Dynamics for a System of Screw Dislocations

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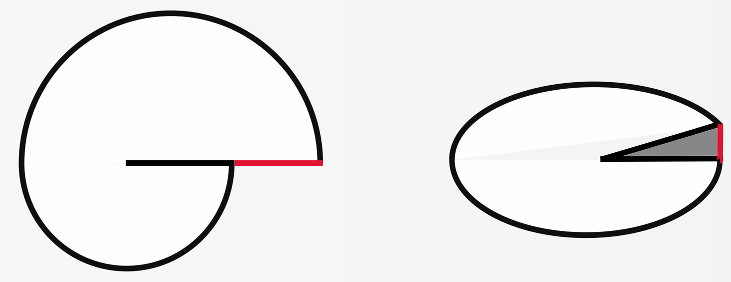
Motivation

Dislocations are point defects in solid crystalline structures. The interest in their study lies in the influence that their presence has on the properties of the material itself. A dislocation is characterized by its *Burgers vector*, which describes the lattice mismatch. There are two main types of dislocations, namely *edge* dislocations and *screw* dislocations. The former are characterized by their Burgers vector being perpendicular to the line direction of the mismatch, while the latter have their Burgers vector parallel to the line of the mismatch.We describe the energy and the dynamics for a system of screw dislocations subject to antiplane shear.

Types of dislocations



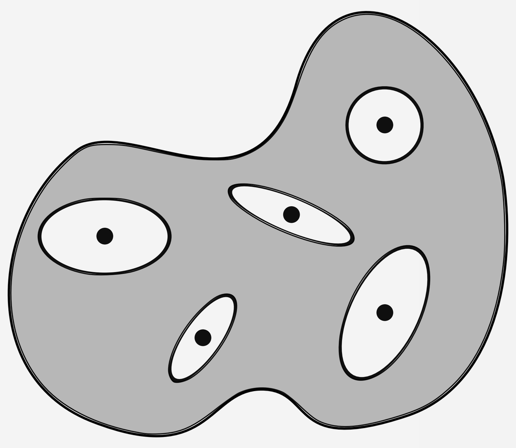
An *edge* dislocation and a *screw* dislocation. The Burgers vectors are colored in red.

The model for screw dislocations

The elastic deformation associated with antiplane shear is described by the field $u:\Omega\to\mathbb{R}$ such that $(x_1,x_2,x_3)\mapsto(x_1,x_2,x_3+u(x_1,x_2))$, whose deformation gradient can be written as $\mathbf{F}=\mathbf{I}+\mathbf{e}_3\otimes(\mathbf{h},0)^\top$, where $\mathbf{h}=\nabla u$. Dislocations in a crystalline elastic solid body are modeled as singularities of the gradient of the displacement, so that $\mathbf{h}$ fails to be a pure gradient and contains a singular part. This is encoded in the curl of $\mathbf{h}$. The system reads [1]

$$\left.\begin{array}{l}\operatorname{curl}\mathbf{h}=\sum_{i=1}^N \mathbf{b}_i\delta_{\mathbf{z}_i}\\ \operatorname{div}\mathbf{Lh}=0\end{array}\right\}\quad\text{in }\Omega,\text{ where }\mathbf{b}_i=b_i\mathbf{e}_3\text{ and }\quad b_i=\int_{\ell_i}\mathbf{h}\cdot\mathrm{d}x; \tag{1}$$

$\mathcal{Z}:=\{\mathbf{z}_1,\dots,\mathbf{z}_N\}$ is the set of dislocations, $\mathcal{B}:=\{\mathbf{b}_1,\dots,\mathbf{b}_N\}$ is the set of the corresponding Burgers vectors, and $\mathbf{L}=\mu\,\mathrm{diag}(1,\lambda^2)$ is the elastic tensor written in terms of the Lamé moduli of the material; finally, ℓ_i is a counterclockwise loop around the dislocation $\mathbf{z}_i$ only.



An open domain $\Omega\subset\mathbb{R}^2$. The dots represent the positions of the dislocations $\mathbf{z}_i$, the white ellipses E_i are the cores to be removed to solve (1) on $\Omega_\varepsilon:=\Omega\setminus(\cup_{i=1}^N\overline{E}_i)$.

There is a unique solution $\mathbf{h}_\varepsilon$ for each Ω_ε.

