

Currents and dislocations at the continuum scale

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Abstract

A striking geometric property of elastic bodies with dislocations is their non-Riemannian nature in the sense that the deformation tensor cannot be written as the gradient of a one-to-one immersion, since its curl must not be zero, but equals to the density of dislocations, a concentrated Radon measure in the dislocation lines. In this work, we discuss the mathematical properties of such constrained deformations and study a variational problem in finite-strain elasticity, where *Cartesian maps* allow us to consider deformations in L^p with $1 \leq p < 2$, as required for dislocation-induced strain singularities. In its first part, this paper addresses the problem of mathematical modeling of dislocations. It is a key purpose of the paper to first build a framework where dislocations are described in terms of *integer rectifiable 1-currents* and to extract from this theoretical setting a series of notions having a mechanical meaning in the theory of dislocations. In particular, the paper aims at classifying rectifiable 1-currents, with modeling purposes. In the second part of the paper, two variational problems are solved by the direct method of the calculus of variations, for two classes of dislocations, at the mesoscopic, and at the continuum scale. By *continuum* it is here meant that a countable family of dislocations is considered, allowing for branching and cluster formation, with possible complex geometric patterns. Therefore, modeling assumption of the defect part of the energy must also be provided, and discussed.

Keywords: Cartesian maps, integer-multiplicity currents, dislocations, finite elasticity, modeling, variational problem.

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1 Introduction

1.1 Physical motivation of the problem

Consider a single dislocation loop \mathcal{L} in a continuum medium $\Omega(t)$ at time t . At the mesoscopic scale it is assumed that $\Omega \setminus \mathcal{L}$ is an elastic body, and thus that all dissipative (i.e., including plastic) effects are concentrated in \mathcal{L} . It is also assumed that \mathcal{L} is a one-dimensional singularity set for the extensive fields such as stress and strain. Moreover, if a linear elastic constitutive law is chosen, classical examples of screw and edge dislocations show that stress and strain are not square integrable [14], and hence that the strain energy is unbounded near \mathcal{L} . This strongly suggests to consider finite elasticity near the line with a less-than-quadratic strain energy, possibly matched with a linear law at some distance from the singularities, since it is also known that linear elasticity and the small strain assumption are perfectly valid to describe the single crystal away from the dislocations [17]. A crucial property of $\Omega(t)$ assumed as a single crystal (as opposed to a polycrystal with internal boundaries) is that the family of dislocations are free to move in the bulk and through part of the boundary, and hence are likely to form geometrically complex structures, called *clusters*. This phenomenon is enhanced if the crystal is considered at high temperature or subjected to high temperature gradients, since the constrained motion of dislocation on predefined glide planes only holds for moderate temperature ranges. Overlooking on purpose the specific inter-dislocation dynamics [25,28,29] which causes attraction/repulsion between dislocations and are responsible for their

aggregation, in this paper we consider the cluster as a mathematical object which must be described in a geometrically unified way together and accordingly with any single dislocation loop.

1.2 Origin and nature of a dislocation singularity

Another intrinsic difficulty of mesoscopic dislocations is that there is no unambiguous definition of the displacement field (whatever the reference configuration) in the whole body, while the jump of any displacement field is a physical field attached to \mathcal{L} and called the *Burgers vector*. In the linear elastic model this amounts to observe that the displacement field as defined by line integration of appropriate combinations of the strain and strain curl is path-dependent, rendering the displacement field multiple valued and hence uneasy to properly handle in a mathematical model [26,27]. This path dependence is expressed by the nonvanishing of the elastic strain incompatibility $\text{inc } \mathcal{E} := \text{Curl} (\text{Curl } \mathcal{E})^T$ with $\mathcal{E} = \mathbb{S}\sigma$, σ the stress tensor and \mathbb{S} the compliance tensor.

Let us assume for a while that there are no dislocations and that the current configuration $\Omega(t)$ is simply connected. In finite elasticity, frame-indifference implies that the strain energy will depend on $C = C(t)$, the *metric tensor* in $\Omega(t)$. Then it is known that C can be written as $C = \nabla\phi^T\nabla\phi$ for some reference configuration Ω and some smooth immersion $\phi : \Omega \rightarrow \mathbb{R}^3$ such that $\phi(\Omega) = \Omega(t)$ if and only if the Riemannian curvature tensor associated to C vanishes identically in $\Omega(t)$ [7]. Let us emphasize that the Riemannian curvature is the finite-elasticity counterpart of the aforementioned incompatibility tensor. By eigendecomposition one has $C = F^T F$ for some F and hence $C = \nabla\phi^T\nabla\phi$ for some ϕ as soon as $\text{Curl } F = 0$ in Ω . In this case the displacement field is defined as $u := \Phi - \text{Id}$ and $F = \nabla\Phi = I + \nabla u$ is called the *deformation gradient* associated to Ω and $\Omega(t)$. Otherwise, $\text{Curl } F$ and the Riemann curvature are nonvanishing, which is a specific *geometrical constraint* for the deformation in the presence of dislocations, and is at the core of the present work. In linear infinitesimal elasticity, incompatibility is directly related to the presence of dislocations [16, 23, 24], and the same property holds in finite elasticity. The dislocations which generate curvature are called *geometrically necessary* [11,19] and will be given a precise mathematical meaning in this paper, together with their companion *geometrically unnecessary* (called “statistically stored” in the engineering literature) which solely contribute to plastic strain in the absence of strain gradients.

