Variational evolution of dislocations in single crystals

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Abstract

In this paper we provide an existence result for the energetic evolution of a set of dislocation lines in a three-dimensional single crystal. The variational problem consists of a polyconvex stored-elastic energy plus a dislocation energy and some higher-order terms. The dislocations are modeled by means of integral one-currents. Moreover, we discuss a novel dissipation structure for such currents, namely the flat distance, that will serve to drive the evolution of the dislocation clusters.

1 Introduction

Origin of the model

Dislocations are one-dimensional singularities in a three-dimensional body, whose motion is ultimately responsible for metal plasticity. Their study is of crucial impact in many technological processes such as the industry of semiconductors, as related to bulk crystal growth [27], since metal toughness and conductivity for instance depend on their density. In this process, a crystal is grown from the melt and dislocations are created from the incorporation of point defects at the solid-liquid interface, and can leave the crystal by its solid-gas interface. The particular feature of this process is that the crystal must be considered on a large range of temperatures and hence the motion of dislocations cannot be assumed as restricted to some pre-established glide planes, as for a crystal at ambient temperature. This is the motivation of our series of works [30–33] whose main feature is to consider dislocations in their three-dimensional generality (based on the pioneering contribution [28]). The second specificity of our approach is to consider finite-strain elasticity, since a dislocation does by essence induce large deformations near its singularity. Therefore, our model choice is to consider polyconvex energies [4], together with higher order terms accounting for the energy of the singularities. In turn, dislocation singularities are described as integral 1-currents, which in order to keep track of the associated Burgers vector, are taken with coefficients in a group (see also, e.g., [12]).

So far, our study was dedicated to a variational approach to the static problem, since difficult issues had to be faced, for instance as related to the closedness of the class of admissible fields. As a matter of fact, we consider a limit-case thermodynamics in which the first and second principle are satisfied by minimizing an energy functional, that, quoting Berdychevski [7] "in crystals with negligible resistance to dislocations motion, like pure copper, [...] can be reached very fast".

If one restricts to the motion of parallel dislocations, the problem becomes two-dimensional, since the dislocations are modelled as points [37]. In this case, the mathematical analysis of dynamics model already exists in the wake of Ginsburg-Landau vortices dynamics, and can be found for instance in [1,2,8,9]. The dynamics of this kind of dislocations have been studied by several authors, see for instance the important contributions [18] and [25] for a rate-independent evolution. See also the more recent paper [26] and references therein. Let us also mention the interesting analysis contained in [38], and the references therein. Nonlocal evolution models can also be considered as in [29]. At the mesoscale, another route is known as the Discrete Dislocations Dynamics model (DDD), see [11, 36, 39], that considers the dynamics of single dislocations segments and their interactions. Though, this approach is computationally expensive and hence restricted to small samples.

Brief exposition of the variational evolution model

The energetic formulation for quasi-static evolutions, due to Mielke and coauthors (see [22] for a survey) has become very popular in the recent years. One reason is that in this theory, the variational approach and its elegant mathematical techniques meet physical principles among which conservation laws. This approach has proved successful, among other, in fracture dynamics, delamination, damage, as well as Ginsburg-Landau-like models (see, e.g., [13, 21, 23, 24, 34, 35]). To the knowledge of the authors, no such energetic evolution was ever considered for three-dimensional dislocation clusters. It is the first purpose of this paper to recall and expose how the ideas developed in [30–33] meet in a very natural way the lines of Mielke and coauthors well-established existence theory for the quasi-static evolution of rate-independent systems. The basic ingredients are the following: (i) a variational model at the statics level, and (ii) an appropriate notion of dissipation distance. Whereas the first point has been addressed in previous papers by the authors, the second is presented as a novel contribution in the present work.

We consider a three-dimensional elastic body represented by a bounded and connected open set Ω. In the presence of dislocations, the main variables of the system are the deformation field $F : \Omega \to \mathbb{R}^{3\times3}$ (which is, locally, the gradient of a displacement $u : \Omega \to \mathbb{R}^3$), and the associated dislocation density $\Lambda_{\mathcal{L}}$, namely a $\mathbb{R}^{3\times3}$-valued Borel measure on Ω defined as

$$\Lambda_{\mathcal{L}} = \tau \otimes b\mathcal{H}^1 \llcorner_L, \tag{1.1}$$

where b is the Burgers vector, L is the dislocation curve with unit tangent vector τ, and $\mathcal{H}^1$ is the one-dimensional Hausdorff measure. Let us already mention that for the existence results we present three scenarios. In the second and third ones, all dislocations lines are assumed to have the same Burgers vector. In the first setting instead, it is possible to consider cluster of dislocations with linearly independent Burgers vectors. The deformation F and the dislocation density $\Lambda_{\mathcal{L}}$ are related by the identity

$$-\operatorname{Curl} F = \Lambda_{\mathcal{L}}^T, \tag{1.2}$$

where symbol T stands for the transpose. We denote $\mathcal{L} := \tau\mathcal{H}^1\llcorner_L$ and in the language of currents we write $\Lambda_{\mathcal{L}}^T = b \otimes \mathcal{L}$, since in our approach the measure $\mathcal{L}$ is identified with a one-dimensional integral current and is called dislocation current.

We consider a quasi-static evolution in the presence of a nonlinear stored-elastic energy following the framework proposed in [31–33], which relies on a polyconvex elastic energy, plus two higher order terms depending on the first derivatives of F, and in particular on the dislocations density. We supplement the system with a time-depending external bulk force f and a traction g acting on the Neumann part of the boundary, which drives the evolution. For the dissipation functional $\mathcal{D}$, we make the choice of the flat distance on the spaces of dislocations currents. Its physical meaning is discussed below. For simplicity, we will consider an isotropic flat distance, even if, in the presence of dislocations an anisotropic version of the flat distance would be more realistic from a physical viewpoint. Lastly, we choose a fixed Dirichlet boundary datum w independent of time. The more involved problem of imposing a time-dependent Dirichlet boundary condition is a challenging issue that we are not able to address at the present stage (see the Open problems section). This is due to additional difficulties deriving from the fact that fixing time-dependent dislocations at the boundary yields a poor regularity in the boundary datum for the displacement field, and this prevents to have control on the time derivative of the energy.

Mathematical modeling of the dissipation

Let us now spend some words on the model. In the spirit of Gurtin [17], we will consider the work expended by a dislocation to change position. This so-called configurational work represents the dissipation produced by this configurational motion. Moreover, any other source of dissipation is assumed negligible with respect to micro-structure dissipation. Let $\mathcal{L} \subset \Omega$ be a dislocation loop with tangent vector τ and Burgers vector $b = |b|B$ where $B \in S^2$. In a first step, we assume that the time-dependent dislocation $t \mapsto \mathcal{L}(t)$ lies and moves on a glide plane Π with unit normal n. We will consider the case when the dislocation moves by a displacement $\overrightarrow{\delta q} \in \mathbb{R}^3$ during the time interval δt, i.e., $\vec{q}(t+\delta t) = \vec{q}(t) + \overrightarrow{\delta q} \in \Omega$. Accordingly, let $\mathcal{L}' := \mathcal{L}(t+\delta t)$. Let us write $\overrightarrow{\delta q}$ in the local base (τ, B), i.e.,

$$\overrightarrow{\delta q} = \overrightarrow{\delta q}_\tau + \overrightarrow{\delta q}_B$$

where $\overrightarrow{\delta q}_\tau$ and $\overrightarrow{\delta q}_B$ are the components of $\overrightarrow{\delta q}$ respectively along τ and B. We write $\overrightarrow{\delta q}_B := (\delta \ell)B$ for $\delta \ell \in \mathbb{R}$ to mean the configurational displacement. If the dislocation changes location, the micro-structure configuration has changed, and configurational work has been expended (in the form of a dissipated energy). Hence, to compute the configurational work, we will consider the force over a displacement $\overrightarrow{\delta q_B}$ purely along B, since the component along τ does not change the defect configuration, hence its associated work is assumed negligible. Define the surface element $\overrightarrow{\delta S} := \overrightarrow{\delta q} \times \tau$ (vanishing if the displacement has no configurational component).

Now, denoting the (symmetric) Cauchy stress tensor σ, the force per unit surface exerted by the crystal on any facet of the glide plane Π is $\vec{t} = \sigma \vec{n}$. In particular $\vec{t}(\delta S) = \sigma_{jl}(\delta S)_l$ represents the configurational force exerted on the planar strip δS with normal n. The associated variation of configurational work, or micro-structure dissipation, is defined as

$$\delta W_c := \vec{t} \cdot \overrightarrow{\delta q_B}.$$

Indicewise, we define the normalized configurational work of a dislocation as $\delta \bar{W}_c := (|b|/\delta\ell)\delta W_c = \sigma_{jl}(\delta S)_l b_j$, representing the work expended for a displacement of $\mathcal{L}$ by b caused by the configurational force $\vec{t}(\delta S)$. By $(\delta S)_l = \epsilon_{lmi}(\delta q)_m \tau_i$, we have $\delta \bar{W}_c := \sigma_{jl} b_j \epsilon_{lmi}(\delta q)_m \tau_i$. Owing to the symmetry of σ, the configurational force F^{PK} is defined componentwise as follows: $F^{\mathrm{PK}}_m := \dfrac{\partial \delta \bar{W}_c}{\partial (\delta q)_m} = \epsilon_{mil}\sigma_{lj} b_j \tau_i$, known as the Peach-Koehler force on $\mathcal{L}$. In compact form, for the motion on the glide plane,

$$\delta \bar{W}_c = \sigma b \cdot n |\delta S|, \tag{1.3}$$

where

$$\begin{aligned} |\delta S| &= \text{the area of the planar strip between } \mathcal{L} \text{ and } \mathcal{L}' \\ &= d_F(\mathcal{L}, \mathcal{L}') \\ &:= \text{the minimum area of the surfaces enclosed by } \mathcal{L} - \mathcal{L}'. \end{aligned} \tag{1.4}$$

