Dynamics for a System of Screw Dislocations

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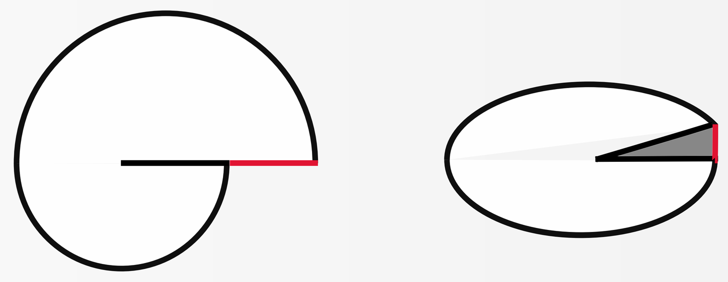
Motivation

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. We describe the energy and the dynamics for a system of screw dislocations subject to antiplane shear.

Types of dislocations



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

Essential references

[1] P. Cermelli and M.E. Gurtin. *Arch. Ration. Mech. Anal.*, 148(1):3–52, 1999.

[2] P. Cermelli and G. Leoni. *SIAM J. Math. Anal.*, 37(4):1131–1160 (electronic), 2005.

[3] A.F. Filippov, Differential equations with discontinuous right-hand sides.

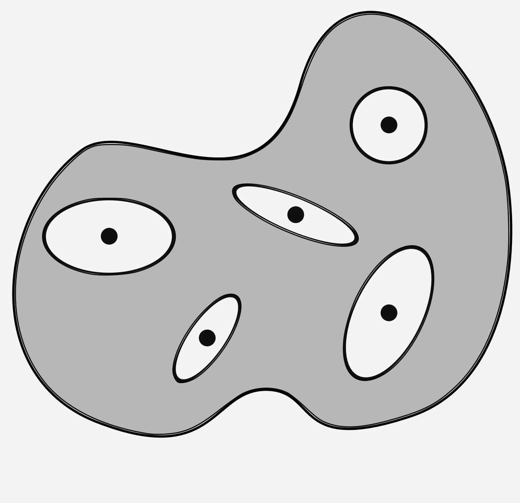
[4] T. Blass, I. Fonseca, G. Leoni, and M. Morandotti. *In preparation.*

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]

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

$\mathcal{Z} := \{\mathbf{z}_1, \dots, \mathbf{z}_N\}$ is the set of the dislocations sites, $\mathcal{B} := \{\mathbf{b}_1, \dots, \mathbf{b}_N\}$ 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 $C_{\varepsilon,i}$ are the cores to be removed to solve (1) on $\Omega_\varepsilon := \Omega \setminus (\cup_{i=1}^N \overline{C}_{\varepsilon,i})$.

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 $W(\mathbf{h}) := \frac{1}{2}\mathbf{h}\cdot\mathbf{L}\mathbf{h}$. The associated energy functional is $J(\mathbf{h}) := \int_\Omega W(\mathbf{h})\,d\mathbf{x}$, which in the perforated domain reads

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

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, if* $\mathbf{h}_\varepsilon \in H_0^{\mathrm{curl}}(\Omega_\varepsilon, \mathcal{Z}, \mathcal{B}) := \{\mathbf{h} \in H^{\mathrm{curl}}(\Omega_\varepsilon) : \operatorname{curl}\mathbf{h} = 0, \int_{\partial C_{\varepsilon,i}} \mathbf{h}\cdot d\mathbf{x} = b_i\}$ *is a minimizer of* J_ε*, it solves the Euler equation*

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

Moreover, the solution is unique.

By letting $\varepsilon \to 0$, $\mathbf{h}_\varepsilon$ converges to $\mathbf{h}_0$ [2, 4], the solution to the problem for the punctured domain $\Omega \setminus \mathcal{Z}$.

Renormalized energy

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

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

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

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

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

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: existence of solutions

Following [1], dislocations can only move along a finite set $\mathcal{G} := \{\mathbf{g}_1, \dots, \mathbf{g}_M\}$ 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

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

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

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

so that the vectors $\mathbf{g}_i$'s represent the glide directions *closest to* $\mathbf{j}_i(\mathbf{Z})$ (see [1]), that is $\mathbf{j}_i(\mathbf{Z})\cdot\mathbf{g}_i \geqslant \mathbf{j}_i(\mathbf{Z})\cdot\mathbf{g}$, 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* $F(\mathbf{Z}) := F_1(\mathbf{Z}) \times \cdots \times F_N(\mathbf{Z}) : \mathcal{D}(F) \to \mathcal{P}(\mathbb{R}^{2N})$ *and let* $\mathbf{Z}_0 \in \mathcal{D}(F)$ *be a given initial configuration of dislocations. Consider the initial value problem*

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

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

The domain $\mathcal{D}(F)$ of the set-valued function F is $\Omega^N \setminus \{\text{collisions}\}$. To prove the local existence theorem it is enough to notice that the set-valued function $\operatorname{co} F$ 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.