The precise expression of $\text{Curl } F$ in the presence of dislocations will now be described with some detail, since the concepts of displacement, deformation and reference configuration become uncomfortable in the presence of dislocations. First, we emphasize that no perfect, that is, dislocation-free reference configuration can be considered. Second, the fundamental issue is that the reference configuration is needed to consider finite elasticity, but the dislocation line is better defined in the current configuration. It is worth writing with some detail what happens in the presence of a dislocation in finite elasticity (the following discussion is illustrated in Fig. 1). Consider the current configuration $\Omega(t)$ (a bounded simply connected set) with a single dislocation L and any dividing surface S_L containing L . The set $\Omega(t) \setminus L$ is not simply connected, but the upper and lower partition of $\Omega(t)$, $\Omega^+(t)$ and $\Omega^-(t)$ divided by S_L , are simply connected and in each it holds $\text{inc } \mathcal{E} = 0$. Thus there exists a linear-elasticity

displacement field $u_{S_L} = u_{S_L}^\pm$ such that $\mathcal{E} = \nabla^S u_{S_L}$ in $\Omega^\pm(t)$. For any smooth one-to-one φ , the map $\phi := \varphi \circ (\text{Id} - u_{S_L})$ defines a reference configuration. We assume that there exists at least a $P_0 \in \partial\Omega(t) \setminus L$ where $\phi(P_0) = \phi_0$ is prescribed. It turns out that in the presence of a dislocation the map ϕ is multivalued, i.e., there is a mismatch in the reference configuration due to presence of the dislocation, which we describe as follows. Let $\Omega^\pm := \phi(\Omega^\pm(t))$ define the lower and upper parts of a reference configuration while $F = F^\pm = \nabla\phi$ are the associated (inverse¹) deformation gradients. Now take two curves α^\pm in $\Omega^\pm(t)$ with startpoint P_0 and endpoints P or Q , respectively outside and inside L in S_L . Integrating F along α^\pm defines the nonzero² Burgers vector b attached to L , $b := \int_{\alpha^+} F^+ dx + \int_{\alpha^-} F^- dx = (\phi^+)(Q) - (\phi^-)(Q)$. Thus S_L is mapped into two surfaces which match outside L (i.e., at P), since α^\pm does not enclose L , but do not coincide inside (i.e., at Q). The region of S_L inside L is denoted by S_L° , and it is observed by Stokes theorem, that b is independent of $Q \in S_L^\circ$.

Summarizing, this procedure "à la Volterra" yields

$$b = \int_{\alpha^\pm} \nabla\phi dl(x) = \int_{\alpha^\pm} F dl, \quad (1.1)$$

otherwise said, ϕ shows a jump of amplitude b in S_L° , while $F = \nabla\phi$ in $S_L \setminus S_L^\circ$. Hence its distributional derivative writes as $D\phi = F + b \otimes n\mathcal{H}_{\setminus S_L^\circ}^2$ and it holds $-\text{Curl } F = \text{Curl}(b \otimes n\mathcal{H}_{\setminus S_L^\circ}^2)$. Thus by Stokes theorem and written in terms of the *dislocation density*

$$\Lambda := \tau \otimes b\mathcal{H}_{\setminus L}^1,$$

as

$$-\text{Curl } F = \Lambda^T. \quad (1.2)$$

whereby (1.1) is equivalent to (1.2). The fact that $\text{Curl } F$ is a concentrated measure in L can therefore be understood as L preventing F to be globally the gradient of a deformation and hence preventing the right Cauchy-Green tensor C to write as $C = \nabla^T \phi \nabla \phi$ for some immersion ϕ . In passing, the Riemann curvature associated to C will be nonvanishing and an interesting open question is to relate this tensor to the density of dislocations.

1.3 The variational framework

Coming back to the physics and the mathematical properties of dislocations, we have already mentioned that in linear elasticity $F \in L^p$ with $1 \leq p < 2$, while specific examples for elastic bodies also show that p cannot be greater or equal to 2 [30]. Moreover, with a view to a global model, cavitation solutions cannot be ruled out, since they are at the origin of the nucleation of dislocations from the growth of micro-voids in the bulk [21]. Here, classical examples show that deformation allowing for radial cavitation are such that $\text{cof } F \in L^q$ with $1 \leq q < 3/2$ [13]. Thus, one cannot restrict to the interval $3/2 \leq p < 2$ where some existence results in finite elasticity exists [20], and must allow $F, \text{cof } F \in L^p$

¹This convention – of considering the inverse deformation gradient, thus defined on the current configuration, can also be found in [1]. It is related to the multivalued nature of the reference configuration, which renders its presence in any mathematical description of dislocations, an issue which we prefer to bypass..

²That it is nonzero is due to crystal atomic mismatch (lack or excess) in the region where the dislocation is created.

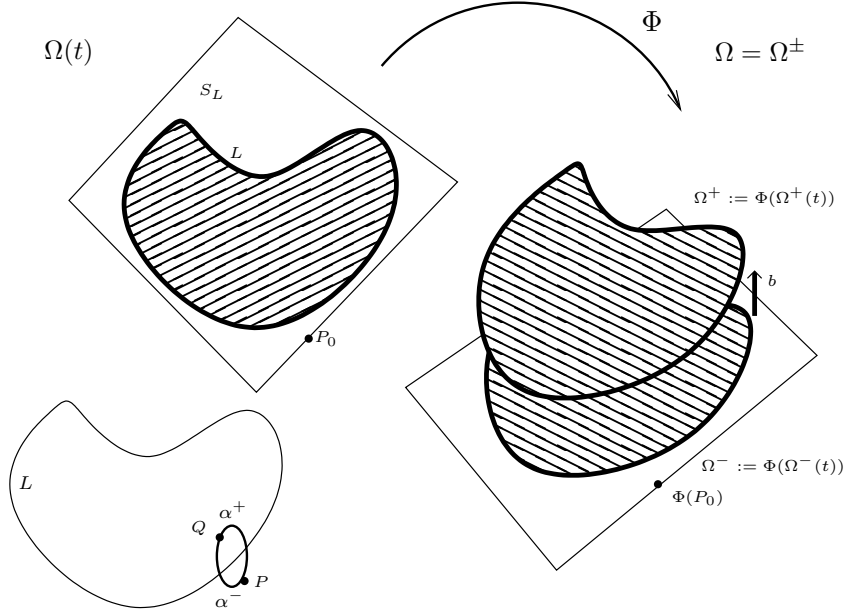


Figure 1: Current and reference configurations showing a jump of the displacement inside the dislocation.