Consider now that the motion is free of any predefined glide plane. The configurational work is again defined by (1.3), with n the unit normal to the strip δS. However, being the motion no more planar, δS is not univoquely defined, since it can be any two-dimensional manifold enclosed by the closed loop $\mathcal{L} - \mathcal{L}'$. Taking such strip of minimal area, we take by definition the configurational dissipation as given by (1.3) and (1.4). By this means, we introduce precisely the notion of flat distance between $\mathcal{L}$ and $\mathcal{L}'$ (see for instance [20]). The key point to observe is that the configurational work, that indeed represents the dissipation produced by the configurational motion [17], is proportional to $d_F(\mathcal{L}, \mathcal{L}')$ for dislocation movements in the glide plane. Therefore we extend this property to be a definition of configurational dissipation for a general motion, i.e.,

$$\text{Dislocation dissipation} = W_c = \gamma d_F(\mathcal{L}, \mathcal{L}'),$$

where $|\delta S| = d_F(\mathcal{L}, \mathcal{L}')$ is indeed the minimal area between $\mathcal{L}$ and $\mathcal{L}'$, and $\gamma > 0$ is a material parameter. It is crucial to have in mind that $\mathcal{L}$ and $\mathcal{L}'$ have an orientation and hence the flat norm between to geometrically closed loops with opposite orientation will not tend to zero. This corresponds to the highly dissipative process required to invert the orientation of a dislocation. Summarizing, our total energy will be

$$\mathcal{E} + \mathcal{D} := \mathcal{W} + \mathcal{P} + W_c,$$

with $\mathcal{W}$ the stored-elastic energy, $\mathcal{P}$ the potential energy equals to minus the work of the external loads, and W_c the configurational work. The problem that we address is to indeed find an evolution $t \mapsto \mathcal{L}(t)$ such that at each time the minimum of $\mathcal{E} + \mathcal{D}$ is achieved (such a minimization is for instance attained for certain crystals such as copper, cf. [7]). This dynamics indeed is a variational evolution in the sense of Mielke and coauthors [22] together with the existence results established by the authors for the statics problem [31–33]. For the sake of exposition, our main result is here stated in a simplified form:

Theorem 1.1. *In the hypotheses given by the settings (D1), (D2), and (D3) (introduced in Section 2.2), and if the energy of the system $\mathcal{E}$ and the dissipation $\mathcal{D}$ satisfy suitable conditions (see assumptions (A1)-(A6) in Section 3.2) then there exists a quasistatic evolution for the deformation field $F : [0, T] \times \Omega \to \mathbb{R}^{3\times 3}$, which is an energetic solution.*

The precise meaning of energetic solution is given in Definition 3.1. Roughly speaking this means that at every time $t \in [0, T]$ the solution $F(t)$ is stable, that is, minimizes the internal energy. Moreover, the energy of the system, namely the internal energy plus the dissipation, is conserved. Let us here stress that in the setting (D1) we can consider dislocation clusters generated by linearly independent Burgers vectors, whereas the scenarios (D2) and (D3) only consider evolution of clusters generated by a single Burgers vector. Furthermore the evolution considers a fixed (in time) Dirichlet boundary datum. The generalizations to the case of (i) evolution of linearly independent Burgers vectors in the settings (D2) and (D3) and (ii) a time-dependent Dirichlet boundary conditions, are discussed in Section 4.

Let us finally emphasize that at the present stage we have considered a dissipation distance which is isotropic, while a generalized anisotropic version of the flat distance should be introduced in order to describe a more realistic physical framework. For simplicity of discussion, we do not cover here this generalization and leave this effort for future contributions.

2 Preliminaries and model description

The crystal is represented by a bounded, connected open set $\Omega \subset \mathbb{R}^3$. We assume that Ω has a Lipschitz boundary $\partial\Omega$ that writes as the union of a Dirichlet and Neumann part, the first one with positive Hausdorff measure, namely

$$\partial\Omega := \Gamma_D \cup \Gamma_N, \qquad \text{with } \mathcal{H}^2(\Gamma_D) > 0. \tag{2.1}$$

It is convenient to assume that there is a Lipschitz bounded and connected open set U such that $\partial\Omega \cap U = \Gamma_D$. We set $\hat{\Omega} := U \cup \Omega$.

Setting and kinematical variables. Referring to the classical nonlinear model for crystals in the presence of dislocations, the main variables of the system are the deformation field F and its induced dislocation current $\mathcal{L}$. The deformation field satisfies $F \in L^p(\Omega; \mathbb{R}^{3\times 3})$ for some $p \in (1, 2)$, while $\mathcal{L} \in \mathcal{D}_1(\Omega)$ is a integer-multiplicity boundaryless 1-current (here $\mathcal{D}_k(\Omega)$ denotes the space of k-currents in Ω). These two variables are related by the equation

$$-\operatorname{Curl} F = b \otimes \mathcal{L}, \tag{2.2}$$

where $b \in 2\pi\mathbb{Z}$ is the Burgers vector associated to the cluster $\mathcal{L}$. Here $\mathcal{L}$ is identified with the Radon measure $\mathcal{L} = \tau\mathcal{H}^1 \llcorner_L$, where $\mathcal{H}^1$ is the one-dimensional Hausdorff measure restricted to L, the support of $\mathcal{L}$, which is a rectifiable 1-set with unit tangent vector τ. For the detailed description and the general properties of these objects we refer to [31, 32].

Following [32, 33], the deformation tensor can be always decomposed as the sum of two gradients, namely

$$F = \nabla\bar{u} + \nabla v = \nabla u, \tag{2.3}$$

where $\bar{u} \in W^{1,p}(\Omega; \mathbb{T}^3)$ (with $\mathbb{T}^3$ being the three dimensional flat torus), $v \in W^{1,p}(\Omega; \mathbb{R}^3)$, satisfying

$$\begin{cases} \Delta\bar{u} & = 0, \\ -\operatorname{Curl} \nabla\bar{u} & = b \otimes \mathcal{L}, \end{cases} \qquad \begin{cases} \Delta v & = \operatorname{Div} F \\ \operatorname{Curl} \nabla v & = 0, \end{cases} \tag{2.4}$$

together with suitable boundary conditions. The maps $\bar{u}$ and v are referred to as incompatible and compatible displacements, respectively. It is always possible to consider v with values in the flat torus as well, in such a way that it is licit to define $u := \bar{u} + v \in W^{1,p}(\Omega; \mathbb{T}^3)$ to be the total displacement field as in (2.3). If the divergence of the deformation F belongs to $L^r(\Omega; \mathbb{R}^3)$ for some $r \geq 1$, then from the second system of equations in (2.4), it is possible to prove (see [32]) that

$$v \in W^{2,r}(\Omega; \mathbb{R}^3).$$

Moreover, as admissible deformation fields always satisfy this regularity condition, the compatible displacement v shows some higher regularity properties than $\bar{u}$.

In the case that the dislocation cluster is generated by more than only one Burgers vector b, the incompatible part of the displacement $\bar{u}$ does satisfy the general equations

$$\begin{cases} \Delta \bar{u} & = 0, \\ -\operatorname{Curl} \nabla \bar{u} & = e_1 \otimes \mathcal{L}^1 + e_2 \otimes \mathcal{L}^2 + e_3 \otimes \mathcal{L}^3, \end{cases},$$

where $\{e_1, e_2, e_3\}$ is the canonical basis of $\mathbb{R}^3$ and $\mathcal{L}^i$ is a 1-dimensional closed integral current, for $i = 1, 2, 3$.

Notice that in the case that the cluster is generated by a single Burgers vector b, up to a change of basis, we can also consider the variable $\bar{u}$ (and then the whole displacement u) with values in $\mathbb{T} \times \mathbb{R}^2 \equiv S^1 \times \mathbb{R}^2$.

Set of admissible variables. When the dislocation cluster is generated by a single Burgers vector b we introduce the space of admissible deformation fields $\mathcal{F}_b$ for the domain Ω as follows

$$\mathcal{F}_b(\Omega) := \{F \in L^p(\Omega; \mathbb{R}^{3\times 3}) : \operatorname{cof} F \in L^{p_2}(\Omega; \mathbb{R}^{3\times 3}),\ \det F \in L^{p_3}(\Omega),\ \operatorname{Div} F \in L^r(\Omega; \mathbb{R}^3), \\ \text{and } -\operatorname{Curl} F = b \otimes \mathcal{L} \text{ for some dislocation current } \mathcal{L}\}, \tag{2.5}$$

where the exponents $p, p_2, p_3, r \geq 1$ will be specified later. If the cluster is general, we use a different notation for the

$$\mathcal{F}^\star(\Omega) := \{F \in L^p(\Omega; \mathbb{R}^{3\times 3}) : \operatorname{cof} F \in L^{p_2}(\Omega; \mathbb{R}^{3\times 3}),\ \det F \in L^{p_3}(\Omega),\ \operatorname{Div} F \in L^r(\Omega; \mathbb{R}^3), \\ \text{and } -\operatorname{Curl} F = e_1 \otimes \mathcal{L}^1 + e_2 \otimes \mathcal{L}^2 + e_3 \otimes \mathcal{L}^3 \\ \text{for three dislocation currents } \mathcal{L}^i,\ i = 1, 2, 3\}, \tag{2.6}$$

