Density gradients driving crystal dislocations

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Dislocations are topological defects known to be crucial in the onset of plasticity and in many properties of crystals. Classical Elasticity still fails to fully explain their dynamics under extreme conditions of high strain gradients and small scales, which can nowadays be scrutinized. By separating conformal and shape deformations, we construct a new formalism for two-dimensional (2D) classical Elasticity and describe edge dislocations as finite disclination dipoles. This lead us to heuristically obtain that dislocations can be driven by a fundamentally new type of force, which is induced by background density (or hydrostatic strain) gradients. The existence of such mechanism is confirmed through atomistic simulations, where we can move and trap individual dislocations using such configurational force. It depends on a small length parameter, has nonlocal character and can provide ground basis for some phenomenological theories of size effects in plasticity.

The idea of dislocation defects was first conceived mathematically, and later applied in the context of plasticity, by considering the movement of defects in a periodic lattice. It soon became a vital feature of investigation in the structure of real three-dimensional (3D) crystals. In addition, since the bubble-raft models, 2D crystals have been widely used as simple models to study dislocation dynamics (for example, using colloids, complex plasmas and vortices in superconductors). Especially in the new 2D materials such as graphene, defects are increasingly showing to be an important factor on the mechanical, electronic, optical, thermal and chemical properties. Therefore, significant effort has been devoted to find different ways of controlling dislocation distributions in 2D.

The individual dislocation movement is generally assumed to be governed by configurational forces which are well known for decades. There are the Peach-Koehler (PK) driving force due to background stresses and the Peierls-Nabarro barrier due to crystal’s discreteness, besides other possible motion’s resistance, climb and diffusion mechanisms. These forces have been widely used to model plastic deformations in Discrete Dislocation Dynamics (DDD) simulations, where the exact locations of all atoms can be ignored and one only needs to consider the dynamics of dislocation lines, in 3D, or points, in 2D. The validity of such mesoscale approach relies on the forces and mobility law that it considers. The PK interactions between dislocations have power law behavior and the resulting dynamics has no intrinsic length scale (thus leading to a “similarity principle”). The size effects and length scales emerging from DDD simulations and from rigorous theories based on PK driving forces are usually associated with the obstacle and dislocation densities. They still cannot explain the full range of new plastic phenomena with technological impact observed, for instance, in micron and sub-micron scales (with a “smaller is stronger” trend) and during shock loadings. Thus, several phenomenological and mechanism-based models have been developed, including corrections to the mobility law, nonlocal Elasticity and strain gradient plasticity.

The aim of our work is to broaden current knowledge about dislocation dynamics. By separating shear deformations and variations in density and orientation, a new formulation of 2D Elasticity is constructed. It shows to be suitable in the problem of configurational forces on edge dislocations, which in real crystals are described as finite disclination dipoles. We heuristically obtain that dislocation glide can be induced by a background density gradient in the glide direction. This new type of driving force have an intrinsic length parameter and nonlocal behavior. Such mechanism cannot be directly predicted by classical continuum Elasticity and provides a more fundamental motivation for strain gradient theories. Finally, using atomistic simulations, we demonstrate its existence and measure its parameter for some systems.

2D Elasticity formalism

In a deformed crystal, the deformation gradient tensor \( F \) relates its particles’ positions \( \{ r \} \) with the ones of a reference perfect crystal \( \{ R \} \) through \( d \mathbf{r} = F \mathbf{r} \mathbf{d} \mathbf{R} \). We are interested in the current configuration of the crystal (that is, an Eulerian description) and consider, as our measure of deformation, the deviation of \( F^{-1} = F^{-1}(\mathbf{r}) \) from identity. This tensor measure can be decomposed in its 3 irreducible parts (that is, the trace, the antisymmetric and the traceless symmetric parts) that do not mix after rotations. We write it as

\[
I - F^{-1} = \frac{1}{2} \left\{ C_x I - C_y \epsilon + \begin{bmatrix} S_x & S_y \\ S_y & -S_x \end{bmatrix} \right\},
\]

where \( I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \) and \( \epsilon = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \). The definitions of the “vectors” \( C = (C_x^*) \) and \( S = (S_x^*) \) are convenient for us since they consistently separate the deformation in parts with different natures. After a rotation of coordinates where normal vectors in the system (such as \( \mathbf{r} \)) are rotated by an angle \( \theta \), \( C \) remains unchanged and \( S \) is rotated by \( 2\theta \) (see Supplementary Information). Therefore, we can say that \( C, r \) and \( S \) behave, respectively, as spin-0 (scalar), spin-1 (true vector) and spin-2 objects, where the spin indicates how much the mathematical object is rotated.

It is useful to directly relate \( C \) and \( S \) in \( \mathbf{r} \) with the displacement field \( \mathbf{u}(\mathbf{r}) = \mathbf{r} - \mathbf{R}(\mathbf{r}) \). We use the definition...
\[ F_{ij}^{-1} = \nabla_j R_i = \delta_{ij} - \nabla_j u_i, \] where \( \nabla = \partial / \partial r \), and define operations \( \circ \) and \( \ast \) such that we can write
\[
C = \nabla \circ u \equiv \begin{pmatrix} \nabla_x u_x + \nabla_y u_y \\ \nabla_x u_y - \nabla_y u_x \end{pmatrix} = \left( \begin{array}{c} \nabla \cdot u \\ \nabla \wedge u \end{array} \right) \tag{2}
\]
and
\[
S = \nabla \ast u \equiv \begin{pmatrix} \nabla_x u_x - \nabla_y u_y \\ \nabla_x u_y + \nabla_y u_x \end{pmatrix} = \nabla u_x - \epsilon \cdot \nabla u_y. \tag{3}
\]
The spin character resulting from the bilinear map \( \circ \ast \) is the spin in the right entry minus (plus) the spin in the left entry. For example, \( \nabla \circ S \) and \( \nabla \ast C \) behave as true vectors (that is, spin-1 fields).

Note that \( S = 0 \) implies in Cauchy-Riemann equations for the components of \( u \) and then \( C \) gives conformal deformations, preserving relative angles. In linear Elasticity (that is, for small deformations), the components in (2) have well-known interpretations: \( C \) is the one after deformation, while \( \rho \) is valid and the interaction energy of deformation is twice the angle of rotation (which does not strain the crystal). In contrast, the traceless symmetric part of \( \nabla \cdot u \) is the deviatoric strain tensor and responsible for pure shear strains (shape changes).

Shear and density variations cost energy. For small deformations in triangular and hexagonal crystals with short-range interactions, isotropic linear Hyperelasticity is valid and the interaction energy of deformation is
\[
U_{int} = \frac{1}{2} \int \left[ BC_x^2(r) + \mu |S(r)|^2 \right] \, d^3r, \tag{4}
\]
where \( B \) and \( \mu \) are the bulk and shear moduli, respectively. The interaction force density within the crystal is obtained from (4) using \( F_{int} = -\frac{\partial U_{int}}{\partial u} = \nabla \circ S + \nabla \ast C \). Thus, the equilibrium condition, when the particles are subjected to an external force field \( F_{ext}(r) \), is given by
\[
B \nabla C_x + \mu \nabla \circ S + \rho_0 F_{ext}(r) = 0. \tag{5}
\]
Note that \( C \) and \( S \) are derivatives of the same \( u \) and then obey some compatibility conditions. Moreover, in the presence of defects, the possibility of \( u \) do not satisfy the commutation of partial derivatives must be taken into account. We define the Burgers vector of a single dislocation \( i \) as \( b_i = \frac{1}{2} \delta \cdot du \), for small counterclockwise closed curves enclosing it, and obtain
\[
\nabla \ast C(r) - \nabla \circ S(r) = 2 \epsilon \cdot B(r) \tag{6}
\]
where \( B(r) = (\nabla \circ \nabla) u(r) = \sum_i b_i \delta (r - r_i) \) is the density of Burgers vectors (see Supplementary Information).

In a crystal where \( B(r) \) and boundary conditions are known, equation (6) can be used to determine \( C(r) \) from \( S(r) \) and vice versa. We can then entirely describe the deformation using only the shape variations (\( S \)) or, alternatively, using only the variations in density (\( C_x \)) and orientation (\( C_y \)). This physical duality originates from the mathematical duality in the definition of the spin-0 field \( C \) and the spin-2 field \( S \). We show in this article that the \( S \)-picture of Elasticity is appropriate for describing PK forces on dislocations in terms of local strains. On the other hand, the \( C \)-picture is suitable for a local description of induced torques on finite disclination dipoles.