in the whole range $1 \leq p < 2$. For this reason, as suggested in [20], *Cartesian maps* will be considered [12]. Moreover, nucleation resulting from the collapse of a void will provoke locally high pressure gradient and hence the behaviour of the Jacobian $J = \det F$ must be controlled. Therefore, classical pointwise conditions on J will be considered: these are the non-negativeness (to ensure orientation preserving deformation and non-interpenetration of matter) or the fact that $J \rightarrow 0^+$ is precluded by finite energy states. Finally, to avoid any spurious, i.e., *concentrated and dissipative*, effects away from the dislocation set we will assume not only that $\det F, \operatorname{cof} F \in L^p$ but also that their distributional counterpart have no s -dimensional ($0 \leq s \leq 3$) singular parts in $\Omega \setminus L$, that is, $\operatorname{Det} F, \operatorname{Cof} F \in L^p$ locally away from L [18]. As a consequence, the strain energy W_e will depend on $F, \operatorname{cof} F$ and $\det F$ and be assumed polyconvex, i.e., convex in each variable separately, and have a growth bounded from below, writing for instance as

$$W_{\text{deforem}}(F) \geq C(|F|^p + |\operatorname{cof} F|^p + |\det F|^p) - \beta$$

for some $C, \beta > 0$. In our problem, strain gradients play a crucial role and thus a strain-gradient elastic energy involving F and $\operatorname{Curl} F$ will apply. This can be achieved by considering an energy of the form $\mathcal{W}(F, \operatorname{Curl} F) = W_{\text{deforem}}(F) + \tilde{W}_{\text{defect}}(\operatorname{Curl} F)$ or equivalently since $-\operatorname{Curl} F = \Lambda^T$ in terms of the *internal thermodynamic variable* Λ as $W(F, \Lambda) = W_e(F) + W_{\text{defect}}(\Lambda)$, with a growth condition of the type

$$W_{\text{defect}}(\Lambda) \geq C\|\Lambda\|_{\mathcal{M}(\Omega)},$$

allowing us to control pathological behaviours of dislocation clusters.

1.4 Scope of the work

The variational framework was inspired by the pioneer paper [20], where a *single and fixed* dislocation loop was considered, and hence minimization was achieved only with respect to the deformation tensor F . The principal aim of this paper is to generalize the problem, and thus minimization is made also w.r.t. to the line location. With the aforementioned type of energy, our aim is twofold. In a first step, to define classes of admissible deformations F and admissible dislocations L satisfying (i) a boundary condition in terms of dislocation density and (ii) the geometric constraint (1.2). In a second step, to prove existence of minimizers of the energy

$$\inf_{\substack{F, \mathcal{L} \\ -\text{Curl } F = \Lambda_{\mathcal{L}}^T}} \mathcal{W}. \quad (1.3)$$

To achieve the proof of existence, a series of preliminary results must be proved and in particular we define and carefully analyze two classes of dislocations, at the *mesoscopic* and at the *continuum* scales. To this respect an important result is Theorem 4.5 which states their equivalence under certain conditions. Let us stress that each of these two classes has a specific interest in terms of modeling, according to choice of the dislocation variable: either the line per se (a current, \mathcal{L}), or its associated density (a measure, $\Lambda_{\mathcal{L}}$). Then, the two existence results are Theorems 7.6 and 7.7, respectively for the class of mesoscopic and continuum dislocations.

1.5 Structure of the paper

This paper is self-contained and can be read without previous notions neither on dislocations nor on currents. In Section 2, we introduce the concepts of currents in general and of their subclasses of integer-multiplicity currents (i.m.c. in abridged) and Cartesian maps, and recall classical results on compact sets. In Section 3 the general notion of dislocations as described by i.m.c. is provided, while in Section 4 special emphasis is given on its two subclasses of so-called *mesoscopic* and *continuum* dislocations. In particular the relation between these two notions is discussed in Theorem 4.5. A modeling discussion is proposed in Section 5. In Section 6, we discuss the admissible deformations satisfying constraint (1.2). In particular, we show that the class of admissible deformations satisfying the boundary conditions given in terms of the dislocation density is well defined and this allows us to solve the two minimum problems of Section 7. Conclusions and plans to further extend the range of applications of this approach are drawn in Section 8.

1.6 A modeling remark

Let us remark that by solving (1.3) we consider a static problem, whereas dislocations are known to be moving defects inside the crystal by the action of mechanical and thermal forces [1,15]. First, we should precise that by considering an equilibrium problem at fixed time t we indeed define a thermodynamical ground-state on the base of which dynamical effects will be added in a second step, beyond the scope of this paper. Second, such minimization states are reached very fast in actual crystals such as pure copper, where resistance to dislocation motion is negligible [3]. Nonetheless we emphasize that the main

objective of this work is not the minimization result *per se*, but rather the mathematical definition of dislocations, which will be achieved by means of *integer-multiplicity currents* [10]. It will be shown that these well-studied mathematical objects are perfectly adapted to describe *countable families* of dislocations each of which can deform and which mutually can be summed, possibly forming complex *transfinite* geometries (in the sense of Cantor [5]), with appropriate laws on their Burgers vectors.