Dynamics: uniqueness of solutions

To discuss uniqueness of solutions, a deep investigation of the set

$$\mathcal{A}_i := \{\mathbf{Z} \in \mathcal{D}(F) : \operatorname{card}(F_i(\mathbf{Z})) = 2\}, \qquad i \in \{1, \dots, N\}, \tag{5}$$

where the direction of motion is not uniquely defined, is required. Note that, if $\mathbf{Z} \in \mathcal{A}_i$, then $F_i(\mathbf{Z}) = \{\mathbf{f}_i^-(\mathbf{Z}), \mathbf{f}_i^+(\mathbf{Z})\}$. Define $\mathbf{f}^\pm(\mathbf{Z}) := (\mathbf{f}_1(\mathbf{Z}), \dots, \mathbf{f}_{i-1}(\mathbf{Z}), \mathbf{f}_i^\pm(\mathbf{Z}), \mathbf{f}_{i+1}(\mathbf{Z}), \dots, \mathbf{f}_N(\mathbf{Z})) \in \mathbb{R}^{2N}$. These results, together with general theorems from [3], yield

Theorem (Right uniqueness [4]). *Let* $\Omega \subset \mathbb{R}^2$ *be a connected open set. Let* $F(\mathbf{Z}) : \mathcal{D}(F) \to \mathcal{P}(\mathbb{R}^{2N})$*, let* $\mathbf{Z}_0 \in \mathcal{I}_i$ *for some* $i \in \{1, \dots, N\}$*, and let* $\mathbf{n}(\mathbf{Z}_0)$ *be the unit normal to* $\mathcal{A}_i$ *at* $\mathbf{Z}_0$*. If either* $\mathbf{f}^-(\mathbf{Z}_0)\cdot\mathbf{n}(\mathbf{Z}_0) > 0$ *or* $\mathbf{f}^+(\mathbf{Z}_0)\cdot\mathbf{n}(\mathbf{Z}_0) < 0$*, then there exists* $T > 0$ *such that the solution to (4) is unique in* $[0, T]$*.*

Here, $\mathcal{I}_i := \mathcal{A}_i \setminus (\mathcal{S}_i \cup \mathcal{E}_{\mathrm{int}} \cup \mathcal{E}_{\mathrm{zero}})$. The previous theorem allows to deal with situations like *cross-slip* and *fine cross-slip*, initially described in [1].

Theorem (Cross-Slip [4]). *Suppose* $\mathbf{Z}(t)$ *is a solution to (4) for* $t \in [0, T]$ *and that* $\exists\, t_1 \in (0, T)$ *and* $\hat{\mathbf{Z}} \in \mathcal{I}_i$ *for some* $i \in \{1, \dots, N\}$ *such that* $\mathbf{Z}(t_1) = \hat{\mathbf{Z}}$*,* $\mathbf{f}^-(\hat{\mathbf{Z}})\cdot\mathbf{n}(\hat{\mathbf{Z}}) > 0$ *and* $\mathbf{f}^+(\hat{\mathbf{Z}})\cdot\mathbf{n}(\hat{\mathbf{Z}}) > 0$*. Furthermore, suppose* $\exists\, \delta_1 > 0$ *such that* $\mathbf{Z}(t) \in V^-$ *for* $t \in (t_1 - \delta_1, t_1)$*. Then* $\exists\, \delta_2 > 0$ *such that* $\mathbf{Z}(t) \in V^+$ *for* $t \in (t_1, t_1 + \delta_2)$*. That is,* $\mathbf{Z}(t)$ *crosses from* V^- *into* V^+*.*

Theorem (Fine Cross-Slip [4]). *Let* $\mathbf{Z}_0 \in \mathcal{I}_i$ *for some* $i \in \{1, \dots, N\}$ *and suppose* $\exists\, r > 0$ *such that for all* $\mathbf{Z} \in B_r(\mathbf{Z}_0)$*,* $\mathbf{f}^-(\mathbf{Z})\cdot\mathbf{n}(\mathbf{Z}) > 0$ *and* $\mathbf{f}^+(\mathbf{Z})\cdot\mathbf{n}(\mathbf{Z}) < 0$*. Then* $\exists\, T > 0$ *and a unique solution* $\mathbf{Z} : [0, T] \to \mathcal{D}(F)$ *to (4). Moreover,* $\exists\, \delta > 0$ *such that* $\mathbf{Z}(t) \in \mathcal{I}_i \subset \mathcal{A}_i$ *for* $t \in [0, \delta)$ *and solves the ordinary differential equation*

$$\dot{\mathbf{Z}} = \mathbf{f}^0(\mathbf{Z}) \in \operatorname{co} F(\mathbf{Z}), \qquad \textit{where} \quad \mathbf{f}^0(\mathbf{Z}) := \alpha\mathbf{f}^+(\mathbf{Z}) + (1-\alpha)\mathbf{f}^-(\mathbf{Z}),$$

and $\alpha \in (0, 1)$ *is defined by* $\alpha := \dfrac{\mathbf{f}^-(\mathbf{Z})\cdot\mathbf{n}(\mathbf{Z})}{\mathbf{f}^-(\mathbf{Z})\cdot\mathbf{n}(\mathbf{Z}) - \mathbf{f}^+(\mathbf{Z})\cdot\mathbf{n}(\mathbf{Z})}$.