We remark that our only assumption about the original configuration \{\( R \)\} was that it represents a perfect periodic crystal. In linear approximation, choosing different density and orientation for that reference crystal is equivalent to adding constants to \( C_x \) and \( C_y \), respectively. On the other hand, the shear field \( S \) is invariant under such conformal transformations of \{\( R \)\}, in linear Elasticity. Since the (nonrelativistic) crystal dynamics must depend on the current configuration \{\( r \)\} only, some local physical quantities at some point cannot depend on the local \( C(r) \) but \( S(r) \) and derivatives of them. This is the case for configurational forces on dislocations.

## Configurational forces on point dislocations
For a single dislocation \( B(r) = b \delta(r) \), we have singular deformation fields inducing regular ones, in order to reach equilibrium \( (\mathbf{b}) \), and the resulting deformation have
\[
C^{(disl)}(r) = \frac{\epsilon \cdot [(B + 2\mu) \mathbf{r} \circ b + B \mathbf{b} \circ \mathbf{r}]}{2\pi(B + \mu)|\mathbf{r}|}, \tag{7}
\]
and
\[
S^{(disl)}(r) = -\frac{B \epsilon \cdot [(\mathbf{r} \circ \mathbf{b} + \mathbf{b} \circ (\mathbf{r} \circ \mathbf{r})]}{2\pi(B + \mu)|\mathbf{r}|}, \tag{8}
\]
where \( \mathbf{r} = r/|\mathbf{r}| \) (see Supplementary Information for details). Fig. 1a shows the shear field \( S^{(disl)}(r) \) when \( \mathbf{b} = \mathbf{b}/|\mathbf{b}| = \hat{x} \). The most energetically favorable and ubiquitous value for \( |\mathbf{b}| \) in the triangular crystal is the lattice spacing \( a_0 = (2/(\sqrt{3}\rho_0))^{1/2} \). The corresponding

![FIG. 1. Strain fields of a dislocation. a. Shear field \( S^{(disl)}(r) \) for a point dislocation with \( \mathbf{b} \parallel \hat{x} \) and the corresponding crystal configuration, represented by light gray circles in the background. b. Field \( \nabla C_x^{(disl)}(r) \), representing the negative of density gradient, near the dislocation core when we consider it as a finite disclination dipole. The disclination particles are represented by filled circles in the background.](image-url)
uum theory has shown to provide useful results. In spite of its divergences, continu-
ous formulations illustrate fivefold (sevenfold) disclinations. The Peach-Koehler force for glide movement
\begin{equation}
\hat{\mathbf{b}} \cdot \mathbf{F}_{\text{Peach-Koehler}}(\mathbf{r}) = \mathbf{\nabla} \cdot \mathbf{C}(\mathbf{r}) = \mathbf{\nabla} C_x(\mathbf{r}) - \epsilon \cdot \mathbf{\nabla} C_y(\mathbf{r}).
\end{equation}
This relation directly shows how lines of discontinuity on $C_x$ or $C_y$ (separating regions with different density or orien-
tation, respectively) require dislocations concentrated on these lines, giving rise to grain boundaries. We remark
that relation (10) suggests yet another trend to $\mathbf{B} \perp \mathbf{\nabla} C_x$.

The nonzero averaged $\mathbf{B}(\mathbf{r})$ in (10) provides a direct illustration of Geometrically Necessary Dislocations (GNDs), which strongly affect the plastic properties of the crystal. The GNDs motivated phenomenological theories of strain gradient plasticity by considering that dislocation distributions must not only depend on strains, as suggested by (9), but also on their gradients. We intend to study how strain gradients can influence dislo-
cation dynamics at a fundamental level, contributing to the emergence of size effects in plasticity.

Fig. 2 shows results from some Molecular Dynamics (MD) simulations where the individual dislocation po-
sitions depend on conservative external forces $\mathbf{F}_{\text{ext}} = -\nabla V_{\text{ext}}$ which do not produce background resolved shear on them. The $S_{\text{res}}$ on each dislocation is produced only by the other one, with the PK forces trying to drive them to annihilate each other. They are

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**FIG. 2. Dislocations with mutual Peach-Koehler attraction and kept separated by the effect of density gradients.** Configurations obtained from MD simulations at low temperatures (see Supplementary Information for details). a, In a perfect triangular crystal with lattice spacing $a_0$ and pairwise interactions of power-law repulsion $V_{\mu}(r) = (a_0/r)^{\delta}$, a pair of dislocations was nucle-
ated and thereafter they were kept separated by the action of a conservative external potential field $V_{\text{ext}}(x, y) = -V_0 e^{-(x^2+y^2)/2\sigma^2}$ centered between them, where $V_0 = 12\epsilon$ and $\sigma = 3.7a_0$. b, Similar simulation but using Lennard-Jones interactions $V_{\mu}(r) = e[(a_0/r)^{12}-(a_0/r)^6]$ and external potential $V_{\text{ext}}(x) = V_0\left[e^{-(x+D+\sigma)^2/2\sigma^2} - e^{-(x-D-\sigma)^2/2\sigma^2} - e^{-(x+D-\sigma)^2/2\sigma^2} + e^{-(x-D+\sigma)^2/2\sigma^2}\right]$ where $V_0 = 2.7\epsilon$, $\sigma = 3.5a_0$ and $D = 12a_0$. The light red (blue) in the background help us to visualize the density gradients, illustrating regions where the density was increased (decreased) due to the action of $V_{\text{ext}}$. Dark red (blue) cells in Voronoi constructions illustrate fivefold (sevenfold) disclinations.
kept separated though, at adjustable distances, due to the effect of external forces which generate \( \varphi_{res}^{(bg)} = 0 \) and \( \hat{b} \cdot \nabla C_x^{(bg)} \neq 0 \) on them. In these cases, point dislocations are weak approximations to real ones. Their \( \nabla C_x^{(disc)} \) is ill-defined inside the dislocation core where, on the real crystal, there is a finite effective density gradient. Such core structure thus needs to be considered.

**Effective torques on finite disclination dipoles**

We look for the outcomes of relating the dislocation in the real crystal with a finite disclination dipole in continuum theory. To do so, we first analyze the deformation fields of a disclination. In this type of defect, the orientation \( C_y^{(disc)} = \nabla \wedge u^{(disc)} \) is the multivalued quantity, that is, \( \oint dC_y^{(disc)} = s \) where \( s \) is the disclination charge. Here again there are singular fields inducing regular ones through (10) and, for a disclination at the origin, we obtain (see Supplementary Information)

\[
\nabla \varphi C^{(disc)}(r) = \frac{B+2\mu}{\mu} \nabla C_x^{(disc)}(r) = -\frac{s(B+2\mu)}{2\pi(B+\mu)} \hat{r}, \quad (11)
\]

This is an irrotational source/sink type of field. Only the irrotational/longitudinal part of \( \nabla \varphi C^{(bg)} \) (or of \( \nabla \varphi S^{(bg)} \)) can couple with the disclination fields. For them (and then for dislocations too), in the \( \mathbf{C} \)-description of Elasticity, the relevant local background strain derivatives are restricted to density gradients.

The dislocation, as a disclination dipole, is a source-sink pair of density singularities. We then expect that the real crystal dislocation has, in its core, regions with high and low densities. Such regions have particles with more or less neighbors. For triangular lattices, we define disclination particles as the ones having more or less than six neighbors in a Voronoi tessellation. They are not necessarily at the same positions of the disclination singularities in continuum theory (which, during dislocation glide, move continuously as in a rigid body translation). In the discrete crystal, the dislocation glide is a change in the disclination particles due to exchanges of neighbors.

The key feature here is that the dipole of disclination particles (or the dipole of regions with high and low densities, in general lattices) can rotate and produce relevant variations in the local density gradient. Fig. 1b shows the field \( \nabla C_x^{(disc)} \) near the core of a dislocation (with \( \hat{b} = \hat{x} \)) which is considered to be a finite disclination dipole. By assigning the properties of (11) to the disclination particles, we can see that a gradient field is produced in the direction of \( \hat{b} \) when such particles move oppositely to each other in this direction (that is, an effective dipole’s rotation).