The chosen approach to minimize jointly the deformation and the line location is more physical, since the fields of deformation and dislocation density are bound. To our knowledge, this is the first generalization in that direction. Of course, to achieve this purpose, modeling assumptions on the defect-part of the energy must be made, since otherwise dense clusters might appear as limit of minimizing sequences, and hence the mesoscopicity assumption would be violated. We attempted to also give a physical understanding on the growth assumptions, but our aim was mainly to set a mathematical framework, where the complete problem could be studied. We are certain that better assumptions exist, but left these considerations for a more model-oriented future work. In this respect, thanks to our minimization result, the dynamics of the lines at optimality could be analysed and discussed in a subsequent paper [22]. Nevertheless, in order to set apart the construction of the mathematical model and the discussion of the definitions and assumptions, we have chosen to defer a large portion of the model discussion to a specific section: about modeling considerations and model justifications, we suggest to read Section 5.

2 Preliminary notions and results

The curl of a tensor A will be defined componentwise as $(\text{Curl } A)_{ij} = \epsilon_{jkl} D_k A_{il}$ where D is a symbol for the distributional derivative; if pointwise and distributional derivative coincide then $(\text{Curl } A)_{ij} = \epsilon_{jkl} \partial_k A_{il}$. In particular one has

$$\langle \text{Curl } A, \psi \rangle = -\langle A_{il}, \epsilon_{jkl} D_k \psi_{ij} \rangle = \langle A_{il}, \epsilon_{lkj} D_k \psi_{ij} \rangle = \langle A, \text{Curl } \psi \rangle. \quad (2.1)$$

Note that with this convention one has $\text{Div } \text{Curl } A = 0$ in the sense of distributions, since componentwise the divergence is classically defined as $(\text{Div } A)_i = D_j A_{ij}$.³ For the remaining of this section, our main references are [10, 12].

2.1 Notations

Let M, n be integers with $0 \leq M \leq n$. We denote by $\Lambda^M \mathbb{R}^n$ and $\Lambda_M \mathbb{R}^n$ the vector spaces of M -covectors and M -vectors respectively. A M -vector ξ is said *simple* if it can be written as a single wedge product of vectors, $\xi = v_1 \wedge v_2 \wedge \dots \wedge v_M$. Let α be a multiindex, i.e., an ordered (increasing) subset of $\{1, 2, \dots, n\}$. We denote by $|\alpha|$ the cardinality of α , and we denote by $\bar{\alpha}$ the complementary set of α , i.e., the multiindex given by the ordered set $\{1, 2, \dots, n\} \setminus \alpha$.

For a $n \times n$ matrix A with real entries and for α and β multiindices such that $|\alpha| + |\beta| = n$, $M_{\bar{\alpha}}^{\beta}(A)$ will denote the determinant of the submatrix of A

³In this paper we therefore follow the transpose of Gurtin's notation convention [6] but care must be paid since the curl and divergence of tensor fields are given alternative definitions in the literature (including the second author references [23]- [27] where it holds $\text{Curl } A = -A \times \nabla$).

given by erasing the i -th columns and the j -th rows, for all $i \in \alpha$ and $j \in \bar{\beta}$. Moreover, symbol $M(A)$ will denote the n -vector in $\Lambda_n \mathbb{R}^{2n}$ given by

$$M(A) := \sum_{|\alpha|+|\beta|=n} \sigma(\alpha, \bar{\alpha}) M_{\bar{\alpha}}^{\beta}(A) e_{\alpha} \wedge \varepsilon_{\beta},$$

where $\{e_i, \varepsilon_i\}_{i \leq n}$ is the Euclidean basis of \mathbb{R}^{2n} and $\sigma(\alpha, \bar{\alpha})$ denotes the sign of the ordered set $\{\alpha, \bar{\alpha}\}$ seen as a permutation of the set $\{1, 2, \dots, n\}$. Accordingly, it holds

$$|M(A)| := \left(1 + \sum_{\substack{|\alpha|+|\beta|=n \\ |\beta|>0}} |M_{\bar{\alpha}}^{\beta}(A)|^2\right)^{1/2}.$$

For a matrix $A \in \mathbb{R}^{3 \times 3}$ it is intended by $\text{adj } A$ and $\text{det} A$ the adjunct, i.e. the transpose of the matrix of the cofactors of A , and the determinant of A , respectively. Explicitely,

$$M_j^i(A) = A_{ij}, \quad M_j^I(A) = M_j^I(A) = (\text{cof } A)_{ij} \quad M_{\{1,2,3\}}^{\{1,2,3\}}(A) = \text{det} A, \quad (2.2)$$

where I and J are the complementary set in $\{1, 2, 3\}$ of $\{i\}$ and $\{j\}$. Moreover,

$$|M(A)| = \left(1 + \sum_{i,j} A_{ij}^2 + \sum_{i,j} \text{cof}(A)_{ij}^2 + \text{det}(A)^2\right)^{1/2}. \quad (2.3)$$

Let also $\mathcal{M}(A) := (A, \text{adj } A, \text{det} A)$ and $|\mathcal{M}(A)| := |M(A)|$.

2.2 Currents

Let Ω be an open set in \mathbb{R}^n . For a non-negative integer $M \leq n$, the space $\mathcal{D}^M(\Omega) = \mathcal{D}(\Omega; \Lambda^M \mathbb{R}^n)$ stands for of C^∞ -differential forms with degree M with compact support in Ω . Moreover $\mathcal{D}_M(\Omega) := (D(\Omega; \Lambda^M \mathbb{R}^n))'$ is the space of M -dimensional currents on Ω . Since $\mathcal{D}_M(\Omega)$ is defined as a dual space, it is endowed with a natural weak topology. More precisely, the currents $T_k \in \mathcal{D}_M(\Omega)$ are said to weakly converge to $T \in \mathcal{D}_M(\Omega)$ if and only if

$$\langle T_k, \omega \rangle \rightarrow \langle T, \omega \rangle$$

for every $\omega \in \mathcal{D}^M(\Omega)$.