The variables of the model being the deformation field $F : \Omega \to \mathbb{R}^{3\times 3}$ and its dislocation density, suitable boundary conditions must be prescribed. The Dirichlet boundary datum, in the spirit of the minimum problem in [31–33], can be given by introducing an admissible deformation field $\hat{F} \in L^p(\hat{\Omega}; \mathbb{R}^{3\times 3})$ and saying that $F \in \mathcal{F}_b$ satisfies the Dirichlet boundary condition if $F \llcorner_{\hat{\Omega}\setminus\Omega} = \hat{F}$. However, since by (2.3), to any admissible field $F \in \mathcal{F}_b$ there exists a displacement $u \in W^{1,p}(\Omega; \mathbb{T}^3)$ such that $\nabla u = F$, we formulate our problem in terms of u and correspondingly we will impose Dirichlet boundary conditions on u. We therefore introduce the class of admissible displacement fields as follows: fix a displacement $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ satisfying the condition

$$\nabla w \in \mathcal{F}_b(\hat{\Omega}),$$

and say that $u \in W^{1,p}(\Omega; \mathbb{T}^3)$ is an admissible displacement if $u \in \mathcal{U}_b(w)$, where

$$\mathcal{U}_b(w) := \{u \in W^{1,p}(\Omega; \mathbb{T}^3) : \nabla u \in \mathcal{F}_b(\Omega) \text{ and } u = w \text{ on } \Gamma_D\}. \tag{2.7}$$

The equality $u = w$ on Γ_D must be understood in the sense of trace, as elements of $W^{1-1/p,p}(\Gamma_D; \mathbb{T}^3)$. In the general case of cluster generated by multiple Burgers vectors we fix

$$\nabla w \in \mathcal{F}^\star(\hat{\Omega}),$$

and we say that $u \in W^{1,p}(\Omega;\mathbb{T}^3)$ is admissible if $u \in \mathcal{U}^\star(w)$ where

$$\hat{\mathcal{U}}^\star(w) := \{u \in W^{1,p}(\Omega;\mathbb{T}^3) : \nabla u \in \mathcal{F}^\star(\Omega) \text{ and } u = w \text{ on } \Gamma_D\}, \tag{2.8}$$

Further we introduce the class of admissible dislocation currents as

$$\mathcal{R} := \{\mathcal{L} \in \mathcal{D}_1(\hat{\Omega}) : \mathcal{L} \text{ has integer multiplicity, } \partial\mathcal{L} = 0,\ |\mathcal{L}| < \infty,\ \text{supp}\mathcal{L} \subset \hat{\Omega}\}. \tag{2.9}$$

It is convenient to introduce the following notation: for any constant $C > 0$ we denote by $\mathcal{R}_C$ the subset of $\mathcal{R}$ defined as

$$\mathcal{R}_C := \{\mathcal{L} \in \mathcal{R} : |\mathcal{L}| \leq C\}. \tag{2.10}$$

2.1 Properties of the energy

The energy of the body depends on the tensor field F and on its derivatives. The stored-elastic energy density is given by the functional $W_e(M(F))$, where $M(F)$ is the vector of minors of F, and hence the stored-elastic energy by

$$\mathcal{W}_e(M(F)) = \int_\Omega W_e(M(F))dx. \tag{2.11}$$

We assume that

(E1) $\mathcal{W}_e$ is polyconvex, i.e. W_e is convex in $M(F)$.

We suppose that W_e fulfills the following growth condition: there are constants $c_1, c_2 > 0$, and $\delta \geq 0$ such that

(E2) $W_e(M(F)) \geq c_1(|F|^p + |\operatorname{cof} F|^{p_2} + \delta|\det F|^{p_3}) - c_2$,

for some coefficients $p, p_2, p_3 > 1$ to be specified later. Notice that polyconvexity together with condition (E2) implies lower semi-continuity with respect to the weak convergences of F, $\operatorname{cof} F$, and $\det F$ in $L^p(\Omega;\mathbb{R}^{3\times3})$, $L^{p_2}(\Omega;\mathbb{R}^{3\times3})$, and $L^{p_3}(\Omega)$, respectively (see, e.g., [4, 14]). It is also assumed that $W(M(F)) \geq h(\det F)$ for a continuous and positive function h satisfying $h(t) \to +\infty$ as $t \to 0$ and $h(t) = +\infty$ for $t \leq 0$. The total energy of the system also depends on the derivatives of F. The microstructure part of the energy related to the presence of dislocations is denoted by $\mathcal{W}_{\text{dislo}}$ and is taken as a function of the dislocation density $\Lambda_\mathcal{L} := (\mathcal{L} \otimes b)^T$ that we recall is related to the curl of deformation tensor, Curl F. We make the following assumption:

(E3) $\mathcal{W}_{\text{dislo}}$ is l.s.c. with respect to the weak star convergence of measures,

and assume the following growth condition:

(E4) $\mathcal{W}_{\text{dislo}}(\Lambda_\mathcal{L}) \geq c_3|\Lambda_\mathcal{L}|(\Omega) - c_4$, for some positive constants c_3 and c_4. Eventually, we assume that the total energy of the system depends on Div F via the higher order term $\mathcal{W}_{\rm d}$ in the form

$$\mathcal{W}_{\rm d}(\text{ Div } F) = \int_\Omega W_{\rm d}(\text{ Div } F)dx,$$

where

(E5) $\mathcal{W}_{\rm d}$ is l.s.c. with respect to the weak topology of $L^r(\Omega;\mathbb{R}^3)$,

(E6) $W_{\rm d}(\text{ Div } F) \geq c_5|\text{ Div } F|^r - c_6$,

for some positive constants c_5 and c_6. Note that the modeling meaning of the term Div F, as explained in [33], is related to the invariants of DF. The presence of such a term is related to the fact that the model being of second-order might depend on all the invariants of DF. Moreover, let us stress that this term can also be seen as a regularization, which at the present stage is necessary in order to characterize the graphs of the displacement as an integral currents, and to gain closedness of the state variables (see also Section 4.2).

Summarizing, the total energy of a deformation field F reads

$$\mathcal{W}(F, DF) = \mathcal{W}_{\rm e}(M(F)) + \mathcal{W}_{\rm dislo}(\text{ Curl } F) + \mathcal{W}_{\rm d}(\text{ Div } F), \tag{2.12}$$

and satisfies the coercivity condition

$$\begin{aligned}\mathcal{W}(F, DF) \geq \\ \geq C\left(\|F\|^p_{L^p} + \|\text{ cof } F\|^{p_2}_{L^{p_2}} + \delta\|\det F\|^{p_3}_{L^{p_3}} + \|\text{ Div } F\|^r_{L^r}\right) + c|\Lambda_{\mathcal{L}}|(\Omega) - \gamma,\end{aligned} \tag{2.13}$$

for suitable positive constant C, c, γ, and $\delta \geq 0$, depending on the material properties. We refer to [33] for more detail on the model, and in particular for explicit examples of energies satisfying these properties.

Time-dependent external load

Let $T > 0$ and let us consider the time interval $[0, T]$. The volume and surface forces are $f \in C^1\left([0,T]; L^{p'}(\Omega, \mathbb{R}^3)\right)$ and $g \in C^1\left([0,T]; W^{1-1/p',p'}(\Gamma_N, \mathbb{R}^3)\right)$, satisfying

$$\int_\Omega f(t)\, dx + \int_{\Gamma_N} g(t)\, d\mathcal{H}^2 = 0, \tag{2.14}$$

for any $t \in [0,T]$. Following the approach introduced in [3], we consider the tensor of external load $\mathbb{K}(t) \in C^1([0,T]; W^{1,p'}(\Omega; \mathbb{R}^{3\times 3}))$, satisfying at each $t \in [0,T]$,

$$\begin{cases} -\text{ Div } \mathbb{K}(t) = f(t) & \text{in } \Omega \\ \mathbb{K}N = g(t) & \text{on } \Gamma_N, \\ \mathbb{K}N = 0 & \text{on } \Gamma_D, \end{cases} \tag{2.15}$$

where N stands for the unit normal vector to the boundary. For the existence of $\mathbb{K}$ we refer to [3]. The justification for this approach is that in the absence of dislocations, one has $u \in W^{1,p}(\Omega, \mathbb{R}^3)$ and one recovers by integration by parts the classical expression of the work of the external forces, namely

$$\langle \mathbb{K}(t), \nabla u \rangle = \langle f(t), u \rangle + \langle g(t), u \rangle_{\Gamma_N}. \tag{2.16}$$

However, in the presence of dislocations, such integration by parts cannot be made in a classical manner[1]. Thus, we define the work of the external forces by the term $\langle \mathbb{K}(t), \nabla u \rangle_{L^{p'}, L^p}$. Therefore, the total energy at a given time $t \in [0, T]$ is given by

$$\mathcal{E}(t, u) = \mathcal{W}(\nabla u, D\nabla u) - \langle \mathbb{K}(t), \nabla u \rangle_{L^{p'}, L^p}. \tag{2.17}$$

By Young inequality $\langle \mathbb{K}(t), F \rangle_{L^{p'}, L^p} \leq \frac{\lambda^{p'}}{p'} \|\mathbb{K}(t)\|_{L^{p'}}^{p'} + \frac{1}{p\lambda^p} \|F\|_{L^p}^p$ for any $\lambda > 0$ and hence one also has, from (2.13),

$$\begin{aligned} &\mathcal{E}(t, u) \geq \\ &\quad \geq C \left(\|F\|_{L^p}^p + \|\operatorname{cof} F\|_{L^{p_2}}^{p_2} + \delta \|\det F\|_{L^{p_3}}^{p_3} + \|\operatorname{Div} F\|_{L^r}^r \right) + c|\Lambda_{\mathcal{L}}|(\Omega) - \gamma, \end{aligned} \tag{2.18}$$

for suitable positive constant C, c, γ, and $\delta \geq 0$, depending on the material properties. Note that

$$\partial_t \mathcal{E}(t, u) = \langle \dot{\mathbb{K}}(t), \nabla u \rangle_{L^{p'}, L^p}, \tag{2.19}$$

and thus again by Young inequality, one obtains

$$|\partial_t \mathcal{E}(t, u)| \leq \frac{1}{p'} \|\dot{\mathbb{K}}(t)\|_{L^{p'}}^{p'} + \frac{1}{p} \|\nabla u\|_{L^p}^p. \tag{2.20}$$

In particular, due to estimate (2.18) and the regularity of $\mathbb{K}$, one recovers the following important bound:

$$|\partial_t \mathcal{E}(t, u)| \leq C_1(\mathcal{E}(t, u) + C_2), \tag{2.21}$$

for suitable constants $C_1, C_2 > 0$.