We propose that a background density gradient parallel to \( \hat{b} \) induces an effective rotation on the dislocation in order to counterbalance such gradient. The effective Burgers vector direction, locally responsible for the strains and obtained from the disclination particles’ positions, is rotated due to \( \hat{b} \cdot \nabla C_x^{(bg)} \). The rotation is accompanied by a dipole’s elongation and becomes a local resolved shear deformation, which induces glide. Such mechanism is observed in simulations, as it is shown in Fig. 3. In this case, on the dislocation, we have the (induced) resolved shear

\[
S_{res}^{(ind)}(r) = L \hat{b} \cdot \nabla C_x^{(bg)}(r) \quad (12)
\]

where \( L \) is an intrinsic length scale for the linear response. Note that between Figs. 3a and 3b (or between Figs. 3c and 3d) \( S_{res}^{(ind)} \) was varied but the disclination particles remained the same due to the Peierls-Nabarro barrier.

**Quantitative investigations**

We use low temperature MD simulations to quantitatively probe the total configurational force

\[
\hat{b} \cdot F^{(tot)}_{disl} \propto S_{res}^{(tot)} = (\hat{b} \cdot \hat{b}) \wedge S^{(bg)} + L \hat{b} \cdot \nabla C_x^{(bg)}. \quad (13)
\]

Considering the same external potential of the system in Fig. 3 (that is, the one in Fig. 2b but with \( \sigma = 10a_0 \)
and \( D = 40a_0 \), we use the condition \( S^{(tot)} = 0 \) to obtain an analytical expression relating the external potential strength \( V_0 \) with the equilibrium distance \( d \) between the dislocations (see Supplementary Information for details). A single fitting parameter remains. It is given by \( B_{\text{ann}} \) and can be viewed as simply an energy scale factor. The analytical curves for \( V_0 \) versus \( d \) have a minimum at \( d \approx 84a_0 \), regardless of the interparticle interaction. For \( V_0 \) less than this minimum, the dislocations annihilate each other, as observed in simulations.

Fig. 4 presents results from simulations for different types of short-range pair interactions: power-law interactions \( V_p^{\text{PL}}(r) = \varepsilon (a_0 / r)^6 \), and Lennard-Jones interactions \( V_{\text{LJ}}^{\text{LJ}}(r) = 0.387323 \varepsilon [(a_0 / r)^{12} - (a_0 / r)^6] \). For these systems, the bulk and shear moduli can be evaluated and then we can obtain \( L \) from the fitting result (see Supplementary Information). The strength of \( V_p^{\text{PL}} \) was chosen in such a way that both systems have the same density profile due to the external force field.

While \( S^{(tot)} \) considers continuous possibilities for the dislocation positions, one can observe in Fig. 4 that \( d \) varies with hops (in steps of \( \approx a_0 \)). This occurs because of our way of considering each dislocation position, approximated as the mean position of its disclination particles. In fact, within some finite ranges of \( V_0 \), the system stay in nearly the same \( d \) due to the Piterls-Nabarro barrier. We believe that this barrier and nonlinear effects are the main reasons for the theoretical fits in Fig. 4 start to fail in the region of large \( d \), where they are most relevant.

The interpolations for \( d < 94a_0 \), shown in Fig. 4, provide \( L^{\text{PL}} \approx 0.683a_0 \) and \( L^{\text{LJ}} \approx 4.43a_0 \) for the power-law and Lennard-Jones interactions, respectively. Note that in the systems of Fig. 4, we have induced shear \( \mathbf{L} \cdot \nabla C_\mathbf{xy}^{(bg)} \) of the order of \( 10^{-3} \) and tiny variations on it are able to induce glide. Therefore, the wavelengths of density variations can be much larger than \( L \) and still drive dislocations.

### Concluding remarks on the new configurational force

On account of the compatibility conditions \( \nabla \mathbf{C} \), the total force \( \mathbf{f}_{\text{tot}} \) can neither be expressed locally in the \( \mathbf{S} \)-picture of Elasticity nor in the \( \mathbf{C} \)-picture. While the glide due to PK forces directly decreases the local energy density, the force due to \( S_{\text{res}} \) has a nonlocal origin. The induced rotation contributes to a decrease in \( \mathbf{S} \cdot \nabla C_x \) and then in the integral of \( C_x^2 \), decreasing the total energy. The induced shear itself costs energy and is compensated by the dislocation glide, as in PK.

In fact, the induced resolved shear appears only near the dislocation core. Fig. 5 shows how much localized it is, along the direction \( \perp \mathbf{b} \), for the system of Fig. 3. In this direction, it changes sign and goes to zero within a few lattice spacings \( a_0 \). Because of this change in sign, we
expect that the new force may not be effective in high-angle grain boundaries but can drive low-angle ones, in which the dislocations are sufficiently apart.

The proposed mechanism driving dislocations to regions with lower particle density has much to be investigated. We can directly observe and measure its effects on atomistic simulations but our theoretical approach still lacks an expression for \( L \) and explicit energetic analysis. It may be possible to construct a generalized continua theory\(^6\) in which the Eschekian formalism of configurational forces\(^8\) provides a more formal derivation of \( (13) \). The consideration of a rotating disclination dipole could not be made within classical continuum theory, which prevents rotation of the dipole by topologically constraining the direction of \( \mathbf{b} (= \mathbf{f} \cdot \mathbf{d} \mathbf{u}) \), even though non-singular treatments of the dislocation core\(^2\) can be made.

We anticipate that expression \( (13) \) could be readily adapted for forces on line elements of edge dislocations in 3D and it can be used in DDD simulations to obtain more reliable results. (Note that, while PK forces between dislocations decay as \( 1/\mathbf{r} \), the new contributions decay as \( \sim L/r^2 \).) Moreover, such fundamental influence of strain gradients must be taken into account in constructing better theoretical models for dislocation phenomena. Finally, we hope that recent experimental advances\(^45;50\) may probe the effects of this new force and measure \( L \) in important materials.

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Supplementary Information for “Density gradients driving crystal dislocations”

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Supplementary References

I. 2D ELASTICITY USING \( C \) AND \( S \)

A. Some properties of \( C \) and \( S \)

After a rotation of coordinates by \( \theta \), the normal vectors and tensors transform as \( \mathbf{r}' = R_{\theta} \cdot \mathbf{r} \) and \( \mathbf{F}' = R_{\theta} \cdot \mathbf{F} \cdot R_{\theta}^{-1} \), respectively, where \( R_{\theta} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \). Thus, equation (1) of the main text directly gives \( \mathbf{C}' = \mathbf{C} \) and \( \mathbf{S}' = R_{2\theta} \cdot \mathbf{S} \). Such rotational properties are related to the operations \( \mathbf{v} \circ \mathbf{w} \equiv (v_x w_y + v_y w_x) \) and \( \mathbf{v} \cdot \mathbf{w} \equiv (v_x w_x + v_y w_y) \). We also have

\[
\nabla \cdot \mathbf{C} = \nabla \cdot \left[ \nabla \circ \mathbf{u}(\mathbf{r}) \right] = \nabla^2 \mathbf{u}(\mathbf{r}) + \varepsilon \cdot \left[ (\nabla_x \nabla_y - \nabla_y \nabla_x) \mathbf{u}(\mathbf{r}) \right]
\]

(S1)

and

\[
\nabla \circ \mathbf{S}(\mathbf{r}) = \nabla \circ \left[ \nabla \cdot \mathbf{u}(\mathbf{r}) \right] = \nabla^2 \mathbf{u}(\mathbf{r}) - \varepsilon \cdot \left[ (\nabla_x \nabla_y - \nabla_y \nabla_x) \mathbf{u}(\mathbf{r}) \right].
\]

(S2)

For a single dislocation at \( \mathbf{r}_0 \), we define its Burgers vector through the line integral \( \mathbf{b} = \oint \mathbf{u}(\mathbf{r}) = \oint d\mathbf{r} \cdot \nabla \mathbf{u}(\mathbf{r}) = \oint d\mathbf{r} (\nabla \times \nabla) \mathbf{u}(\mathbf{r}) \) for any counterclockwise closed curve enclosing \( \mathbf{r}_0 \) and then \( (\nabla_x \nabla_y - \nabla_y \nabla_x) \mathbf{u}(\mathbf{r}) = \mathbf{b} \delta(\mathbf{r} - \mathbf{r}_0) \). For general distributions of dislocations, we define the density of Burgers vectors by \( \mathbf{B}(\mathbf{r}) = (\nabla \times \nabla) \mathbf{u}(\mathbf{r}) = \sum_i \mathbf{b}_i \delta(\mathbf{r} - \mathbf{r}_i) \). Therefore, by taking equation (S1) minus equation (S2), we find the compatibility conditions

\[
\nabla \cdot \mathbf{C}(\mathbf{r}) - \nabla \circ \mathbf{S}(\mathbf{r}) = 2\varepsilon \cdot \mathbf{B}(\mathbf{r}).
\]