If S is a M -dimensional oriented submanifold in \mathbb{R}^n and $\vec{S} : S \rightarrow \Lambda_M(\mathbb{R}^n)$ is a M -vector giving the orientation, symbol $\llbracket S \rrbracket \in \mathcal{D}_M(\mathbb{R}^n)$ will denote the current obtained by integration on S , i.e.,

$$\llbracket S \rrbracket(\omega) = \int_S \langle \omega, \vec{S} \rangle d\mathcal{H}^M \quad \text{for } \omega \in \mathcal{D}^M(\Omega), \quad (2.4)$$

where $\langle \cdot, \cdot \rangle$ stands classically for the duality product between M -vectors and M -covectors, and \mathcal{H}^M the M -dimensional Hausdorff measure.

The *boundary* of a current $\mathcal{D}_M(\Omega)$ is the current $\partial T \in \mathcal{D}_{M-1}(\Omega)$ defined by

$$\partial T(\omega) := T(d\omega) \quad \text{for } \omega \in \mathcal{D}^{M-1}(\Omega),$$

where $d\omega$ is the external derivative of ω . Using again the duality with M -forms, if $U \subset \mathbb{R}^n$ and $V \subset \mathbb{R}^m$ are open sets and $F : U \rightarrow V$ is a smooth map, it is possible to define the *push forward* of a current $T \in \mathcal{D}_M(U)$ through F as

$$F_{\#} T(\omega) := T(\zeta F^{\sharp} \omega) \quad \text{for } \omega \in \mathcal{D}^M(V),$$

where $F^\sharp\omega$ is the standard pull back of ω and ζ is any C^∞ function that is equal to 1 on $\text{spt}T \cap \text{spt}F^\sharp\omega$. It turns out that $F_\sharp T \in \mathcal{D}_M(V)$ does not depend on ζ and satisfies

$$\partial F_\sharp T = F_\sharp \partial T. \quad (2.5)$$

The *mass* of a current $T \in \mathcal{D}_M(\Omega)$ is defined by

$$|T| := \sup_{\omega \in \mathcal{D}^M(\Omega), |\omega| \leq 1} T(\omega), \quad (2.6)$$

and if $V \subset \Omega$ is an open set, we can consider the *mass of T in V* , i.e.,

$$|T|_V := \sup_{\substack{\omega \in \mathcal{D}^M(\Omega), |\omega| \leq 1, \\ \text{spt}\omega \subset V}} T(\omega). \quad (2.7)$$

Not to weight up some formulas in the following, the following notation

$$N(T) := |T| + |\partial T|, \quad N_U(T) := |T|_U + |\partial T|_U,$$

will be employed whenever $T \in \mathcal{D}_M(\Omega)$ and $U \subset \Omega$ is open. Remark that this number, which measures both the mass of a current and of its boundary, is not a norm. Moreover, with a little abuse of notation, expression $T \subseteq A$ will mean in the sequel that the support of the current T is a subset of the closed set A .

2.3 Rectifiable currents

A set $S \subset \mathbb{R}^n$ is said \mathcal{H}^M -*rectifiable* if it is contained in the union of a negligible set and a countable family of C^1 -submanifolds. The current S is said locally finite if for each compact set $K \subset \mathbb{R}^n$ we have $\mathcal{H}^M(S \cap K) < \infty$, and that a \mathcal{H}^M -rectifiable set is a M -set if it has finite \mathcal{H}^M -measure. It is well known that at \mathcal{H}^M -a.e. point x of a \mathcal{H}^M -rectifiable set S , there exists an approximate tangent space defined as the M -dimensional plane $T_x S$ in \mathbb{R}^n such that

$$\lim_{\lambda \rightarrow 0} \int_{\eta_{x,\lambda}(S)} \varphi(y) d\mathcal{H}^M(y) = \int_{T_x S} \varphi(y) d\mathcal{H}^M(y),$$

for all $\varphi \in C_c^0(\mathbb{R}^n)$, where $\eta_{x,\lambda} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is the map defined by $\eta_{x,\lambda}(y) = \lambda^{-1}(y - x)$ with $x, y \in \mathbb{R}^n$ and $\lambda > 0$.

Moreover, if $\tau : S \rightarrow \Lambda_M(\mathbb{R}^n)$ and $\theta : S \rightarrow \mathbb{R}$ are \mathcal{H}^M -integrable and such that $\tau(x) \in T_x S$ is a simple unit M -vector for \mathcal{H}^M -a.e. $x \in S$, then we can define the current T as

$$T(\omega) = \int_S \langle \omega(x), \tau(x) \rangle \theta(x) d\mathcal{H}^M(x) \quad \text{for } \omega \in \mathcal{D}^M(\Omega). \quad (2.8)$$

Every current for which there exists S , τ , and θ as before is said *rectifiable current*. If also its boundary ∂T is rectifiable, then to denote T , the short notation

$$T \equiv \{S, \tau, \theta\} \quad (2.9)$$

will be adopted.

2.4 Integer-multiplicity currents and graphs of Sobolev functions

The current $T \in \mathcal{D}_M(\Omega)$ is *rectifiable with integer multiplicity* if it is rectifiable with rectifiable boundary, and S , τ , and θ in (2.8) satisfy also the property that θ is integer valued. Integer multiplicity currents are also said *integral currents*. The following compactness theorem for integer multiplicity currents holds:

Theorem 2.1 (Compactness for i.m. currents). *Let $\{T_i\} \subset \mathcal{D}_M(\Omega)$ be a sequence of integer multiplicity currents such that*

$$N_U(T) < C \quad \text{for all } i \text{ and } U \subset\subset \Omega,$$

with $C > 0$. Then there exist an integer multiplicity current $T \in \mathcal{D}_M(\Omega)$ and a subsequence $\{T_{k(i)}\}_i$ such that $T_{k(i)} \rightarrow T$ weakly in Ω as $i \rightarrow \infty$.