2.2 Static problem

Let us discuss several possible hypotheses according to the results contained in [31–33]:

(D1) Continuum dislocations as in [31]. In this setting we assume (E1), (E2), and (E3), and consider general dislocation clusters generated by multiple Burgers vectors. Moreover, the regularizing term $W_{\mathrm{d}} = 0$, whereas the dislocation singularities energy $\mathcal{W}_{\mathrm{dislo}}$ satisfies the following condition, replacing (E4):

(E4)' $\mathcal{W}_{\mathrm{dislo}}(\Lambda_{\mathcal{L}}) \geq \kappa \inf_{\mathcal{K}} \left(\mathcal{H}^1(\mathcal{K}) + \sharp\mathcal{K} \right) - C$, where the infimum is computed on all rectifiable and closed 1-sets containing the support of $\Lambda_{\mathcal{L}}$; here $\sharp\mathcal{K}$ represents the number of connected components of $\mathcal{K}$, $C > 0$ and $\kappa > 0$ are material parameters.

[1] However, in order to define the external forces as in (2.16) a possibility might be to fix a suitable lifting for the map u (which takes values in the torus) and to prove that the obtained expression does not depend on the chosen lifting. We thank the anonymous referee for this suggestion.

The infimum in this condition is assumed to attain the value $+\infty$ if the family of continuum sets $\mathcal{K}$ is empty. Notice that the energy is finite only if the dislocation density $\Lambda_{\mathcal{L}}$ is a continuum dislocation, according to [31]. A physical interpretation of this assumption is also proposed in [31]. Moreover we assume the following conditions on the coefficients in (E2): $\delta > 0$, $p_2, p_3 > 1$, and $1 < p < 2$. The class of admissible displacements $\mathcal{U}^\star(w)$ is defined by

$$\mathcal{U}^\star(w) := \{u \in \hat{\mathcal{U}}^\star(w) : \text{if } B \subset \Omega \text{ is a ball not intersecting the support of } \Lambda_{\mathcal{L}}, \\ u \in \text{Cart}(B;\mathbb{T}^3) \text{ is a Cartesian map on } B\}. \quad (2.22)$$

Recall that w is such that $\nabla w \in \mathcal{F}^\star(\Omega)$ and then allows for the presence of dislocations with linearly independent Burgers vectors. The fact that u restricted to any ball is Cartesian means that its graph, seen as a integral current, is boundaryless (see [31] and [16] for general treatment of Cartesian currents). We emphasize that this hypothesis was first introduced in [28].

Remark 2.1. Let us stress out that in this case the dislocation currents, being well included in continuum sets, can be proved to be equivalent of simple Lipschitz curves. The use of currents is however useful to give direct proofs of existence and to give a general description which is uniform with the other scenarios (see also [31] for the usefulness of the tool of currents).

(D2) Regular compatible displacement v, as in [32]. We assume (E1)-(E6). In this scenario, the compatible deformation part v of the displacement is smooth enough, i.e., $v \in \mathcal{C}^1(\Omega, \mathbb{R}^3)$, due to the assumption $r > 3$ in (E6). Moreover we set $\delta > 0$, $p_2, p_3 > 1$, and $1 < p < 2$.

(D3) Singular compatible displacement v, as in [33]. We assume (E1)-(E6). We suppose that the coefficients in (E2) satisfy $1 < p < 2$, $p_2 \geq 2$, $p_3 > 1$, $r > \frac{12}{7}$. Moreover, one of the following two technical conditions are required

(E7) $\delta > 0$;

(E7)' $\delta = 0$ and either $r > \frac{6p}{5p-3}$ or $\frac{1}{p} + \frac{1}{p_2} > 1$.

In the scenarios (D2) and (D3) we consider dislocation clusters generated by a single Burgers vector denoted by b. Therefore the class of admissible displacements $\mathcal{U}_b(w)$ has been introduced in (2.7) for a fixed w such that $\nabla w \in \mathcal{F}_b(\Omega)$.

We introduce the following notation: in the case of multiple Burgers vectors (and then in scenario (D1)) the set of admissible variables is

$$\mathcal{A}^\star(w) := \{(u, \mathcal{L}^1, \mathcal{L}^2, \mathcal{L}^3) \in \mathcal{U}^\star(w) \times \mathcal{R}^3 : -\,\text{Curl } \nabla u = e_1 \otimes \mathcal{L}^1 + e_2 \otimes \mathcal{L}^2 + e_3 \otimes \mathcal{L}^3\}, \quad (2.23)$$

while the set of admissibility in the case of a single Burgers vector is defined as follows:

$$\mathcal{A}_b(w) := \{(u, \mathcal{L}) \in \mathcal{U}_b(w) \times \mathcal{R} : -\,\text{Curl } \nabla u = b \otimes \mathcal{L}\}. \quad (2.24)$$

This last notation will be adopted for scenarios (D2) and (D3).

Remark 2.2. Notice that by [33, Lemma 1.1 and Lemma 1.2] (see also the discussion in Section 4 of [33]) in the case (E7)' then the energy satisfies, even if $\delta = 0$ in hypothesis (E2), the following coercivity condition:

$$\mathcal{W}(F, DF) \geq c_7 \| \det F\|^t_{L^t} - c_8, \tag{2.25}$$

for some positive constants c_7 and c_8 and for $\frac{1}{t} = \frac{6-2r}{3r} + \frac{1}{p}$.

Let us discuss the conditions in (D2) and (D3). In the first case, thanks to the results in [32], the fact that $r > 3$ allows us to characterize the graph of the displacement field u, seen as an integer multiplicity 3-current in $\Omega \times \mathbb{T}^3$. In particular, it turns out that its boundary is an integer multiplicity 2-current in $\Omega \times \mathbb{T}^3$, given by

$$\begin{aligned}\partial\mathcal{G}_u(\omega) &= \mathcal{L} \wedge \vec{b}(\omega) + \mathcal{C}_v(\omega) := \\ &= -\frac{1}{2\pi}\int_L \int_0^{2\pi} \langle \omega(x, \frac{b\theta}{2\pi}), \bar{\tau} \wedge \bar{b}\rangle d\theta d\mathcal{H}^1(x) \\ &\quad + \frac{1}{2\pi}\int_L \int_0^{2\pi} \langle \omega(x, \frac{b\theta}{2\pi} + v(x)), \frac{\partial \bar{v}}{\partial \tau} \wedge \bar{b}\rangle d\theta d\mathcal{H}^1(x),\end{aligned} \tag{2.26}$$

for any 2-form $\omega \in \mathcal{D}^2(\Omega \times \mathbb{R}^3)$ being 2π-periodic in the second variable. In the formula above τ is the oriented tangent vector to the dislocation line L, and $\bar{\tau} = (\tau, 0) \in \mathbb{R}^6$, $\bar{b} = (b, 0) \in \mathbb{R}^6$, $\frac{\partial \bar{v}}{\partial \tau} = (0, \frac{\partial v}{\partial \tau}) \in \mathbb{R}^6$, and $v \in \mathcal{C}^1(\Omega, \mathbb{R}^3)$ is the compatible displacement associated to u. In particular, it is proven in [32, Theorem 4.6] that

$$M(\partial\mathcal{G}_{u+v}) \leq C(1 + \|Dv\|_{L^\infty(\Omega)})|\mathcal{L} \otimes b|(\Omega),$$

in such a way that a bound on the dislocation density provides a bound on the mass of the boundary, as required to have compactness (see next theorem). The condition Div $F \in L^r$ with $r > 3$ together with $F \in L^p$ with $p < 2$ might appear as a strong assumption. In the setting (D3) the requirement $r > 3$ is relaxed (and indeed $r < 2$ is admissible), but we add the hypothesis that $p_2 \geq 2$ in order to control the part of the current $\partial\mathcal{G}_u$ given by $\mathcal{C}_v$. Indeed, if $p_2 \geq 2$ it is proved that $\mathcal{C}_v$ vanishes, and again it is possible to control the mass of $\partial\mathcal{G}_u$ (see [33]). It is also discussed in [33] why the hypothesis $p_2 \geq 2$ is rather natural from a modeling viewpoint. It is now possible to prove that the energy has compact sublevels. To this aim, in the following theorem we rephrase the compactness results that were proved in [31–33].

Theorem 2.3. *Assume that one of the working hypotheses (D1), (D2) or (D3) holds. For all $t \in [0, T]$ the energy $\mathcal{E}(t, \cdot) : \mathcal{U}(w) \to \mathbb{R} \cup \{+\infty\}$ has compact sublevels. Namely, let $(u_k, \mathcal{L}_k)_k \in \mathcal{A}(w)$ be a sequence such that*

$$\mathcal{E}(t, u_k) < C < +\infty,$$

for all $k > 0$, then there exists a (not relabelled) subsequence such that $(u_k, \mathcal{L}_k) \rightharpoonup (u, \mathcal{L}) \in \mathcal{A}(w)$, and $\mathcal{E}(t, u) \leq \liminf_{k\to\infty} \mathcal{E}(t, u_k)$.