(S3)

We can use the Green’s function for the 2D Laplacian, given by \( G(\mathbf{r} - \mathbf{r}') = \ln |\mathbf{r} - \mathbf{r}'|/2\pi \) with \( \nabla^2 G(\mathbf{r} - \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \) and \( (\nabla \times \nabla) G(\mathbf{r} - \mathbf{r}') = 0 \), to obtain solutions for inhomogeneous differential equations of \( \nabla \cdot \) and \( \nabla \circ \). We have

\[
\mathbf{C}(\mathbf{r}) = \nabla \circ \int G(\mathbf{r} - \mathbf{r}') [\nabla \cdot \mathbf{C}(\mathbf{r}')] d^2r' + \mathbf{C}^{(bc)}(\mathbf{r})
\]

(S4)

\[
= \int \nabla G(\mathbf{r} - \mathbf{r}') \circ [\nabla \cdot \mathbf{C}(\mathbf{r}')] d^2r' + \mathbf{C}^{(bc)}(\mathbf{r})
\]

(S5)

which is a 2D Helmholtz decomposition since \( \nabla \cdot \mathbf{C}(\mathbf{r}) = \nabla \cdot \mathbf{C}_x(\mathbf{r}) - \varepsilon \cdot \nabla \cdot \mathbf{C}_y(\mathbf{r}) \), and

\[
\mathbf{S}(\mathbf{r}) = \nabla \circ \int G(\mathbf{r} - \mathbf{r}') [\nabla \times \mathbf{S}(\mathbf{r}')] d^2r' + \mathbf{S}^{(bc)}(\mathbf{r})
\]

(S6)

\[
= \int \nabla G(\mathbf{r} - \mathbf{r}') \times [\nabla \times \mathbf{S}(\mathbf{r}')] d^2r' + \mathbf{S}^{(bc)}(\mathbf{r})
\]

(S7)
where \( \mathbf{C}^{(bc)} \) and \( \mathbf{S}^{(bc)} \) are solutions to the homogeneous equations \( \nabla \ast \mathbf{C}^{(bc)}(\mathbf{r}) = 0 \) and \( \nabla \circ \mathbf{S}^{(bc)}(\mathbf{r}) = 0 \), respectively, such that the total fields satisfy the boundary conditions. Since the superposition principle is valid in linear Elasticity, we can separately analyze the deformation by contributions from defects, external forces and boundary conditions.

### B. Deformation fields of a point dislocation

The deformation fields of defects can be separated in a regular part, with \( \nabla_x \nabla_y \mathbf{u}^{(reg)} = \nabla_y \nabla_x \mathbf{u}^{(reg)} \), and singular one, with \( \nabla_x \nabla_y \mathbf{u}^{(sing)} \neq \nabla_y \nabla_x \mathbf{u}^{(sing)} \). A single dislocation with Burgers vector \( \mathbf{b} \) at the origin have, from \( \text{[S1]} \) and \( \text{[S2]} \), singular deformation fields satisfying \( \nabla \ast \mathbf{C}^{(sing)}(\mathbf{r}) = -\nabla \circ \mathbf{S}^{(sing)}(\mathbf{r}) = \epsilon \cdot \mathbf{b} \delta(\mathbf{r}) = \mathbf{b} \delta(\mathbf{r}) \) where \( \mathbf{b} = \epsilon \cdot \mathbf{b} \). For deformation fields going to zero at infinity, we use \( \text{[S1]} \) and \( \text{[S2]} \) to obtain

\[
\mathbf{C}^{(sing)}(\mathbf{r}) = \nabla \mathbf{G}(\mathbf{r}) \circ \mathbf{b} = \frac{\mathbf{r} \circ \mathbf{b}}{2\pi|\mathbf{r}|} \quad \text{and} \quad \mathbf{S}^{(sing)}(\mathbf{r}) = -\nabla \mathbf{G}(\mathbf{r}) \ast \mathbf{b} = -\frac{\mathbf{r} \ast \mathbf{b}}{2\pi|\mathbf{r}|} \tag{S8}
\]

where \( \mathbf{r} = \mathbf{r}/|\mathbf{r}| \). These singular fields alone cannot satisfy the mechanical equilibrium equation without external forces (that is, \( B \nabla \mathbf{C}^{(sing)} + \mu \nabla \circ \mathbf{S}^{(sing)} \neq 0 \)). Regular fields, satisfying \( \nabla \ast \mathbf{C}^{(reg)}(\mathbf{r}) = \nabla \circ \mathbf{S}^{(reg)}(\mathbf{r}) \), are thus induced in such a way that

\[
0 = B \nabla \left( \mathbf{C}^{(sing)} + \mathbf{C}^{(reg)} \right) + \mu \nabla \circ \left( \mathbf{S}^{(sing)} + \mathbf{S}^{(reg)} \right)
\]

or simply

\[
\mathbf{C}^{(reg)}(\mathbf{r}) = \frac{\mu}{B + \mu} \nabla \mathbf{G}(\mathbf{r}) \circ \mathbf{b} - B \frac{\mathbf{b} \circ \nabla \mathbf{G}(\mathbf{r})}{B + \mu} \tag{S9}
\]

One can see that such regular field is derived from a regular displacement field (that is, \( \mathbf{C}^{(reg)} = \nabla \circ \mathbf{u}^{(reg)} \)) given by

\[
\mathbf{u}^{(reg)}(\mathbf{r}) = \frac{2\mu \ln|\mathbf{r}| - B \mathbf{b} \circ (\mathbf{r} \ast \mathbf{b})}{4\pi(B + \mu)} \tag{S10}
\]

which gives a regular shear field that can be written as

\[
\mathbf{S}^{(reg)}(\mathbf{r}) = \nabla \ast \mathbf{u}^{(reg)}(\mathbf{r}) = \frac{\mu}{B + \mu} \nabla \mathbf{G}(\mathbf{r}) \ast \mathbf{b} + B \frac{\mathbf{b} \circ [\mathbf{r} \ast \mathbf{r} \ast \nabla \mathbf{G}(\mathbf{r})]}{B + \mu} \tag{S11}
\]

Note that the multiplication \( \ast \) is commutative and associative. Finally, we can write the total deformation fields \( \mathbf{C}^{(disl)} = \mathbf{C}^{(sing)} + \mathbf{C}^{(reg)} \) and \( \mathbf{S}^{(disl)} = \mathbf{S}^{(sing)} + \mathbf{S}^{(reg)} \) as

\[
\mathbf{C}^{(disl)}(\mathbf{r}) = \frac{(B + 2\mu)}{B + \mu} \nabla \mathbf{G}(\mathbf{r}) \circ \mathbf{b} - B \frac{\mathbf{b} \circ \nabla \mathbf{G}(\mathbf{r})}{B + \mu} = \frac{\epsilon \cdot [(B + 2\mu) \mathbf{r} \circ \mathbf{b} + B \mathbf{b} \circ \mathbf{r}]}{2\pi(B + \mu)|\mathbf{r}|} \tag{S12}
\]

and

\[
\mathbf{S}^{(disl)}(\mathbf{r}) = -\frac{B}{B + \mu} \frac{\nabla \mathbf{G}(\mathbf{r}) \ast \mathbf{b} - \mathbf{b} \circ [\mathbf{r} \ast \mathbf{r} \ast \nabla \mathbf{G}(\mathbf{r})]}{B + \mu} = -\frac{B \epsilon \cdot [\mathbf{r} \ast \mathbf{b} + \mathbf{b} \circ (\mathbf{r} \ast \mathbf{r} \ast \mathbf{r})]}{2\pi(B + \mu)|\mathbf{r}|} \tag{S13}
\]

In particular,

\[
\mathbf{C}^{(disl)}_x(\mathbf{r}) = \frac{\mu \mathbf{r} \wedge \mathbf{b}}{\pi(B + \mu)|\mathbf{r}|} \quad \text{and} \quad \nabla \mathbf{C}^{(disl)}_x(\mathbf{r}) = -\frac{\mu \epsilon \cdot [\mathbf{b} \circ (\mathbf{r} \ast \mathbf{r})]}{\pi(B + \mu)|\mathbf{r}|^2}. \tag{S14}
\]
C. Net variation of the number of particles when the dislocation moves