An integer-multiplicity current $T \in \mathcal{D}_M(\mathbb{R}^n)$ is said *indecomposable* if there exists no integral current R such that $R \neq 0 \neq T - R$ and

$$N(T) = N(R) + N(T - R).$$

The following theorem provides the decomposition of every integral current and the structure of integer-multiplicity indecomposable 1-current (see [10, Section 4.2.25]).

Theorem 2.2. *For every integer-multiplicity current T there exists a sequence of indecomposable integral currents T_i such that*

$$T = \sum_i T_i \quad \text{and} \quad N(T) = \sum_i N(T_i).$$

Suppose T is an indecomposable integer multiplicity 1-current on \mathbb{R}^n . Then there exists a Lipschitz function $f : [0, |T|] \rightarrow \mathbb{R}^n$ with $\text{Lip}(f) = 1$ such that

$$f \llcorner [0, |T|) \text{ is injective and } T = f \# [0, |T|].$$

Moreover $\partial T = 0$ if and only if $f(0) = f(|T|)$.

Approximately differentiability almost everywhere is readily fulfilled if the function u belongs to $W^{1,p}(\Omega, \mathbb{R}^n)$. This will always be the case for the functions considered in the sequel. We refer to [12, Section 3.1.5, Theorem 4] for the proof of this fact and of Theorem 2.3. Given $u \in W^{1,p}(\Omega, \mathbb{R}^n)$, we define its *graph* $\mathcal{G}_u \subset \Omega \times \mathbb{R}^n$ as

$$\mathcal{G}_u := \{(x, u(x)) : x \in R_u \cap \Omega\}.$$

The following theorem provides a sufficient condition to guarantee that the graph is a rectifiable set.

Theorem 2.3. *Let $u \in L^1(\Omega; \mathbb{R}^n)$ be approximately differentiable almost everywhere. Then the graph \mathcal{G}_u is a \mathcal{H}^n -rectifiable set. Moreover it holds that if all the minors of Du are integrable, then $\mathcal{H}^n(\mathcal{G}_u) < \infty$.*

Let us consider the map $(\text{Id} \times u) : \Omega \rightarrow \Omega \times \mathbb{R}^n$ defined by $(\text{Id} \times u)(x) := (x, u(x))$. If $u \in W^{1,p}(\Omega; \mathbb{R}^n)$ and $\omega \in \mathcal{D}^n(\Omega \times \mathbb{R}^n)$, we can extend the definition of pull-back also to the map $\text{Id} \times u$, i.e.,

$$(\text{Id} \times u)^\# \omega = \sum_{|\alpha|+|\beta|=n} \sigma(\alpha, \bar{\alpha}) \omega_{\alpha\beta}(u, u(x)) M_{\bar{\alpha}}^\beta(Du(x)) dx_1 \wedge dx_2 \wedge \cdots \wedge dx_n$$

where

$$\omega(x, y) = \sum_{|\alpha|+|\beta|=n} \omega_{\alpha\beta}(x, y) dx^\alpha \wedge dy^\beta. \quad (2.10)$$

This allows us to extend the definition of push-forward of a current T also throughout the map $\text{Id} \times u$, provided $u \in W^{1,p}(\Omega; \mathbb{R}^n)$. Let us consider the current $[[\Omega]]$, the canonical current given by integration on Ω , we set $G_u := (\text{Id} \times u)_\# [[\Omega]]$, so that, for all ω satisfying (2.10), we have

$$\begin{aligned} G_u(\omega) &= \int_{\Omega} \langle \omega(x, u(x)), M(Du(x)) \rangle dx \\ &= \sum_{|\alpha|+|\beta|=n} \int_{\Omega} \sigma(\alpha, \bar{\alpha}) \omega_{\alpha\beta}(x, u(x)) M_{\bar{\alpha}}^\beta(Du(x)) dx. \end{aligned}$$

2.5 Cartesian maps

Let $u \in W^{1,p}(\Omega; \mathbb{R}^3)$, and suppose $u_1(\text{adj} Du) \in L^1(\Omega, \mathbb{R}^3)$, we define the *distributional cofactor* of Du , the distribution $\text{Cof} Du$ writing componentwise

$$(\text{Cof} Du)_{ij} := \partial_{j+1}(u_{i+1} Du_{(i+2)(j+2)}) - \partial_{j+2}(u_{i+1} Du_{(i+2)(j+1)})$$

with indices $i, j \in \{1, 2, 3\}$ (taken mod 3 when summed and with the derivatives intended in the distribution sense). Moreover, $\text{Adj} Du$ is the *distributional adjunct* of Du , that is the transpose matrix of the distributional cofactors $\text{Cof} Du$. Note that in general it is not true that the pointwise and distributional adjuncts coincide. The *distributional determinant* of Du is the distribution $\text{Det} Du$ given taking the distributional divergence of $u_1(\text{adj} Du)_1$, i.e.,

$$(\text{Det} Du, \varphi) := \int_{\Omega} u_1(\text{adj} Du)_1 D\varphi dx, \quad \forall \varphi \in C_c^\infty(\Omega, \mathbb{R}^3),$$

with $(\text{adj} Du)_1 := (\text{adj}(Du)_{11}, \text{adj}(Du)_{12}, \text{adj}(Du)_{13})$. As for the adjunct, in general $\text{Det} Du$ and $\det Du$ differ. Let us define for $p \geq 1$

$$\mathcal{A}^p(\Omega, \mathbb{R}^n) := \{u \in W^{1,p}(\Omega, \mathbb{R}^3) : M_{\bar{\alpha}}^\beta(Du) \in L^p(\Omega) \forall \alpha, \beta \text{ with } |\alpha| + |\beta| = 3\},$$

and set

$$\|u\|_{\mathcal{A}^p} := \|u\|_p + \|M(Du)\|_p,$$

which is not a norm on $\mathcal{A}^p(\Omega, \mathbb{R}^n)$. In other words, a function $u \in \mathcal{A}^p(\Omega, \mathbb{R}^3)$ if and only if $u \in W^{1,p}(\Omega, \mathbb{R}^3)$, and $\text{adj} Du, \det Du$ belong to $L^p(\Omega)$.