Variational formulation

To tackle system (1) by means of a variational approach, we follow [2] and consider the energy density $W(\mathbf{h}):=\frac12\mathbf{h}\cdot\mathbf{Lh}$. The associated energy functional is $J(\mathbf{h}):=\int_\Omega W(\mathbf{h})\,\mathrm{d}x$, which at the level ε reads

$$J_\varepsilon(\mathbf{h})=\int_{\Omega_\varepsilon}W(\mathbf{h})\,\mathrm{d}x.$$

Define the space $H^{\mathrm{curl}}(\Omega_\varepsilon):=\{\mathbf{h}\in L^2(\Omega_\varepsilon,\mathbb{R}^2):\operatorname{curl}\mathbf{h}\in L^2(\Omega_\varepsilon)\}$. Then, by computing the first variation of J_ε, it is possible to prove the following

Theorem ([4]). *Assume* $\mathbf{L}$ *is positive definite. Then* $\mathbf{h}_\varepsilon\in H_0^{\mathrm{curl}}(\Omega_\varepsilon,\mathcal{Z},\mathcal{B}):=\{\mathbf{h}\in H^{\mathrm{curl}}(\Omega_\varepsilon):\operatorname{curl}\mathbf{h}=0,\int_{\partial E_i}\mathbf{h}\cdot\mathrm{d}x=b_i\}$ *is a minimizer of* J_ε *if and only if it solves the Euler equation*

$$\begin{cases}\operatorname{div}(\mathbf{Lh}_\varepsilon)=0 & \text{in }\Omega_\varepsilon,\\ \mathbf{Lh}_\varepsilon\cdot\hat{\mathbf{n}}=0 & \text{on }\partial\Omega_\varepsilon.\end{cases}$$

Moreover, the solution is unique.

By letting $\varepsilon\to0$, $\mathbf{h}_\varepsilon$ converges to $\mathbf{h}_0$ [2, 4], the solution to the problem for the punctured domain $\Omega\setminus\mathcal{Z}$.

Dynamics: existence of solutions

Following [1], dislocations can only move along a finite set $\mathcal{G}:=\{\mathbf{e}_1,\dots,\mathbf{e}_M\}$ of *glide directions*, with a velocity determined by the force acting on each dislocation. The Peach-Köhler force $\mathbf{j}_i$ acting on the i-th dislocation is the derivative of the energy (2), at a minimum point, with respect to the position of the dislocation $\mathbf{z}_i$. Let $\mathbf{Z}:=(\mathbf{z}_1,\dots,\mathbf{z}_N)\in\Omega^N$. The equations of motion read

$$\dot{\mathbf{z}}_i\in G_i(\mathbf{Z}),\qquad \mathbf{z}_i(0)=\mathbf{z}_{i,0}, \tag{3}$$

for given initial conditions $\mathbf{Z}_0:=(\mathbf{z}_{1,0},\dots,\mathbf{z}_{N,0})$. Here

$$G_i(\mathbf{Z}):=\Big\{(\mathbf{j}_i(\mathbf{Z})\cdot\mathbf{e})\,\mathbf{e}:\mathbf{e}\in\arg\max\{\mathbf{j}_i(\mathbf{Z})\cdot\mathbf{g},\ \mathbf{g}\in\mathcal{G}\}\Big\},$$

so that the vectors $\mathbf{e}$'s represent the glide directions *closest to* $\mathbf{j}_i(\mathbf{Z})$ (see [1]), that is $\mathbf{j}_i(\mathbf{Z})\cdot\mathbf{e}\geqslant\mathbf{j}_i(\mathbf{Z})\cdot\mathbf{g}$, for all $\mathbf{g}\in\mathcal{G}$. To solve (3), we use a technique introduced by Filippov [3].