Proof. Assume $\mathcal{E}(t, u_k) < C$ for all $k > 0$. Then by the equi-coercivity (2.18), which actually holds in the scenarios (D2) and (D3), there exist $u \in W^{1,p}(\Omega; \mathbb{T}^3)$, $A \in L^{p_2}(\Omega; \mathbb{R}^{3\times 3})$, $D \in L^{p_3}(\Omega)$, $G \in L^r(\Omega; \mathbb{R}^3)$, and $\mathcal{L} \in \mathcal{D}_1(\Omega)$, such that

$$u_k \rightharpoonup u \quad \text{weakly in } W^{1,p}(\Omega; \mathbb{T}^3), \tag{2.27}$$

$$\operatorname{cof} F_k \rightharpoonup A \quad \text{weakly in } L^{p_2}(\Omega; \mathbb{R}^{3\times 3}), \tag{2.28}$$

$$\det F_k \rightharpoonup D \quad \text{weakly in } L^{p_3}(\Omega), \tag{2.29}$$

$$\operatorname{Div} F_k \rightharpoonup G \quad \text{weakly in } L^r(\Omega; \mathbb{R}^3), \tag{2.30}$$

$$\mathcal{L}_k \rightharpoonup \mathcal{L} \quad \text{weakly in } \mathcal{D}_1(\Omega). \tag{2.31}$$

Moreover, by the identities $-\operatorname{Curl} \nabla u_k = b \otimes \mathcal{L}_k$ and (2.30)-(2.31), it is easy to see that $-\operatorname{Curl} \nabla u = b \otimes \mathcal{L}$ and $\operatorname{Div} \nabla u = G$. Denote $F := \nabla u$. Notice that in the case (D1) the convergence of the divergence is missing while the convergence of the curl is easily adapted. In order to prove the statement we have to show that $\operatorname{cof} F = A$, and $\det F = D$. Let us discuss the three cases (D1), (D2) or (D3) separately. For (D3), we apply [33, Theorem 3.3] (this actually is the Federer-Fleming closure theorem for integral currents, see also [16, Theorem 3.2.2] for Cartesian maps), so that we have to check that the maps u_k have the properties that their graphs $\mathcal{G}_{u_k}$ are integral currents in $\mathcal{D}_3(\Omega; \mathbb{T}^3)$ with equibounded boundaries. But this is guaranteed by [33, Theorem 4.9] which in turn characterizes the boundary of $\mathcal{G}_{u_k}$ thanks to the fact that $p_2 \geq 2$, and that the dislocation currents $\mathcal{L}_k$ are equibounded. Eventually, the lower-semicontinuity of the energy follows from (E1), (E3), and (E5).

In the case (D2) the required closeness of admissible states is ensured again by Theorem [33, Theorem 3.3], but in order to control the boundaries of the graphs of u_k we have to employ [32, Theorem 4.6]. Let us stress that in this case the hypothesis $r > 3$ compensates the lack of integrability of the cofactor (namely we only have $p_2 > 1$). Again the lower-semicontinuity of the energy derives from (E1), (E3), and (E5).

In the case (D1) we have to argue differently. Actually, the proof relies on suitable application of Golab Theorem, as in [31, Theorem 5.6]. We refer to this for the complete discussion. □

2.3 Dissipation

We introduce the concept of dissipation distance between two internal admissible states. Let us first discuss the case of displacement related to clusters generated by a single Burgers vector. Let $u_1, u_2 \in \mathcal{U}_b(w)$ for a Dirichlet datum $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ with $\nabla w \in \mathcal{F}_b(\hat{\Omega})$. Being admissible, u_1 and u_2 satisfy

$$-\operatorname{Curl} \nabla u_i = b \otimes \mathcal{L}_i, \quad i = 1, 2, \tag{2.32}$$

for some integral 1-currents $\mathcal{L}_i \in \mathcal{D}_1(\Omega)$. Then the dissipation distance between the two states $(u_1, \mathcal{L}_1)$ and $(u_2, \mathcal{L}_2)$ is given by

$$\hat{\mathcal{D}}((u_1, \mathcal{L}_1), (u_2, \mathcal{L}_2)) = \mathcal{D}(\mathcal{L}_1, \mathcal{L}_2) = \gamma d_F(\mathcal{L}_1, \mathcal{L}_2), \tag{2.33}$$

where $\gamma > 0$ is a constant and d_F is the flat distance in $\mathcal{D}_1(\Omega)$ (see [20]). Keeping into account that $\mathcal{L}_i$ are closed 1-currents, this is defined in the following equivalent way:

$$d_F(\mathcal{L}_1, \mathcal{L}_2) := \inf\{|\mathcal{S}| : \mathcal{S} \in \mathcal{D}_2(\Omega) \text{ with } \partial\mathcal{S} = \mathcal{L}_1 - \mathcal{L}_2\}. \tag{2.34}$$

The flat distance satisfies, by definition,

$$d_F(\mathcal{L}_1, \mathcal{L}_2) = d_F(\mathcal{L}_1 - \mathcal{L}_2, 0). \tag{2.35}$$

Remark 2.4. As already pointed out in the introduction, a suitable notion of anisotropic dissipation would be physically more interesting. For simplicity we here consider only this specific case of standard flat distance.

In the case of clusters generated by multiple Burgers vectors the concept of dissipation is similar but should take into account that the dislocation decomposes in three integral currents $(\mathcal{L}^1, \mathcal{L}^2, \mathcal{L}^3)$. Let $u_1, u_2 \in \mathcal{U}^\star(w)$ for a Dirichlet datum $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ with $\nabla w \in \mathcal{F}^\star(\hat{\Omega})$. Being admissible, u_1 and u_2 satisfy

$$-\operatorname{Curl} \nabla u_i = e_1 \otimes \mathcal{L}_i^1 + e_2 \otimes \mathcal{L}_i^2 + e_3 \otimes \mathcal{L}_i^3, \quad i = 1, 2, \tag{2.36}$$

for some integral 1-currents $(\mathcal{L}_i^1, \mathcal{L}_i^2, \mathcal{L}_i^3) \in \mathcal{D}_1(\Omega)^3$. Then the dissipation distance between the two states $(u_1, \mathcal{L}_1^1, \mathcal{L}_1^2, \mathcal{L}_1^3)$ and $(u_2, \mathcal{L}_2^1, \mathcal{L}_2^2, \mathcal{L}_2^3)$ is given by

$$\begin{aligned}\hat{\mathcal{D}}((u_1, \mathcal{L}_1^1, \mathcal{L}_1^2, \mathcal{L}_1^3),(u_2, \mathcal{L}_2^1, \mathcal{L}_2^2, \mathcal{L}_2^3)) &= \mathcal{D}(\mathcal{L}_1^1, \mathcal{L}_2^1) + \mathcal{D}(\mathcal{L}_1^2, \mathcal{L}_2^2) + \mathcal{D}(\mathcal{L}_1^3, \mathcal{L}_2^3) \\ &= \gamma d_F(\mathcal{L}_1^1, \mathcal{L}_2^1) + \gamma d_F(\mathcal{L}_1^2, \mathcal{L}_2^2) + \gamma d_F(\mathcal{L}_1^3, \mathcal{L}_2^3). \end{aligned} \tag{2.37}$$

Notice that, up to a change of basis of $\mathbb{R}^3$, the dissipation in the case of a single Burgers vector can be identified with the last one, just because in the latter case $\mathcal{L}_i^2 = \mathcal{L}_i^2 = \mathcal{L}_i^3 = \mathcal{L}_i^3 = 0$ $(i = 1, 2)$ and we have only the nonnegligible currents $(\mathcal{L}_1, \mathcal{L}_2) = (\mathcal{L}_1^1, \mathcal{L}_2^1)$.

The following well-known result (see, e.g., [20]) will be crucial for our subsequent discussion.

Theorem 2.5. *Let $\mathbb{L} = \{\mathcal{L}_i\}_i \subset \mathcal{D}_1(\Omega)$ be a family of boundaryless integral 1-currents such that*

$$\sup_i |\mathcal{L}_i| \leq C < \infty. \tag{2.38}$$

Then the family $\mathbb{L}$ is relatively compact with respect to the weak topology of $\mathcal{D}_1(\Omega)$; namely, for any sequence $(\mathcal{L}_k)_k \subset \mathbb{L}$ there is an integral 1-current $\mathcal{L}$ such that, up to a further subsequence, $\mathcal{L}_k \rightharpoonup \mathcal{L}$ weakly in $\mathcal{D}_1(\Omega)$.

Moreover, for any sequence $(\mathcal{L}_k)_k \subset \mathbb{L}$ and $\mathcal{L} \in \mathbb{L}$ satisfying (2.38), the following equivalence holds true:

$$d_F(\mathcal{L}_k, \mathcal{L}) \to 0 \text{ iff } \mathcal{L}_k \rightharpoonup \mathcal{L} \text{ weakly in } \mathcal{D}_1(\Omega). \tag{2.39}$$

The last assertion can be found in [20, Theorem 8.2.1]. As a consequence of Theorem 2.5, the set $\mathcal{R}_C$ introduced in (2.10) is a sequentially weakly compact subset of $\mathcal{D}_1(\Omega)$.

Definition 2.6 (Total dissipation for clusters with one Burgers vector)**.** The total dissipation of a process $u : [t_1, t_2] \to W^{1,p}(\Omega; \mathbb{T}^3)$ such that $(u(t), \mathcal{L}(t)) \in \mathcal{A}_b(w)$ for any $t \in [t_1, t_2]$, is defined as follows:

$$\mathrm{Diss}_{\mathcal{D}}(\mathcal{L}; [t_1, t_2]) := \sup \sum_{i=1}^{n-1} \mathcal{D}(\mathcal{L}(r_{i+1}), \mathcal{L}(r_i)), \tag{2.40}$$

where the supremum is computed over all partitions $t_1 = r_1 < r_2 < \cdots < r_n = t_2$ and all $n > 1$.

In the case of general clusters generated by linearly independent Burgers vectors (that will be used only under the scenario (D1)) we define

Definition 2.7 (Total dissipation for clusters with general Burgers vectors)**.** The total dissipation of a process $u : [t_1, t_2] \to W^{1,p}(\Omega; \mathbb{T}^3)$ such that $(u(t), \mathcal{L}^1(t), \mathcal{L}^2(t), \mathcal{L}^3(t)) \in \mathcal{A}^\star(w)$ for any $t \in [t_1, t_2]$, is defined as follows:

$$\mathrm{Diss}^\star_{\mathcal{D}}(\mathcal{L}^1, \mathcal{L}^2, \mathcal{L}^3; [t_1, t_2]) := \sup \sum_{i=1,2,3} \Big(\sum_{i=1}^{n-1} \mathcal{D}(\mathcal{L}(r_{i+1}), \mathcal{L}(r_i)) \Big), \tag{2.41}$$

where the supremum is computed over all partitions $t_1 = r_1 < r_2 < \cdots < r_n = t_2$ and all $n > 1$.