Theorem 2.4. *If $u \in \mathcal{A}^1(\Omega, \mathbb{R}^n)$ then G_u is an integer multiplicity current with multiplicity 1 and support given by the rectifiable set \mathcal{G}_u whose orientation is given by the n -form*

$$\vec{G}_u(x, u(x)) := \frac{M(Du(x))}{|M(Du(x))|},$$

which turns out to be almost everywhere orthogonal to the approximate tangent plane to \mathcal{G}_u .

In symbols,

$$G_u(\omega) = \int_{\Omega} \langle \omega, \frac{M(Du(x))}{|M(Du(x))|} \rangle d\mathcal{H}^n \llcorner \mathcal{G}_u, \quad (2.11)$$

whereby for $p \geq 1$, the class of *Cartesian maps* is defined as the function set

$$\text{Cart}^p(\Omega, \mathbb{R}^n) := \{u \in \mathcal{A}^p(\Omega; \mathbb{R}^n) : \partial G_u \llcorner (\Omega \times \mathbb{R}^n) = 0\}. \quad (2.12)$$

The following closure theorem for Cartesian maps holds (see [12, Section 3.3.3]):

Theorem 2.5. *Let $u_k \in \text{Cart}^p(\Omega, \mathbb{R}^n)$ a sequence such that*

$$\begin{aligned} u_k &\rightharpoonup u \quad \text{weakly in } L^p(\Omega, \mathbb{R}^n), \\ M_{\alpha}^{\beta}(Du_k) &\rightharpoonup v_{\alpha}^{\beta} \quad \text{weakly in } L^p(\Omega), \end{aligned}$$

for all α, β with $|\alpha| + |\beta| = n$, then $u \in \text{Cart}^p(\Omega, \mathbb{R}^n)$ and $v_{\alpha}^{\beta} = M_{\alpha}^{\beta}(Du)$.

The crucial point for our purposes is that for Cartesian maps it is always true that $\text{Det}Du = \det Du$ and $\text{Adj}Du = \text{adj}Du$. In particular $\text{Det}Du \in L^p(\Omega)$ and $\text{Adj}Du \in L^p(\Omega, \mathbb{R}^{n \times n})$.

2.6 Compact sets

Let C be a bounded compact set in \mathbb{R}^n . We define $\mathcal{K}(C)$ as the family of compact and non-empty subsets of C . We define the Gromov-Hausdorff distance $d_H(\cdot, \cdot)$ in $\mathcal{K}(C)$ by

$$d_H(A, B) := \max\{\sup_{a \in A} d(a, B), \sup_{b \in B} d(A, b)\},$$

for all $A, B \in \mathcal{K}(C)$. If A is a Borel set in \mathbb{R}^n , we denote by A_{ϵ} the set of points at distance less than ϵ from A , i.e.,

$$A_{\epsilon} := \{x \in \mathbb{R}^n : d(x, A) < \epsilon\}.$$

It is known that the Gromov-Hausdorff distance satisfies

$$d_H(A, B) = \inf\{\epsilon > 0 : A \subset B_{\epsilon} \text{ and } B \subset A_{\epsilon}\},$$

for all $A, B \in \mathcal{K}(C)$, and hence the latter can be taken as an equivalent definition. The following theorem is a standard result, whose proof can be found, for instance, in [2, 4].

Theorem 2.6. (*Blaschke*) *Let $C \subset \mathbb{R}^n$ be a bounded compact set. Then the space $\mathcal{K}(C)$ endowed with the Gromov-Hausdorff distance d_H is sequentially compact.*

In particular, if K_n is a sequence in $\mathcal{K}(C)$ converging to K , then K is a compact set. Moreover, it holds (for the proof see, e.g., [2, 4]):

Theorem 2.7. (*Golab*) *Let $\{K_n\}$ be a sequence of connected sets in $\mathcal{K}(C)$ converging to K , such that $\mathcal{H}^1(K_n) < \lambda < \infty$. Then K is connected, has Hausdorff dimension 1, and*

$$\mathcal{H}^1(K) \leq \liminf_{n \rightarrow \infty} \mathcal{H}^1(K_n). \quad (2.13)$$

3 Dislocations as currents

A dislocation in an elasto-plastic body arises as a closed arc, or a path connecting two points of the boundary, to which a Burgers vector $b \in \mathbb{R}^3$ and a measure concentrated on the dislocation line (the dislocation density) are associated. Since dislocation densities fulfill linear additivity when dislocation lines overlap, and since to each dislocation 2 preferential directions are associated, which also define its density, we will describe dislocations by the tool of integer-multiplicity 1-currents with coefficients in a group, that in the crystallographic case is assumed isomorphic to \mathbb{Z}^3 . The coefficient θ represents the Burgers vector with its multiplicity, and the fact that it is constant on any dislocation and that the dislocations are closed correspond to the requirement that such currents are boundaryless (i.e., that the density is divergence free). Moreover, integer-multiplicity 1-currents, thanks to Theorem 3.18, are essentially Lipschitz curves, and hence a description of dislocations without using the notion of currents is also possible. However the notion of currents, as we will see, simplifies some descriptions and provides more direct proofs of some of the following statements. In the sequel, we will introduce and discuss two families of dislocations emphasizing the equivalence between them.

Let Ω be a bounded and connected open set in \mathbb{R}^3 , with smooth boundary. Let $\mathcal{I} \subset \mathbb{N}$ be a family of indices.