If the dislocation of the previous subsection moves from the origin to \( r_0 \), from (S14) we have

\[
\Delta C_x^{(\text{disl})}(r) = \frac{\mu}{\pi(B + \mu)} \left( \frac{r - r_0}{|r - r_0|^2} - \frac{r}{|r|^2} \right) \wedge b. \tag{S15}
\]

We consider the dislocation far from the crystal’s edges. In this case, the integral of \( C_x^{(\text{disl})}(r) \) for a fixed dislocation is conditionally convergent. Still, we can estimate the net variation of the number of particles after the dislocation moves

\[
\Delta N = \int \Delta \rho(r)d^2r \approx -\rho_0 \int \Delta C_x^{(\text{disl})}(r)d^2r. \tag{S16}
\]

We use \( \int_{-\infty}^{\infty} \frac{1}{h+y^2}dy = \frac{\pi}{\sqrt{h}} \) to obtain

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{x} \cdot \left( \frac{r - r_0}{|r - r_0|^2} - \frac{r}{|r|^2} \right) dy dx = \pi \int_{-\infty}^{\infty} \left[ \text{sgn}(x - x_0) - \text{sgn}(x) \right] dx = -2\pi x_0 \tag{S17}
\]

where the sign function \( \text{sgn}(x) \) gives \(-1, 0 \) and 1 when \( x < 0, x = 0 \) and \( x > 0 \), respectively. Similarly,

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{y} \cdot \left( \frac{r - r_0}{|r - r_0|^2} - \frac{r}{|r|^2} \right) dx dy = -2\pi y_0. \tag{S18}
\]

Note that we used principal value integrals. Using (S15) in (S16) and then using (S17) and (S18), we obtain

\[
\Delta N \approx \frac{2\rho_0 \mu}{B + \mu} r_0 \wedge b. \tag{S19}
\]

D. Deformation fields of a disclination

Consider a disclination with topological charge \( s \) at the origin. In a C-picture of deformation, the singular field comes from \( \oint dC_y^{(\text{sing})} = s \), which implies in \( (\nabla_x \nabla_y - \nabla_y \nabla_x)C_y^{(\text{sing})} = s \delta(r) \), and the x-component is regular (that is, \( C_x^{(\text{sing})} = 0 \)). We can use this and (S21) in the evaluation of \( \nabla \otimes [\nabla \cdot C^{(\text{sing})}(r)] \) and then use (S20) to obtain

\[
\nabla \cdot C^{(\text{sing})}(r) = \varepsilon \cdot \nabla C_y^{(\text{sing})}(r) = s \nabla G(r). \tag{S20}
\]

The regular fields that are necessary to reach equilibrium must satisfy

\[
0 = B\nabla C_x^{(\text{reg})} + \mu \nabla \cdot (S^{(\text{reg})} + S^{(\text{sing})}) = B\nabla C_x^{(\text{reg})} + \mu \nabla \cdot (C^{(\text{reg})} - C^{(\text{sing})}) \]

\[
= B\nabla C_x^{(\text{reg})} + \mu \nabla \cdot (C^{(\text{reg})} - C^{(\text{sing})}) \]

\[
= (B + \mu)\nabla C_x^{(\text{reg})} - \mu \varepsilon \cdot \nabla C_y^{(\text{reg})} + \mu \varepsilon \cdot \nabla C_y^{(\text{sing})} \]

Then we have

\[
\nabla C_x^{(\text{reg})}(r) = -\frac{\mu s}{B + \mu} \nabla G(r) = -\frac{\mu s}{B + \mu} \frac{\hat{r}}{2\pi|r|} \quad \text{and} \quad C_y^{(\text{reg})} = 0. \tag{S21}
\]

The result of (S14) for \( \nabla C_x^{(\text{disl})} \) is obtained by adding another disclination with charge \(-s\) at \( r_0 \) and then taking the limits \( |r_0| \to 0 \) and \( s \to \infty \) with \( s r_0 = \varepsilon \cdot b \) constant. Note that our convention is the same of Ref. [1], where sevenfold and fivefold disclinations in a triangular crystal have positive and negative charges, respectively.

Finally, for the total disclination deformation field in the C-picture,

\[
\nabla \cdot C^{(\text{disc})}(r) = \nabla C^{(\text{disl})}(r) - \varepsilon \cdot \nabla C_y^{(\text{disl})}(r) \]

\[
= \nabla C_x^{(\text{reg})}(r) - \varepsilon \cdot \nabla C_y^{(\text{sing})}(r) = -\frac{(B + 2\mu)s}{(B + \mu)} \frac{\hat{r}}{2\pi|r|}. \tag{S22}
\]

For the shear field, \( \nabla \cdot S^{(\text{disc})} = \nabla \cdot C^{(\text{reg})} - \nabla \cdot C^{(\text{sing})} \) is also a gradient (irrotational) field.
E. Deformation fields due to external forces

In the presence of an external potential field $V_{\text{ext}}(\mathbf{r})$, regular deformation fields $C^{(\text{ext})}$ and $S^{(\text{ext})}$ appear in order to compensate the conservative external forces $\mathbf{F}_{\text{ext}} = -\nabla V_{\text{ext}}$ and reach the equilibrium

$$0 = B \nabla C^{(\text{ext})}_x + \mu \nabla \cdot S^{(\text{ext})} + \rho_0 \mathbf{F}_{\text{ext}} = B \nabla C^{(\text{ext})}_x + \mu \left( \nabla C^{(\text{ext})}_y - \mathbf{e} \cdot \nabla C^{(\text{ext})}_y \right) - \rho_0 \nabla V_{\text{ext}}.$$ 

Therefore $C^{(\text{ext})}_y = 0$ and

$$\nabla \cdot S^{(\text{ext})}(\mathbf{r}) = \nabla C^{(\text{ext})}_x(\mathbf{r}) = \frac{\rho_0}{B + \mu} \nabla V_{\text{ext}}(\mathbf{r}). \quad (S23)$$

Similarly, for nonconservative forces $\mathbf{F}_{\text{ext}} = -\mathbf{e} \cdot \nabla V^{(\text{nc})}_{\text{ext}}$, we have

$$0 = B \nabla C^{(\text{ext})}_x + \mu \nabla \cdot S^{(\text{ext})} + \rho_0 \mathbf{F}_{\text{ext}} = B \nabla C^{(\text{ext})}_x + \mu \left( \nabla C^{(\text{ext})}_y - \mathbf{e} \cdot \nabla C^{(\text{ext})}_y \right) - \rho_0 \mathbf{e} \cdot \nabla V^{(\text{nc})}_{\text{ext}}.$$ 

Therefore $C^{(\text{ext})}_y = 0$ and

$$\nabla \cdot S^{(\text{ext})}(\mathbf{r}) = -\mathbf{e} \cdot \nabla C^{(\text{ext})}_y(\mathbf{r}) = \frac{\rho_0}{\mu} \mathbf{e} \cdot \nabla V^{(\text{nc})}_{\text{ext}}(\mathbf{r}). \quad (S24)$$

Solutions for the density field in the conservative case $(S23)$ is direct, given by

$$C^{(\text{ext})}_x(\mathbf{r}) = \frac{\rho_0 V_{\text{ext}}(\mathbf{r})}{B + \mu}. \quad (S25)$$

Here, the boundary conditions contributions are also left to be considered later. In general, solutions for the shear field are more complicated and can be evaluated from $(S7)$. In the special case of a one-dimensional conservative external force in the direction of $\hat{x}$ (and then $V_{\text{ext}} = V_{\text{ext}}(x)$), for example, we have

$$S^{(\text{ext})}_y = 0 \quad \text{and} \quad S^{(\text{ext})}_x = S^{(\text{ext})}_x(x) = \frac{\rho_0 V_{\text{ext}}(x)}{B + \mu}. \quad (S26)$$