We are now in position to prove the following result valid for a fixed Burgers vector b:

Theorem 2.8. *Set $(\bar{u}, \bar{\mathcal{L}}) \in \mathcal{A}_b(w)$. Under the assumptions of Theorem 2.3, there exists a minimum $(u, \mathcal{L}) \in \mathcal{A}_b(w)$ of the energy*

$$(u, \mathcal{L}) \mapsto \mathcal{E}(t, u) + \mathcal{D}(\mathcal{L}, \bar{\mathcal{L}}).$$

Proof. By the direct method of the calculus of variation, this is an immediate corollary of Theorem 2.3, once it is proven that the flat distance is lower-semicontinuous (see also the discussion in Section 3.2 of [22]). Let us verify that $d_F : \mathcal{R}_C \times \mathcal{R}_C \to [0, +\infty)$ is lower-semicontinuous. Let $\mathcal{L}_k$ and $\hat{\mathcal{L}}_k$ be two sequences in $\mathcal{R}_C$ converging weakly to $\mathcal{L}$ and $\hat{\mathcal{L}}$ respectively. Let $\mathcal{S}_k \in \mathcal{D}_2(\Omega)$ be a quasi-minimizer for the distance $d_F(\mathcal{L}_k, \hat{\mathcal{L}}_k)$, that is, it holds

$$\partial \mathcal{S}_k = \mathcal{L}_k - \hat{\mathcal{L}}_k, \qquad |\mathcal{S}_k| < d_F(\mathcal{L}_k, \hat{\mathcal{L}}_k) + \frac{1}{k}, \tag{2.42}$$

It is easy to see that the sequence $\{\mathcal{S}_k\}_k$ admits a (not relabeled) subsequence such that $\mathcal{S}_k \rightharpoonup \mathcal{S}$, and it is clear that $\partial \mathcal{S} = \mathcal{L} - \hat{\mathcal{L}}$, so that we infer $d_F(\mathcal{L}, \hat{\mathcal{L}}) \leq |\mathcal{S}|$. Moreover, from (2.42) and the lower-semicontinuity of the mass, it follows that

$$|\mathcal{S}| \leq \liminf_{k \to \infty} |\mathcal{S}_k| \leq \liminf_{k \to \infty} d_F(\mathcal{L}_k, \hat{\mathcal{L}}_k). \tag{2.43}$$

Hence, we conclude $d_F(\mathcal{L}, \hat{\mathcal{L}}) \leq \liminf_{k \to \infty} d_F(\mathcal{L}_k, \hat{\mathcal{L}}_k)$, that is the claim. □

The extension of this result to the case of general clusters with linearly independent Burgers vectors is easily obtained as a corollary, using simply the fact that the dissipation $\mathcal{D}(\mathcal{L}, \bar{\mathcal{L}})$ is replaced by the sum

$$\mathcal{D}(\mathcal{L}^1, \bar{\mathcal{L}}^1) + \mathcal{D}(\mathcal{L}^2, \bar{\mathcal{L}}^2) + \mathcal{D}(\mathcal{L}^3, \bar{\mathcal{L}}^3). \tag{2.44}$$

3 Quasi-static evolution

In this section we study the problem of existence of a quasi-static evolution related to the energy $\mathcal{E}$ with dissipation distance $\mathcal{D}$ in the settings introduced in the three scenarios (D1), (D2), and (D3). Let us introduce the concept of stable states: fix $t \in [0, T]$ we define

$$\mathcal{S}_b(t) := \{(u, \mathcal{L}) \in \mathcal{A}_b(w) : \text{ for all } (\hat{u}, \hat{\mathcal{L}}) \in \mathcal{A}_b(w), \;\; \mathcal{E}(t, u) \leq \mathcal{E}(t, \hat{u}) + \mathcal{D}(\mathcal{L}, \hat{\mathcal{L}})\}. \tag{3.1}$$

and

$$\mathcal{S}^\star(t) := \{(u, \mathcal{L}^1, \mathcal{L}^2, \mathcal{L}^3) \in \mathcal{A}^\star(w) : \text{ for all } (\hat{u}, \hat{\mathcal{L}}^1, \hat{\mathcal{L}}^2, \hat{\mathcal{L}}^3) \in \mathcal{A}^\star(w), \\ \mathcal{E}(t, u) \leq \mathcal{E}(t, \hat{u}) + \sum_{i=1}^{3} \mathcal{D}(\mathcal{L}^i, \hat{\mathcal{L}}^i)\}. \tag{3.2}$$

Moreover, set

$$\mathcal{S}^b_{[0,T]} := \cup_{t \in [0,T]} (t, \mathcal{S}_b(t)) \subset [0, T] \times \mathcal{A}_b(w). \tag{3.3}$$

and

$$\mathcal{S}^\star_{[0,T]} := \cup_{t \in [0,T]} (t, \mathcal{S}^\star(t)) \subset [0, T] \times \mathcal{A}^\star(w). \tag{3.4}$$

Following the classical theory of energetic formulation for quasi-static rate-independent processes [23], we introduce the definition of solution as follows:

Definition 3.1 (Energetic solution for clusters with a single Burgers vector)**.** Given a Dirichlet condition $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ such that $\nabla w \in \mathcal{F}_b(\hat{\Omega})$ and an external force $\mathbb{K} \in C^1([0, T]; W^{1,p'}(\Omega; \mathbb{R}^{3\times 3}))$ we say that a function $(u, \mathcal{L}) : [0, T] \to \mathcal{A}_b(w)$ is an energetic solution with initial datum $(u_0, \mathcal{L}_0) \in \mathcal{S}_b(0)$ if $u(0) = u_0$, $\mathcal{L}(0) = \mathcal{L}_0$, and the two following conditions are satisfied

(S) Stability condition: for all $t \in [0, T]$ and any $(\hat{u}, \hat{\mathcal{L}}) \in \mathcal{A}_b(w)$ it holds

$$\mathcal{E}(t, u(t)) \leq \mathcal{E}(t, \hat{u}) + \mathcal{D}(\mathcal{L}(t), \hat{\mathcal{L}}). \tag{3.5}$$

(E) Energy balance: for all $t \in [0, T]$ it holds

$$\mathcal{E}(t, u(t)) + \mathrm{Diss}_{\mathcal{D}}(u; [0, t]) = \mathcal{E}(0, u_0) + \int_0^t \partial_s \mathcal{E}(s, u(s)) ds. \tag{3.6}$$

In terms of stable states, condition (S) is equivalent to say that, for all $t \in [0,T]$, we have $(u(t), \mathcal{L}(t)) \in \mathcal{S}(t)$. In the case of evolution of clusters with multiple Burgers vectors we introduce the notion:

Definition 3.2 (Energetic solution for clusters with general Burgers vectors)**.** Given a Dirichlet condition $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ such that $\nabla w \in \mathcal{F}^\star(\hat{\Omega})$ and an external force $\mathbb{K} \in C^1([0,T]; W^{1,p'}(\Omega; \mathbb{R}^{3\times 3}))$ we say that a function $(u, \mathcal{L}^1, \mathcal{L}^2, \mathcal{L}^3) : [0,T] \to \mathcal{A}^\star(w)$ is an energetic solution with initial datum $(u_0, \mathcal{L}_0^1, \mathcal{L}_0^2, \mathcal{L}_0^3) \in \mathcal{S}^\star(0)$ if $u(0) = u_0$, $\mathcal{L}^i(0) = \mathcal{L}_0^i$, $i = 1,2,3$, and the two following conditions are satisfied

(S*) Stability condition: for all $t \in [0,T]$ and any $(\hat{u}, \hat{\mathcal{L}}^1, \hat{\mathcal{L}}^2, \hat{\mathcal{L}}^3) \in \mathcal{A}^\star(w)$ it holds

$$\mathcal{E}(t, u(t)) \leq \mathcal{E}(t, \hat{u}) + \sum_{i=1}^{3} \mathcal{D}(\mathcal{L}^i(t), \hat{\mathcal{L}}^i). \tag{3.7}$$

(E*) Energy balance: for all $t \in [0,T]$ it holds

$$\mathcal{E}(t, u(t)) + \mathrm{Diss}^\star_{\mathcal{D}}(u; [0,t]) = \mathcal{E}(0, u_0) + \int_0^t \partial_s \mathcal{E}(s, u(s)) ds. \tag{3.8}$$

3.1 Helly's selection principle

In order to prove existence of an energetic solution, we rely on the general results provided by Mielke and coauthors (see, e.g., [22, 23]). In particular, we need a suitable version of the Helly's selection principle. To this aim we must check that our chosen framework is compatible with the hypotheses of the theory of rate-independent systems [21]. First, let us recall that the dissipation distance, namely the flat distance, is defined on the topological Hausdorff space of closed 1-dimensional integral currents. The lower semicontinuity of the flat distance was proved in Theorem 2.8. Moreover, by [20, Theorem 8.2.1], the continuity of the flat norm for a fixed $\mathcal{L}$ holds, namely (2.39). Thus the following continuity property holds true:

Lemma 3.3 (Continuity of the flat distance)**.** *Let $\mathcal{L}_k$ and $\hat{\mathcal{L}}_k$ be two sequences in $\mathcal{R}_C$ converging in the sense of currents to $\mathcal{L}, \hat{\mathcal{L}} \in \mathcal{R}_C$, respectively. Then*

$$\lim_{k\to\infty} d_F(\mathcal{L}_k, \hat{\mathcal{L}}_k) = d_F(\mathcal{L}, \hat{\mathcal{L}}).$$