Theorem (Local existence [4]). *Let* $\Omega\subset\mathbb{R}^2$ *be a connected open set. Let* $G(\mathbf{Z}):=G_1(\mathbf{Z})\times\dots\times G_N(\mathbf{Z}):\mathcal{D}(G)\to\mathcal{P}(\mathbb{R}^{2N})$ *and let* $\mathbf{Z}_0\in\mathcal{D}(G)$ *be a given initial configuration of dislocations. Finally, let* $F(\mathbf{Z}):=\operatorname{co}G(\mathbf{Z})$ *be the convex hull of the set valued function* G. *Consider the initial value problem*

$$\dot{\mathbf{Z}}\in F(\mathbf{Z}):=\operatorname{co}G(\mathbf{Z}),\qquad \mathbf{Z}(0)=\mathbf{Z}_0. \tag{4}$$

Then there exists a solution $\mathbf{Z}:[0,T]\to\mathcal{D}(G)$ *to problem (4), for a maximal existence time* T *depending only on* $\mathbf{Z}_0$, $\mathcal{D}(G)$, *and* $|\mathbf{j}_i(\mathbf{Z})|$*'s.*

The domain $\mathcal{D}(G)$ of the set-valued function G is $\Omega^N\setminus\{\text{collisions}\}$. To prove the local existence theorem it is enough to notice that the set-valued function F defined in (4) satisfies the hypotheses of Theorem 1 in [3, page 77]. Finally, notice that solutions to (4) exist as long as the dislocations stay away from the boundary $\partial\Omega$ and do not collide.

Renormalized energy

Theorem ([4]). *Let* $\mathbf{h}_\varepsilon$ *be a minimizer of* J_ε. *Then*

$$J_\varepsilon(\mathbf{h}_\varepsilon)=\int_{\Omega_\varepsilon}\frac12\mathbf{h}_\varepsilon\cdot\mathbf{Lh}_\varepsilon=\sum_{i=1}^N\frac{\mu\lambda b_i^2}{4\pi}\log\frac1\varepsilon+U(\mathcal{Z})+O(\varepsilon), \tag{2}$$

where $U(\mathcal{Z})=U_S(\mathcal{Z})+U_I(\mathcal{Z})+U_E(\mathcal{Z})$ *is the renormalized energy, where*

$$U_S(\mathcal{Z})=\sum_{i=1}^N\frac{\mu\lambda b_i^2}{4\pi}\log R+\sum_{i=1}^N\int_{\Omega\setminus E_{j,R}}W(\mathbf{k}_i)\,\mathrm{d}x,\quad U_I(\mathcal{Z})=\sum_{i=1}^{N-1}\sum_{j=i+1}^N\int_\Omega\mathbf{k}_j\cdot\mathbf{Lk}_i\mathrm{d}x,$$

$$U_E(\mathcal{Z})=\int_\Omega W(\nabla u_0)\mathrm{d}x+\sum_{i=1}^N\int_{\partial\Omega}u_0\mathbf{Lk}_i\cdot\hat{\mathbf{n}}\,\mathrm{d}s.$$

The term U_S is the *"self"* energy associated with the presence of the dislocations themselves; the term U_I is the energy given by the *interaction* between the dislocations; the term U_E is the energy associated with the presence of the *elastic* medium: it contains the contribution of the medium and the influence of the tractions of the dislocations on the boundary.

Dynamics: uniqueness of solutions

To discuss uniqueness of solutions a deep investigation of the set

$$\mathcal{M}:=\{\mathbf{Z}\in\mathcal{D}(G):G(\mathbf{Z})\subsetneq\operatorname{co}G(\mathbf{Z})\}, \tag{5}$$

where the direction of motion is not uniquely defined, is required.

Proposition ([4]). *The functions* $\mathbf{j}_i$*'s are analytic.*

By means of the Implicit Function Theorem, one can prove the following

Proposition ([4]). *The set* $\mathcal{M}$ *defined in (5) is contained in a countable union of analytic manifolds of dimension less than or equal to* $2N-1$.

These result, together with general theorems from [3], allow to prove a right uniqueness result for the initial value problem (4).

Theorem (Right uniqueness [4]). *Let* $\Omega\subset\mathbb{R}^2$ *be a connected open set. Let* $G(\mathbf{Z}):\mathcal{D}(G)\to\mathcal{P}(\mathbb{R}^{2N})$ *and let* $\mathbf{Z}_0\in\mathcal{D}(G)$ *be a given* well prepared *initial configuration of dislocations. Then the solution* $\mathbf{Z}:[0,T]\to\mathcal{D}(G)$ *to initial value problem (4) provided by the local existence theorem is unique.*

The previous theorem allows to deal with situations like *cross-slip* and *fine cross-slip*, initially described in [1]. By *well prepared* initial condition we mean one in which no dislocation is at a *source point*. Collisions and dislocations hitting the boundary $\partial\Omega$ are not comprised in the theorem.

References

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