In the case of radial conservative external forces (that is, $V_{\text{ext}} = V_{\text{ext}}(|\mathbf{r}|) \equiv V_{\text{ext}}(r)$), the solution for the shear field is given by

$$S^{(\text{ext})}(\mathbf{r}) = \frac{\rho_0}{B + \mu} \left[ V_{\text{ext}}(r) - \frac{2}{r^2} \int_0^r r' V_{\text{ext}}(r') dr' \right] \hat{r} \cdot \hat{r} \quad (S27)$$

whose magnitude is radial (isotropic). The above result has the property $S^{(\text{ext})}(\mathbf{r}) = S^{(\text{ext})}(-\mathbf{r})$. For the gaussian-like external potential $V_{\text{ext}}(r) = V_0 e^{-r^2/2\sigma^2}$, $(S27)$ gives $S^{(\text{ext})}(\mathbf{r}) = \frac{\rho_0 V_0}{B + \mu} \left[ e^{-r^2/2\sigma^2} - \frac{2\sigma^2}{r^2} (1 - e^{-r^2/2\sigma^2}) \right] \hat{r} \cdot \hat{r}$ whose magnitude is zero at the origin, reaches a maximum at $r \approx 1.89\sigma$ and returns to zero at infinity.
II. MAIN SYSTEMS OF OUR SIMULATIONS

A. Simulational methods

We perform MD simulations with identical interacting particles inside a box with \(-l_x/2 < x \leq l_x/2\) and \(-l_y/2 < y \leq l_y/2\) using periodic boundary conditions, thus simulating an infinite system. The box has \(l_x = 312a_0\) and \(l_y = 180\sqrt{3}a_0 \approx 311.77a_0\), which is approximately a square box and can accommodate a perfect triangular lattice with 112,320 particles and spacing \(a_0 = (2/(\sqrt{3}\rho_0))^{1/2}\), where \(\rho_0\) is the mean density. We use soft isotropic pairwise interactions \(V_p(r)\) that have an energy scale \(\varepsilon\) and are further described in the next subsection. The temperature is fixed to \(k_BT = 0.0000005\varepsilon\) which equilibrates the system in crystalline configurations. At such low temperature, the particles weakly fluctuate around their equilibrium positions and the theoretical approaches can ignore thermal effects.

The time evolution is modeled by overdamped Langevin equations of motion. These are integrated via Euler finite difference steps following the algorithm for the position of particle \(i\) (see Ref. [S2])

\[
\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \frac{\mathbf{F}_i(t)\Delta t}{\gamma} + \mathbf{g}_i\sqrt{\frac{2k_BT\Delta t}{\gamma}},
\]

(S28)

where \(\mathbf{F}_i = -\nabla_{\mathbf{r}}[V_{\text{ext}}(\mathbf{r}_i) + \sum_{j \neq i} V_p(|\mathbf{r}_i - \mathbf{r}_j|)]\) is the total force, \(\gamma\) is the friction coefficient, \(\Delta t\) is the time step and the components of the 2D vector \(\mathbf{g}_i\) are independent random variables with standard normal distribution of zero mean and unity variance which accounts for the Langevin kicks. In general, for our systems, \(\Delta t/\gamma \sim 10^{-3}\sigma_0^2/\varepsilon\) is sufficiently small. The simulation time required to reach equilibrium varied according to the system.

We start with a perfect triangular crystal configuration, with some slip direction (or lines of particles) parallel to \(\hat{\mathbf{x}}\). We then apply a localized external shear stress at \((x, y) = (0, 0)\) in order to nucleate a pair of dislocations. There are many ways to do so. In the following, we describe a procedure which is an illustrative use of our elasticity formalism.

The localized shear can be generated, for example, using a conservative external potential given by \(V_{\text{ext}}^{\text{ini}}(\mathbf{r}) = V_0^{\text{ini}}(e^{-(r-r_0)^2/2\sigma_0^2} + e^{-(r+r_0)^2/2\sigma_0^2})\), where \(r_0 = 1.89\sigma_0(\cos\pi/4)\) and \(\sigma_0\) is equal to a few lattice spacings. As we can see from the results in the end of Sec. 1E, this superposition of two gaussians produces a shear with maximum magnitude at the origin. It has only \(y\)-component there and then the resolved component \((\mathbf{b} \cdot \hat{\mathbf{b}}) \wedge S^{\text{ext}}(0)\) is maximized for \(\hat{\mathbf{b}} = \pm \hat{\mathbf{x}}\) or \(\hat{\mathbf{b}} = \pm \hat{\mathbf{y}}\). Since \(\hat{\mathbf{x}}\) is a slip direction in our triangular crystal and \(\hat{\mathbf{y}}\) is not, a pair of dislocations with \(\mathbf{b} = \pm a_0\hat{\mathbf{x}}\) is nucleated after the resolved shear reaches a critical value. For positive \(V_0^{\text{ini}}\), the dislocation with \(\mathbf{b} = a_0\hat{\mathbf{x}}\) goes to the right and the other one goes to the left, equilibrating at \(x = \pm d/2\) where \(d\) is the distance between them. Thereafter, we use other types of external potential to control their equilibrium positions, considering the configurational forces described in the main text, and turn off \(V_{\text{ext}}^{\text{ini}}(\mathbf{r})\).

In the case of Fig. 2a in the main text, we use a single gaussian \(V_{\text{ext}}(|\mathbf{r}|) = -V_0 e^{-|\mathbf{r}|^2/2\sigma_0^2}\) centered between the dislocations. From (S27) and (S28), we have that this external force field produces \((\mathbf{b} \cdot \hat{\mathbf{b}}) \wedge S^{\text{ext}}(\mathbf{r}) = 0\) and \(\mathbf{b} \cdot \nabla C_{\text{ext}}^{\text{ext}}(\mathbf{r}) > 0\) for \(\mathbf{r} = \pm \hat{\mathbf{x}} d/2\) and \(\mathbf{b} = \pm \hat{\mathbf{x}}\).

B. Elastic constants for systems with interactions that are combinations of power-law terms

In general, the system has isotropic elastic response described by high-frequency (instantaneous) bulk and shear moduli [S3] which depend on temperature and, for 2D, can be evaluated using [S4]

\[
B_\infty = 2\rho_0 k_B T - \frac{\pi \rho_0^2}{4} \int_0^{\infty} r^2 g(r) \left[V_p'(r) - r V_p''(r)\right]dr
\]

(S29)

and

\[
\mu_\infty = \rho_0 k_B T + \frac{\pi \rho_0^3}{8} \int_0^{\infty} r^2 g(r) \left[3V_p'(r) + r V_p''(r)\right]dr
\]

(S30)

where \(g(r)\) is the radial distribution function and the primes indicate derivatives. The simulations were carried out at a very low temperature and we can ignore thermal effects on the crystalline configuration. Within this approximation, we have

\[
2\pi \rho_0 \int r g(r) f(r) dr \approx \sum_i f(r_i)
\]

(S31)
where $\sum_i$ is a lattice sum. It is convenient to define the Madelung energy (the total interaction potential on a particle of the lattice with spacing $a$)

$$\Phi(a) = \sum_i V_p(r_i) = \sum_i V_p(ap_i)$$  \hspace{1cm} (S32)

where $p_i = r_i/a$ are factors of proportionality which depend on the lattice geometry. We can then use the analytical formulas

$$B = \frac{\rho_0}{8} \sum_i \left[ -r_i V_p''(r_i) + r_i^2 V_p''(r_i) \right]$$

$$= \frac{\rho_0}{8} \left[ -a_0 \sum_i p_i V_p'(a_0 p_i) + a_0^2 \sum_i p_i^2 V_p''(a_0 p_i) \right]$$

$$= \frac{\rho_0}{8} \left[ -a_0 \Phi'(a_0) + a_0^2 \Phi''(a_0) \right]$$ \hspace{1cm} (S33)

and

$$\mu = \frac{\rho_0}{16} \sum_i \left[ 3r_i V_p'(r_i) + r_i^2 V_p''(r_i) \right]$$

$$= \frac{\rho_0}{16} \left[ 3a_0 \Phi'(a_0) + a_0^3 \Phi''(a_0) \right].$$ \hspace{1cm} (S34)