Proof. We have that $\mathcal{L}_k - \hat{\mathcal{L}}_k$ weakly converges to $\mathcal{L} - \hat{\mathcal{L}}$, and

$$\limsup_{k\to\infty} d_F(\mathcal{L}_k, \hat{\mathcal{L}}_k) = \limsup_{k\to\infty} d_F(\mathcal{L}_k - \hat{\mathcal{L}}_k, 0) \leq$$
$$\limsup_{k\to\infty} d_F(\mathcal{L}_k - \hat{\mathcal{L}}_k, \mathcal{L} - \hat{\mathcal{L}}) + d_F(\mathcal{L} - \hat{\mathcal{L}}, 0) = d_F(\mathcal{L}, \hat{\mathcal{L}}),$$

the first inequality deriving from the triangle inequality, and the last equality being in force by (2.39). Hence we get upper-semicontinuity, which together with the lower-semicontinuity established in Theorem 2.8 provides the desired continuity. □

After this check, we observe that we are under the hypotheses of [22, Theorem 5.1] with $\mathcal{V}(t) = \mathcal{R}_C$, and thus infer the following statement:

Proposition 3.4. *Let $\mathcal{L}_n : [0,T] \to \mathcal{R}_C$ for some constant $C > 0$, and assume that*

$$Diss_{\mathcal{D}}(\mathcal{L}_n; [0,T]) \leq C', \tag{3.9}$$

for all $n > 0$ and for a constant $C' > 0$. Then there exist a function $\varphi \in BV([0,T];\mathbb{R})$ and $Y \in BV_{\mathcal{D}}([0,T];\mathcal{R}_C)$ such that, up to a subsequence,

(a) $\varphi_n(t) := Diss_{\mathcal{D}}(\mathcal{L}_n; [0,t]) \to \varphi(t)$ *for all* $t \in [0,T]$,

(b) $\mathcal{L}_n(t) \rightharpoonup \mathcal{L}(t)$ *for all* $t \in [0,T]$,

(c) $Diss_{\mathcal{D}}(\mathcal{L} : [t_1,t_2]) \leq \varphi(t_2) - \varphi(t_1)$ *for all* $0 \leq t_1 < t_2 \leq T$.

3.2 Quasi-statics existence result

The proof of existence of a quasi-static evolution relies on the fact that our model [31–33] indeed applies to the framework of energetic evolution for nonconvex problems. Specifically, in order to prove our main result Theorem 3.5, stating the existence of an energetic solution to the quasi-static evolution of dislocation clusters in single crystals, we consider the standard scheme introduced in [22, Theorem 5.2]. To this aim, we collect here some useful properties of the dissipation and the energy functional. For the sake of generality we use the notation

$$\mathcal{U}(w) = \begin{cases} \mathcal{U}_b(w) & \text{in the settings (D2) and (D3),} \\ \mathcal{U}^\star(w) & \text{in the setting (D1).} \end{cases} \tag{3.10}$$

(A1) The dissipation distance satisfies

$$\begin{aligned} &(i)\ \forall \mathcal{L}_1, \mathcal{L}_2 \in \mathcal{D}_1(\Omega): \quad d_F(\mathcal{L}_1,\mathcal{L}_2) = 0 \Leftrightarrow \mathcal{L}_1 = \mathcal{L}_2, \\ &(ii)\ \forall \mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3: \quad d_F(\mathcal{L}_1,\mathcal{L}_2) \leq d_F(\mathcal{L}_1,\mathcal{L}_3) + d_F(\mathcal{L}_3,\mathcal{L}_2). \end{aligned}$$

(A2) There exist constants $C_1, C_2 > 0$ such that for all $u^* \in \mathcal{U}(w)$: if for all $t \in [0,T]$ we have $\mathcal{E}(t,u^*) < \infty$, then

$$\begin{aligned} &\partial_t \mathcal{E}(\cdot, u^*) : [0,T] \to \mathbb{R} \text{ is measurable and} \\ &|\partial_t \mathcal{E}(t,u^*)| \leq C_1(\mathcal{E}(t,u^*) + C_2). \end{aligned} \tag{3.11}$$

(A3) For all $t \in [0,T]$ the energy $\mathcal{E}(t,\cdot) : \mathcal{U}(w) \to \mathbb{R} \cup \{+\infty\}$ has compact sublevels and $\mathcal{D} : \mathcal{R}_C \times \mathcal{R}_C$ is lower semicontinuous for any $C > 0$.

(A4) Let $C > 0$ be a constant. Whenever $\mathcal{L}_k$ is a sequence in $\mathcal{R}_C$ and $\mathcal{L} \in \mathcal{R}_C$, then property (2.39) holds true.

(A5) The following uniform continuity of the power holds true: $\forall C > 0$, $\forall \epsilon > 0$, $\exists \delta > 0$:

$$\mathcal{E}(t,u) < C, \quad |t-s| < \delta \quad \Rightarrow |\partial_t \mathcal{E}(t,u) - \partial_t \mathcal{E}(s,u)| \leq \epsilon. \tag{3.12}$$

(A6) The dissipation distance d_F is continuous on $\mathcal{R}_C \times \mathcal{R}_C$.

Let us check the validity of such hypotheses in our setting: property (A1) is immediate from the properties of the distance. Fixing a boundary Dirichlet datum, property (A2) is (2.21). Similarly (A5) follows from (2.19) and the regularity of the external load $\dot{\mathbb{K}}$ which belongs to $C^0([0,T]; W^{1,p'}(\Omega; \mathbb{R}^{3\times3}))$. Property (A3) has been proved in Theorem 2.8, whereas property (A4) is the content of Theorem 2.5. Finally property (A6) is guaranteed by Lemma 3.3. The abstract existence result for energetic solution is given by the following theorem that we first state in the case of a single Burgers vector:

Theorem 3.5 (Existence result; Theorem 5.2 in [22])**.** *Consider the setting (D2) or (D3). Fix $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ with $\nabla w \in \mathcal{F}_b(\Omega)$. Assume that the energy and dissipation $\mathcal{E}$ and $\mathcal{D}$ satisfy conditions (A1)-(A6). Then, for each $(u_0, \mathcal{L}_0) \in \mathcal{S}(0)$ there exists an energetic solution $(u, \mathcal{L}) : [0,T] \to \mathcal{U}_b(w) \times \mathcal{R}$ as in Definition 3.1.*

The proof follows the lines of [22, Theorem 5.2] For completeness, we sketch it with our notations.

Proof. Let us choose a sequence of partitions $0 = t_0 < t_1 < \cdots < t_n = T$ whose fineness $\eta_n := \max_i |t_i - t_{i-1}|$ tends to 0 as $n \to \infty$. Recursively we solve the time-incremental minimization problem $(u_i, \mathcal{L}_i) \in \operatorname{argmin} \ \mathcal{E}(t_i, \cdot) + \mathcal{D}(\cdot, \mathcal{L}_{i-1})$, which is solvable thanks to Theorem 2.8 (consequence of (A3)). The piecewise constant interpolation function $(U_n, \mathcal{L}_n)$ defined via

$$u_n(t) := u_i \ \text{ if } t \in [t_i, t_{i+1}), \qquad \mathcal{L}_n(t) := \mathcal{L}_i \ \text{ if } t \in [t_i, t_{i+1}), \tag{3.13}$$

satisfies the a-priori estimates

$$\forall t \in [0,T] \ \ \mathcal{E}(t, u_n(t)) < C, \quad \text{and} \quad \mathrm{Diss}_{\mathcal{D}}(\mathcal{L}_n; [0,T]) < C, \tag{3.14}$$

for a constant $C > 0$ independent of n. These are consequence of (A2) and (A5), see [22, Section 3.2]. We set $\theta_n(t) := \partial_t \mathcal{E}(t, u_n(t))$. Now, we apply the generalized Helly's selection principle and passing to a subsequence we get the existence of functions δ, $\mathcal{L}$, and θ, such that

$$\delta_n(t) := \mathrm{Diss}_{\mathcal{D}}(\mathcal{L}_n; [0,t]) \to \delta(t) \ \ \forall t \in [0,T], \tag{3.15}$$

$$\mathcal{L}_n(t) \rightharpoonup \mathcal{L}(t) \ \forall t \in [0,T], \tag{3.16}$$

$$\theta_n \rightharpoonup \theta \text{ weakly star in } L^\infty([0,T]). \tag{3.17}$$

The function $\theta_{\sup}(t) := \limsup_{n\to\infty} \theta_n(t)$ for any $t \in [0,T]$ belongs to $L^\infty([0,T])$ and satisfies $\theta \leq \theta_{\sup}$ by Fatou's Lemma. For any fixed $t \in [0,T]$ it holds $\mathcal{E}(t, u_n(t)) < C$

so that by compactness of the sublevels of the energy there are a subsequence of n denoted by k_n^t (dependent on t) and a function $u(t) \in \mathcal{U}_b(w)$ such that

$$\theta_{k_n^t}(t) \to \theta_{\sup}(t) \quad \text{and} \quad u_{k_n^t}(t) \rightharpoonup u(t) \text{ in } \mathcal{U}_b(w). \tag{3.18}$$

We will now see that the defined function $t \mapsto (u(t), \mathcal{L}(t))$ satisfies (S) and (E). First we observe that condition (A6) implies that the equibounded (in energy) stable states are weakly closed, and this is sufficient to conclude that the couple $(u(t), \mathcal{L}(t))$ is stable. Again, as in [22, Theorem 5.2], we infer that $\theta_{\sup}(t) = \partial_t \mathcal{E}(t, u(t))$ and the upper energy estimate

$$\mathcal{E}(t, u(t)) + \mathrm{Diss}_{\mathcal{D}}(\mathcal{L}; [0, t]) \leq \mathcal{E}(0, u_0) + \int_0^t \partial_t \mathcal{E}(s, u(s)) ds. \tag{3.19}$$

