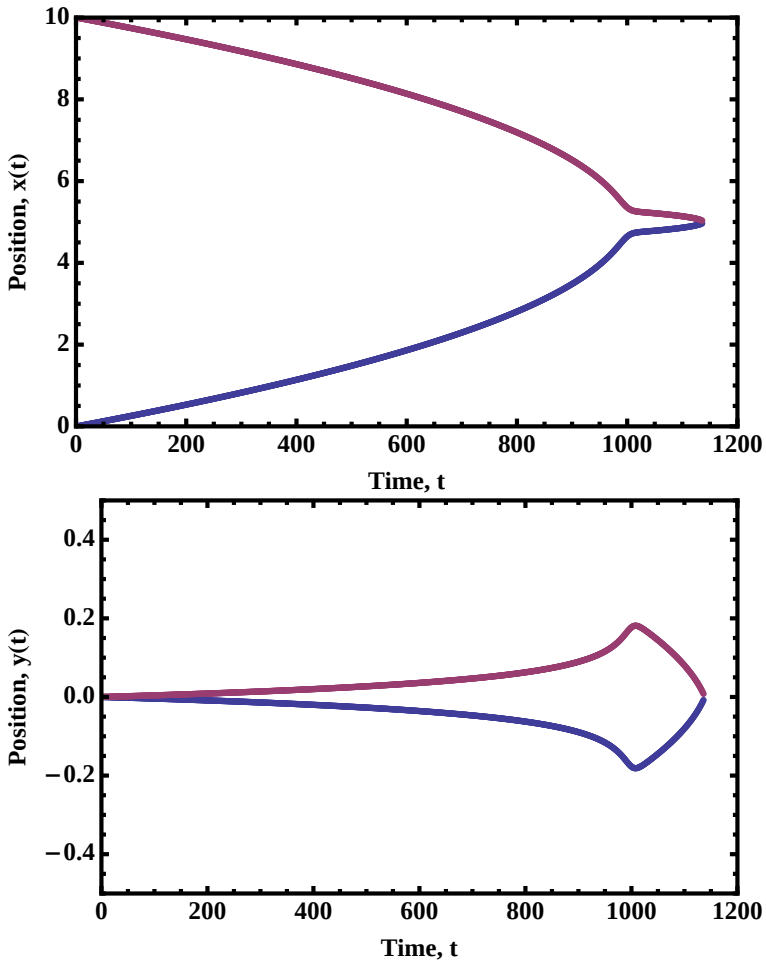

FIG. 3. a.) The dislocation position, $x\,(t)$, as a function of time, t, for the case in which both lattice rotations and climb are operative. In this case, $D_c/D_g = 0.02$. The dipolar configuration seen in the previous figure is unstable and annihilation results. b.) The corresponding dislocation position, $y\,(t)$, as a function of time, t.

example, we have used isotropic results to compute interaction defect energies and lattice rotation, while retaining motion along two privileged slip axes. The results of Secs. III and IV are free of these limitations, but are considerably more involved, necessitating a fully numerical approach for their analysis.

We conclude by mentioning that we expect that the methods described above provide a first step into incorporating kinetic lattice effects into continuum (coarse-grained) descriptions of defect motion. We have done so by allowing directional defect mobilities along distinguished slip systems in weakly distorted systems. The case of a square lattice is somewhat simpler as the number of slip systems equals the dimensionality of the lattice. For

a hexagonal lattice, on the other hand, linear elasticity is that of an isotropic system -a simplification- whereas the coarse-grained model requires the introduction of geometrically unnecessary dislocations -a complication. In this latetr case, and for large coarse-graining volumes, a fully isotropic theory is expected albeit with separate climb and glide diffusivities. Unfortunately, the governing equations which we have obtained are quite complex and need to be evaluated numerically. Such a numerical solution could be compared to direct coarse-graining of Molecular Dynamics simulations of two-dimensional lattices. Alternatively, our results can be verified against numerical solutions of Phase Field Crystal models which hold at the same level of coarse graining as our theory. Finally, for the simple example of two point edge dislocations that we have described in Sec. V, we have shown dynamical arrest in dislocation motion that arises from mismatches in the local slip planes as the defects approach each other. Such an effect is absent in a purely continuum theory.

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