We simulated systems with power-law type $V_p^{PL}(r) = \varepsilon (a_0/r)^6$ and Lennard-Jones type $V_p^{LJ}(r) = \Lambda \varepsilon [(a_0/r)^{12} - (a_0/r)^6]$ interactions, where $\Lambda$ is a numerical factor. For these cases, we have the Madelung energies

$$\Phi^{PL}(a) = \varepsilon M_6 \left( \frac{a_0}{a} \right)^6$$ \hspace{1cm} and \hspace{1cm} $$\Phi^{LJ}(a) = \Lambda \varepsilon \left[ M_{12} \left( \frac{a_0}{a} \right)^{12} - M_6 \left( \frac{a_0}{a} \right)^6 \right]$$ \hspace{1cm} (S35)

where $M_n = \sum_i 1/p_i^n$ are lattice constants. The constants can be calculated for the triangular lattice and we obtain $M_6 \approx 6.37588$ and $M_{12} \approx 6.00981$. Therefore, the bulk and shear moduli for these systems can be readily evaluated. In particular, we have

$$B^{PL} = 6M_6 \rho_0 \varepsilon \hspace{1cm} \text{and} \hspace{1cm} B^{LJ} = 3(7M_{12} - 2M_6) \Lambda \rho_0 \varepsilon.$$ \hspace{1cm} (S36)

In order to have the Lennard-Jones system with the same $B + \mu$ of the power-law one, we use

$$B^{PL} + \mu^{PL} = B^{LJ} + \mu^{LJ} \hspace{1cm} \Rightarrow \hspace{1cm} \Lambda = \left( \frac{57M_{12}}{15M_6} - 1 \right)^{-1} \approx 0.38732.$$ \hspace{1cm} (S37)

With such factor, we have two different systems with the same elastic response $\varepsilon$ to conservative external forces.

C. External forces and the induced resolved shear strain

The system starts as a perfect triangular crystal with lattice spacing $a_0 = (2/\sqrt{3})^{1/2}$. By applying a localized shear stress, a pair of dislocations was nucleated and thereafter they were kept symmetrically separate, with $b = \pm a_0 \hat{x}$ at $x = \pm d/2$, solely by the effect of the external potential field

$$V_{ext}(x) = V_0 \left[ e^{-(x+D+\sigma)^2/2\sigma^2} - e^{-(x+D-\sigma)^2/2\sigma^2} - e^{-(x-D+\sigma)^2/2\sigma^2} + e^{-(x-D-\sigma)^2/2\sigma^2} \right]$$ \hspace{1cm} (S38)

acting on the crystal. Fig. S1 presents the plots of this potential and of its derivative

$$\nabla_x V_{ext}(x) = (V_0/\sigma^2) \left[ -(x+D+\sigma)e^{-(x+D+\sigma)^2/2\sigma^2} + (x+D-\sigma)e^{-(x+D-\sigma)^2/2\sigma^2} + (x-D+\sigma)e^{-(x-D+\sigma)^2/2\sigma^2} - (x-D-\sigma)e^{-(x-D-\sigma)^2/2\sigma^2} \right]$$ \hspace{1cm} (S39)

for $\sigma = 10a_0$ and $D = 40a_0$. The regions in gray represent the regions where the dislocations can stay in equilibrium. They stay there by the mechanism in which the density gradients (provoked by the external forces) induce resolved shear strains on them. Note that only two of the gaussian exponential terms in (S39) effectively acts on each dislocation, as it can be seen in Fig. S1.
FIG. S1. **External potential field and its derivative.** Plots of $V_{\text{ext}}(x)/V_0$ and $(a_0/V_0) \nabla_x V_{\text{ext}}(x)$, given in (S38) and (S39), for $\sigma = 10a_0$ and $D = 40a_0$. The gray regions indicate where the dislocations can be trapped (that is, kept apart) when the external force field is sufficiently strong.

Besides the external potential contribution, the background deformation fields on each dislocation have contributions due to the other one and to the boundary conditions. From (S14), we have that each dislocation produces a density gradient that, in the position of the other one, is perpendicular to $\hat{b}$. Since the external potential already satisfies the periodicity of boundary conditions (we have $V_{\text{ext}}(-l_x/2) = V_{\text{ext}}(l_x/2)$ and the derivatives going to zero at these borders), the contribution to deformation due to the periodic boundary conditions is only the effect of repeated dislocations, which are more investigated in the next subsection. This contribution also gives a density gradient that is $\perp \hat{b}$ and therefore the total induced resolved shear is only

$$S_{\text{res}}^{(\text{ind})} = L \hat{b} \cdot \nabla C_x^{(bg)} = \pm L \nabla_x C_x^{(\text{ext})}(\pm d/2) = \pm \frac{L\rho_0}{B + \mu} \nabla_x V_{\text{ext}}(\pm d/2)$$

$$\approx \frac{L\rho_0 V_0}{(B + \mu)\sigma^2} \left[ \left( \frac{d}{2} - D + \sigma \right) e^{-(d/2-D+\sigma)^2/2\sigma^2} - \left( \frac{d}{2} - D - \sigma \right) e^{-(d/2-D-\sigma)^2/2\sigma^2} \right]$$

on the dislocations at $x = \pm d/2$. Since $S_{\text{res}}^{(\text{ind})} > 0$ and $\hat{b} \cdot F_{\text{disl}} \propto S_{\text{res}}$, the induced forces on the dislocations contribute to push them apart.

**D. Boundary conditions and the background resolved shear strain**

The external potential contribution to shear, which has the form of (S26), do not produce background resolved shear strain on the dislocations, which is simply $S_{\text{res}}^{(bg)}(\mathbf{r}) = (\hat{b} \cdot \hat{b}) \wedge S^{(bg)}(\mathbf{r}) = S_y^{(bg)}(\mathbf{r})$ since $\hat{b} = \pm \hat{x}$. In a first approximation, the background resolved shear that the dislocations directly produce on each other is equally negative.
FIG. S2. Repetition of dislocations due to the periodic boundary conditions. The contribution to deformation fields originated from the (periodic) boundary conditions is equivalent to infinitely repeated dislocation pairs.

and, using (S13), given by

\[ S^{(bg)}_{\text{res}} \approx - \frac{Ba_0}{\pi(B + \mu)d} \]  \hspace{1cm} (S41)

where \( d \) is the distance between them. However, as it is shown in Fig. S2, the periodic boundary conditions create lattices of dislocations, with periodicities \( l_x \) and \( l_y \), that contribute to deformation. Note that each dislocation does not interact with its own lattice but with the one formed by the other.

The lattices of dislocations can then be approximated by square lattices with spacing \( l = l_x \approx l_y \). On the dislocation with \( b = a_0 \hat{x} \) at \( x = d/2 \) (that is, the central open circle in Fig. S2), the total \( S^{(bg)}_{\text{res}} \) can be calculated from the lattice produced by the other one, with \( b = -a_0 \hat{x} \) at \( x = -d/2 \) (that is, from all filled circles in the figure). Numbering these dislocations by \((n, m)\), where \((0, 0)\) is the central one and \( \Delta r_{(n,m)} = a_0 \hat{x} - r_{(n,m)} = \left( \frac{d+nl}{ml} \right) \), and using (S13), we have

\[
S^{(bg)}_{\text{res}} = \sum_{n,m=-\infty}^{\infty} \frac{Ba_0}{2\pi(B + \mu)} \left( \hat{x} \cdot \hat{x} \right) \wedge \mathbf{\epsilon} \cdot \left( \frac{\Delta r_{(n,m)} \cdot \hat{x}}{|\Delta r_{(n,m)}|^2} + \frac{\Delta r_{(n,m)} \cdot \Delta r_{(n,m)} \cdot \Delta r_{(n,m)}}{|\Delta r_{(n,m)}|^4} \right)
\]

\[
= -\frac{Ba_0}{2\pi(B + \mu)} \sum_{n,m=-\infty}^{\infty} \hat{x} \cdot \left( \frac{\Delta r_{(n,m)} \cdot \hat{x}}{|\Delta r_{(n,m)}|^2} + \frac{\Delta r_{(n,m)} \cdot \Delta r_{(n,m)} \cdot \Delta r_{(n,m)}}{|\Delta r_{(n,m)}|^4} \right)
\]

\[
= -\frac{Ba_0}{2\pi(B + \mu)} \sum_{n,m=-\infty}^{\infty} \left( \frac{d + nl}{(d + nl)^2 + m^2l^2} + \frac{(d + nl)^2 - 3(d + nl)m^2l^2}{[(d + nl)^2 + m^2l^2]^2} \right)
\]

\[
= -\frac{Ba_0}{\pi(B + \mu)l} \sum_{n,m=-\infty}^{\infty} \left[ \frac{d/l + n}{(d/l + n)^2 + m^2} \left( 1 - \frac{2m^2}{(d/l + n)^2 + m^2} \right) \right]
\]

\[
= -\frac{Ba_0}{\pi(B + \mu)l} \sum_{n=-\infty}^{\infty} \left[ \frac{d/l + n}{(d/l + n)^2 + m^2} \left( -\frac{2(d/l + n)m^2}{[(d/l + n)^2 + m^2]^2} \right) \right]. \hspace{1cm} (S42)
\]
FIG. S3. Approximations for the background resolved shear. Curves obtained by considering only the nearest dislocation, by adding of the second nearest one and by considering some terms in the total result (S46). As in Fig. S1, the gray region indicate where the dislocations can be trapped in our systems.