Since $\theta_{\sup} = \partial_t \mathcal{E}(\cdot, u(\cdot)) \in L^\infty([0, T])$ we are in position to apply [22, Proposition 5.7] to infer the opposite inequality, concluding the proof of (E). □

Eventually, as in [22, Theorem 5.2], we infer the following auxiliary result:

Theorem 3.6. *For any sequence of partitions* $\{\Pi_l\}_l$, $\Pi_l := \{0 = t_0^l < t_1^l < \cdots < t_{n_l}^l = T\}$ *whose fineness* η_l *tends to* 0 *as* $l \to \infty$, *the corresponding interpolant solutions* $(u_l(t), \mathcal{L}_l(t))$, *up to a subsequence, converge to an energetic solution* $(u(t), \mathcal{L}(t))$, *in the following sense*

$$\begin{aligned}
&(i) \quad \forall t \in [0, T] \;\; \mathcal{L}_l(t) \rightharpoonup \mathcal{L}(t), \\
&(ii) \quad \forall t \in [0, T] \;\; \mathit{Diss}_{\mathcal{D}}(\mathcal{L}_l; [0, t]) \to \mathit{Diss}_{\mathcal{D}}(\mathcal{L}; [0, t]), \\
&(iii) \quad \forall t \in [0, T] \;\; \mathcal{E}(t, u_l(t)) \to \mathcal{E}(t, u(t)), \\
&(iv) \quad \partial_t \mathcal{E}(\cdot, u_l(\cdot)) \to \partial_t \mathcal{E}(\cdot, u(\cdot)) \text{ in } L^1([0, T]).
\end{aligned}$$

We now state the existence result for the framework (D1) where we can allow the dislocation cluster to be generated by multiple Burgers vectors. The proof is a straightforward adaptation of the one of Theorem 3.5.

Theorem 3.7. *Consider the setting (D1). Fix* $w \in W^{1,p}(\hat{\Omega}; \mathbb{T}^3)$ *with* $\nabla w \in \mathcal{F}^\star(\Omega)$. *Assume that the energy and dissipation* $\mathcal{E}$ *and* $\mathcal{D}$ *satisfy conditions (A1)-(A6). Then, for each* $(u_0, \mathcal{L}_0^1, \mathcal{L}_0^2, \mathcal{L}_0^3) \in \mathcal{S}^\star(0)$ *there exists an energetic solution* $(u, \mathcal{L}^1, \mathcal{L}^2, \mathcal{L}^3) : [0, T] \to \mathcal{U}^\star(w) \times \mathcal{R}^3$ *as in Definition 3.2.*

4 Open problems

We list here some interesting generalizations we are not able to cover at the present stage.

4.1 Time-dependent Dirichlet boundary condition

The validity of (3.14) relies on the fact that u_j and u_{j-1} have the same boundary conditions, since it is crucial that the following inequality can be written

$$\mathcal{E}(t_j, u_j) + \mathcal{D}(\mathcal{L}_j, \mathcal{L}_{j-1}) \leq \mathcal{E}(t_j, u_{j-1}),$$

by minimality of u_j at time $t = t_j$ in the time incremental problem. At the present stage it is only possible to consider Dirichlet boundary condition w that are independent of time. We see two possible approach to the general case:

Approach 1. We follow the approach as suggested in, for instance, [19, 21]. If we consider a non-constant boundary condition $t \mapsto w(t)$, we must first correct u_{j-1} by adding $\delta w_{j-1} = w_j - w_{j-1}$ in such a way that $u_{j-1} + \delta w_{j-1}$ has the same boundary condition as u_j. Therefore we are led to estimate

$$\delta W := |\mathcal{W}(\nabla u_{j-1}) - \mathcal{W}(\nabla u_{j-1} + \nabla \delta w_{j-1})|. \tag{4.1}$$

We see two ways for proceeding. Letting $W(F) := W_\mathrm{e}(M(F))$, the first consists in making a standard assumption of the type $F^T DW(F) \leq C(W(F)+1)$, as in [5, 6] (see also [19]), where DW stands for the Fréchet differential of W. Then, following [5, 6], one has (see [19, Eq. (14)])

$$\begin{aligned} \delta W &:= |\mathcal{W}(\nabla u_{j-1}) - \mathcal{W}\left(\nabla u_{j-1}(\mathbb{I} + (\nabla u_{j-1})^{-1} \nabla \delta w_{j-1})\right)| \\ &\leq C(W(\nabla u_{j-1}) + 1)|(\nabla u_{j-1})^{-1} \nabla \delta w_{j-1}|. \end{aligned} \tag{4.2}$$

Due to the integrability of $(\nabla u_{j-1})^{-1} = \mathrm{cof}\,^T \nabla u_{j-1} (\det \nabla u_{j-1})^{-1}$ (at best L^{p_2} with $p_2 \geq 2$) and $\nabla \delta w_{j-1} \in L^p$ with $p < 2$, we were not able to bound the right-hand side of (4.2) by Hölder's-like inequalities. Note that in [19, 21], in the absence of dislocations, this estimate was possible in view of the better regularity of the strains.

The second way consists in writing $DW(F)[\nabla \delta w_{j-1}]$ as $\partial_F W_\mathrm{e}(M(F))[\nabla \delta w_{j-1}] + \partial_C W_\mathrm{e}(M(F)) DC(F)[\nabla \delta w_{j-1}] + \partial_J W_\mathrm{e}(M(F)) DJ(F)[\nabla \delta w_{j-1}]$, where we have noted $C := \mathrm{cof}\ F$, $J = \det F$. For simplicity take the last term zero (see Remark 2.2). Then the first term is bounded, since $\partial_F W_\mathrm{e} \sim |F|^{p-1} \in L^{p'}$. As for the second one, let us first compute the differential of the cofactor. According to [10] one has

$$C := \mathrm{cof}\ F = \frac{1}{2} F \times F, \quad \text{with } (A \times B)_{il} = \epsilon_{ijk} \epsilon_{lmn} A_{jm} B_{kn}.$$

and hence

$$D\,\mathrm{cof}\ F[H] = F \times H, \tag{4.3}$$

for any direction $H \in \mathbb{R}^{3\times 3}$. Thus

$$\partial_C W_\mathrm{e}(M(F)) DC(F)[\nabla \delta w_{j-1}] := \partial_C W_\mathrm{e}(M(F)) F \times \nabla \delta w_{j-1}. \tag{4.4}$$

Again one has $\partial_C W_\mathrm{e}(M(F)) \sim |C|^{p_2-1} \in L^{p_2'}$ but $F \times \nabla \delta w_{j-1}$ does not belong to $L^{p_2}, p_2 \geq 2$, since $F, \nabla w_{j-1} \in L^p, 1 \leq p < 2$.

Approach 2. A multiplicative decomposition of the displacement $u(t) = w(t) \circ v$ as suggested in [15], here v satisfying $v = Id$ on Γ_D, does not help in our setting. At the present stage we see that the main difficulty relies in the fact that, if we want to impose the presence of dislocation at the boundary Γ_D (which is essential to guarantee that the dislocation cluster in Ω is not null), one has to assume that $\nabla w(t)$ is singular on Γ_D, and in particular is not square-integrable.

4.2 Generalization to linearly independent Burgers vectors

In the scenarios (D2), and (D3), the admissible deformation fields F are assumed to satisfy the condition

$$- \operatorname{Curl} F = b \otimes \mathcal{L}. \tag{4.5}$$

Since b is fixed we see that all the Burgers vector of the related cluster have the same direction. The generalization of this setting would include all the possible directions, and hence we would obtain a formula like

$$- \operatorname{Curl} F = e_1 \otimes \mathcal{L}_1 + e_2 \otimes \mathcal{L}_2 + e_3 \otimes \mathcal{L}_3, \tag{4.6}$$

for three integral currents $\mathcal{L}_1$, $\mathcal{L}_2$, and $\mathcal{L}_3$. The main problem in this case arises from the closedness of the sublevels of the energy, which in the cases discussed here is ensured by the characterization of the graphs of the involved displacement field u, where $F = \nabla u$. Such characterization under the general condition (4.6) is currently missing. Some partial results are available in [33], but only in some constrained geometric setting on the dislocation locations. Hence, also the statics case in the setting (4.6) is yet an open problem.

In [33] we conjecture that for a general $F = \nabla u$, with $u \in W^{1,p}(\Omega; \mathbb{T}^3)$, satisfying (4.6), the graph of u is an integer multiplicity current in $\Omega \times \mathbb{T}^3$ with integral boundary as soon as the cofactor of F turns out to be square integrable. More specifically, if $\operatorname{cof} F \in L^2(\Omega; \mathbb{R}^{3\times 3})$, then we expect that the graph $\mathcal{G}_u$ of u has boundary $\partial \mathcal{G}_u$ satisfying

$$\begin{aligned} \partial \mathcal{G}_u(\omega) &= \sum_{i=1}^{3} \mathcal{L}_i \wedge e_i(\omega) \\ &= \sum_{i=1}^{3} \int_0^{2\pi} \int_{S^i} \langle d\omega(x, e_i\theta + \hat{u}_i(x)), (s_1, 0) \wedge (s_2, 0) \wedge \vec{e_i} \rangle d\mathcal{H}^2(x) d\theta, \end{aligned}$$

for all 3-forms $\omega \in \mathcal{D}^3(\Omega \times \mathbb{R}^3)$ that are 2π-periodic in the second variable. In this formula the functions $\hat{u}_i$ are specific harmonic maps defined via

$$\hat{u}_i(x) = -e_i \int_{S^i} \nabla \Phi(x' - x) \cdot N(x') d\mathcal{H}^2(x'), \tag{4.7}$$

where Φ is the the fundamental solution of the Laplacian in $\mathbb{R}^3$, with $\Delta \Phi = \delta_0$, and S^i is any closed surface with boundary $\mathcal{L}_i$ and unit normal N. In the formula above the vectors s_1 and s_2 form an orthonormal basis of the tangent plane to S^i.

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