Now we use (see the series no. (886) in Ref. [S5])

$$\sum_{n=1}^{\infty} \frac{h}{(nz)^2 + h^2} = \frac{\pi}{z} \left[ \frac{1}{e^{2\pi h/z} - 1} + \frac{1}{2} - \frac{z}{2\pi h} \right] = \frac{\pi}{2z} \coth \left( \frac{\pi h}{z} \right) - \frac{1}{2h}$$  \hspace{1cm} (S43)

and

$$\sum_{n=1}^{\infty} \frac{2zhn^2}{((nz)^2 + h^2)^2} = \frac{\partial}{\partial z} \left[ \sum_{n=1}^{\infty} \frac{h}{(nz)^2 + h^2} \right] = \frac{\pi}{2z^2} \left[ \coth \left( \frac{\pi h}{z} \right) - \frac{\pi h}{z} \mathrm{csch}^2 \left( \frac{\pi h}{z} \right) \right]$$  \hspace{1cm} (S44)

to obtain

$$\sum_{m=1}^{\infty} \left( \frac{d/l + n}{(d/l + n)^2 + m^2} - \frac{2(d/l + n)m^2}{(d/l + n)^2 + m^2} \right) = \frac{\pi^2}{2(d/l + n)} \mathrm{csch}^2 \left[ \pi(d/l + n) \right] - \frac{1}{2(d/l + n)}$$  \hspace{1cm} (S45)

and then

$$S_{\text{res}}^{(bg)} = -\frac{B_0}{(B + \mu)l} \sum_{n=-\infty}^{\infty} \left[ \frac{1}{d/l + n} + 2 \left( \frac{\pi^2}{2(d/l + n)} \mathrm{csch}^2 \left[ \pi(d/l + n) \right] - \frac{1}{2(d/l + n)} \right) \right]$$

$$= -\frac{B_0}{(B + \mu)l} \sum_{n=-\infty}^{\infty} (d/l + n) \mathrm{csch}^2 \left[ \pi(d/l + n) \right].$$  \hspace{1cm} (S46)

Fig. S3 presents a graph which compares some approximations for $S_{\text{res}}^{(bg)}$. Within our region of interest, the consideration of just the nearest dislocation (the one in the central box of Fig. S2) as in (S41), or even when adding the second nearest one (which is in the box on the right side of Fig. S2), do not give good approximation. The more correct evaluation is given by the infinite series (S46) which is rapidly convergent and very well approximated by

$$S_{\text{res}}^{(bg)} \approx -\frac{B_0}{(B + \mu)l} \left[ \frac{d}{l} \mathrm{csch}^2 \left( \frac{\pi d}{l} \right) + \left( \frac{d}{l} + 1 \right) \mathrm{csch}^2 \left( \frac{\pi d}{l} + \pi \right) + \left( \frac{d}{l} - 1 \right) \mathrm{csch}^2 \left( \frac{\pi d}{l} - \pi \right) \right].$$  \hspace{1cm} (S47)
E. Equilibrium positions of the dislocations

Finally, with the results (S47) and (S40), and using (S39), we find that the equilibrium condition \( \mathbf{b} \cdot \mathbf{F}_{\text{disl}}^{(\text{tot})} \propto S_{\text{res}}^{(\text{tot})} = S_{\text{res}}^{(\text{ind})} + S_{\text{res}}^{(bg)} = 0 \) gives

\[
V_0 \approx \frac{B a_0 \pi \sigma}{L \rho_0^2} \left[ \frac{d \operatorname{csch}^2 \left( \frac{\pi d}{a} \right) + (d + 1) \operatorname{csch}^2 \left( \frac{\pi d}{a} + \pi \right) + (d - 1) \operatorname{csch}^2 \left( \frac{\pi d}{a} - \pi \right)}{\left( \frac{d}{a} - D + \sigma \right) e^{-\left(\frac{d}{a} - D + \sigma\right)^2/2\sigma^2} - \left( \frac{d}{a} - D - \sigma \right) e^{-\left(\frac{d}{a} - D - \sigma\right)^2/2\sigma^2}} \right]
\]

or, substituting our parameters,

\[
V_0 \approx \frac{B a_0}{L \rho_0} \frac{25\pi}{12168} \left[ \frac{d \operatorname{csch}^2 \left( \frac{\pi d}{312a_0} \right) + \left( \frac{d}{a_0} + 312 \right) \operatorname{csch}^2 \left( \frac{\pi d}{312a_0} + \pi \right) + \left( \frac{d}{a_0} - 312 \right) \operatorname{csch}^2 \left( \frac{\pi d}{312a_0} - \pi \right)}{\left( \frac{d}{a_0} - 60 \right) e^{-\left(\frac{d}{a_0} - 60\right)^2/800} - \left( \frac{d}{a_0} - 100 \right) e^{-\left(\frac{d}{a_0} - 100\right)^2/800}} \right].
\]

The above equation relates the external potential strength with the distance between the dislocations. It can be directly compared with the simulation results and has only one fitting parameter, given by \( B a_0/(L \rho_0) \) which can be viewed as an energy scale for \( V_0 \).

In simulations we use positive values of \( V_0 \). At \( d \approx 84a_0 \), the curve \( V_0 = V_0(d) \) for \( V_0 = V_0(d) \) has a minimum, then increases with \( d \) and blows up at \( d \approx 104a_0 \). This is our region of interest, since elsewhere \( V_0(d) \) is either negative or decreasing. When, in simulation, \( V_0 \) is decreased bellow that minimum, at which \( d \approx 84a_0 \), the configurational force due to the density gradient can no longer kept the dislocations apart and the PK forces drive them to annihilate each other. Indeed, we observed that \( d \approx 84a_0 \) is the minimum distance that the dislocations can be trapped by the action of the external potential. In Fig. 4 of the main text, we can see that our theoretical predictions for the configurational force has a good agreement with the MD results, mainly for smaller \( d \) (possible reasons for this are described in the main text). From the fits, we estimate the values \( L^{PL} \approx 0.683a_0 \) and \( L^{L}\approx 4.43a_0 \) for the length parameter in the power-law and Lennard-Jones systems, respectively.

Finally, it is important to point out that, for the system analyzed here, \( C_x^{(bg)} = S_x^{(bg)} = (\mathbf{b} \cdot \hat{\mathbf{b}}) \cdot \mathbf{S}^{(bg)} \) on the dislocations. This leaves an ambiguity in interpreting the observed results as consequences of “unresolved” shear gradients or density ones. Such ambiguity disappears in radial external potentials, for which \( C_x^{(ext)} \neq S_x^{(ext)} \) as we can see from (S25) and (S27). Therefore, we can consider the simulation result shown in Fig. 2a of the main text to analyze \( S_{\text{res}}^{(bg)} \) in comparison with \( L^{PL} \mathbf{b} \cdot \nabla C_x^{(bg)} \) and \( L^{PL} \mathbf{b} \cdot \nabla S_x^{(bg)} \). Nonlinear (and other) effects are strong in that case but linear Elasticity still provides useful estimations. We have \( d \approx 14.27a_0 \) and then linear Elasticity provides \( L^{PL} \mathbf{b} \cdot \nabla C_x^{(bg)} \approx 0.0139 \) and \( L^{PL} \mathbf{b} \cdot \nabla S_x^{(bg)} \approx -0.000414 \), which must compensate the background resolved shear \( S_{\text{res}}^{(bg)} \approx -0.0177 \). This indicates that \( \mathbf{b} \cdot \nabla \left[ (\mathbf{b} \cdot \hat{\mathbf{b}}) \cdot \mathbf{S}^{(bg)} \right] \) have, in a fundamental level of configurational forces, small effects (if any) on the dislocations, while \( \mathbf{b} \cdot \nabla C_x^{(bg)} \) strongly affect them.

SUPPLEMENTARY REFERENCES

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