Definition 3.1. *A dislocation is a couple $\mathcal{L}_{\mathcal{I}} := (\mathcal{L}_i, b_i)_{i \in \mathcal{I}}$, where \mathcal{L}_i are integer-multiplicity currents in $\bar{\Omega}$ and b_i are vectors. We define $\mathcal{B}_{\mathcal{I}} = \{b_i\}_{i \in \mathcal{I}}$. Each $\mathcal{L}_{\mathcal{I}}$ can be represented by means of the quadruple $\{L_i, \tau_i, \theta_i, b_i\}_{i \in \mathcal{I}}$. The current associated to the dislocation $\mathcal{L}_{\mathcal{I}}$ is $\mathcal{L} = \sum_{i \in \mathcal{I}} \mathcal{L}_i$.*

In many applications, the Burgers vector is constraint by crystallographic properties to belong to a lattice. For simplicity this lattice will be assumed isomorphic to \mathbb{Z}^3 . Let the lattice vector $\bar{b} = (\bar{b}_1, \bar{b}_2, \bar{b}_3)$ be fixed, and define the set of *admissible Burgers vectors* as

$$\mathcal{B} := \{b \in \mathbb{R}^3 : \exists \beta \in \mathbb{Z}^3 \text{ such that } b_i = \beta_i \bar{b}_i, \text{ for } i = 1, 2, 3\}. \quad (3.1)$$

Accordingly if $\mathcal{B}_{\mathcal{I}} \subset \mathcal{B}$ then $\mathcal{L}_{\mathcal{I}}$ is called a *crystallographic dislocation*. With this definition we can identify each dislocation with a current with coefficients in the group $\mathcal{B} \cong \mathbb{Z}^3$. However we will need some specific characterization of dislocations which are physically admissible. This is why we need to introduce finer classes of dislocations in the sequel.

The *density of a dislocation* is a key measure associated to the dislocation current.

Definition 3.2. *The density associated to $\mathcal{L}_{\mathcal{I}}$ is the linear functional $\Lambda_{\mathcal{L}}$ defined by*

$$\langle \Lambda_{\mathcal{L}}, w \rangle := \sum_{i \in \mathcal{I} \subset \mathbb{N}} \mathcal{L}_i((wb^i)^*), \quad (3.2)$$

for every $w \in C^\infty(\bar{\Omega}, \mathbb{R}^{3 \times 3})$, where in the right-hand side $\omega := (wb)^*$ is the covector writing componentwise $(wb)^* := w_{kj} b_j dx_k$ (with Einstein summation convention on repeated indices).

If $\sum_{i \in \mathcal{I}} |\mathcal{L}_i| \|b_i\| < \infty$ then $\Lambda_{\mathcal{L}}$ is well defined as a Radon measure, and we write $\Lambda_{\mathcal{L}} \in \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3})$.

Definition 3.3 (Equivalence between dislocations). *Two dislocations $\mathcal{L}_{\mathcal{I}}$ and $\mathcal{L}'_{\mathcal{I}}$ are said geometrically equivalent if*

$$\Lambda_{\mathcal{L}} = \Lambda_{\mathcal{L}'}. \quad (3.3)$$

Definition 3.4 (Geometrically necessary dislocation set). *The geometric necessary dislocation set L^* is the support of $\Lambda_{\mathcal{L}}$. In particular there are τ^* and \mathcal{I}^* , such that $\{L^*, \tau^*, 1, \mathcal{B}_{\mathcal{I}^*}\}$ is said the minimal dislocation equivalent to $\mathcal{L}_{\mathcal{I}}$.*

Under suitable assumptions L^* turns out to be a \mathcal{H}^1 -rectifiable compact set. In the sequel we discuss some sufficient assumptions in order for L^* to have this regularity.

3.1 Regular dislocations

Definition 3.5 (b -dislocation currents). *Let $b \in \mathcal{B}$. A b -dislocation current is a dislocation $\mathcal{L}_{\mathcal{I}}$ such that (i) $b_i = b$, (ii) \mathcal{I} is finite with cardinality k_b , (iii) there exist k_b Lipschitz functions $\varphi_j^b : [0, T_j] \rightarrow \bar{\Omega}$ with $\text{Lip}(\varphi_j^b) \leq 1$ such that*

$$\mathcal{L}^b = \sum_{i \in \mathcal{I}} \mathcal{L}_i = \sum_{j=1}^{k_b} \varphi_{j\#}^b \llbracket [0, T_j] \rrbracket. \quad (3.4)$$

Moreover, for all $j \leq k_b$ we have either $\varphi_j^b(0) = \varphi_j^b(T_j)$ or $\varphi_j^b(0), \varphi_j^b(T_j) \in \partial\Omega$. The current \mathcal{L}^b is called a b -dislocation current.

In particular, with this definition, we require that a b -dislocation is always closed in Ω .

From Theorem 2.2, one can always decompose \mathcal{L}^b as follows

$$\mathcal{L}^b = \sum_{i \in \mathcal{I}^b} \mathcal{L}_i^b, \quad (3.5)$$

with \mathcal{L}_i^b indecomposable 1-current such that $\sum_{i \in \mathcal{I}^b} N(\mathcal{L}_i^b) = N(\mathcal{L}^b)$. The components \mathcal{L}_i^b are called *current loops*. Thanks to the Lipschitzianity of the functions

φ_j^b one has $\sum_{j=1}^{k_b} l_j^b := \sum_{j=1}^{k_b} \int_0^{T_j} \|\dot{\varphi}_j^b\| dt < \infty$, meaning that the total length of the

supporting set of the current \mathcal{L}^b counted with overlapping is finite, where l_j^b is the length of the current given by φ_j^b .

We remark that even if the word loop usually refers to a closed path, we use the same word when referring to a non-closed current. This follows from the fact that we are only interested to describe the behaviour of loops inside $\bar{\Omega}$, so that if their ranges intersect both Ω and Ω^c , the restriction of the loop to the interior part is not a closed current, and has a non-vanishing boundary supported in $\partial\Omega$. Note also that by definition, a b -dislocation current satisfies $\partial\mathcal{L}^b \subseteq \partial\Omega$.

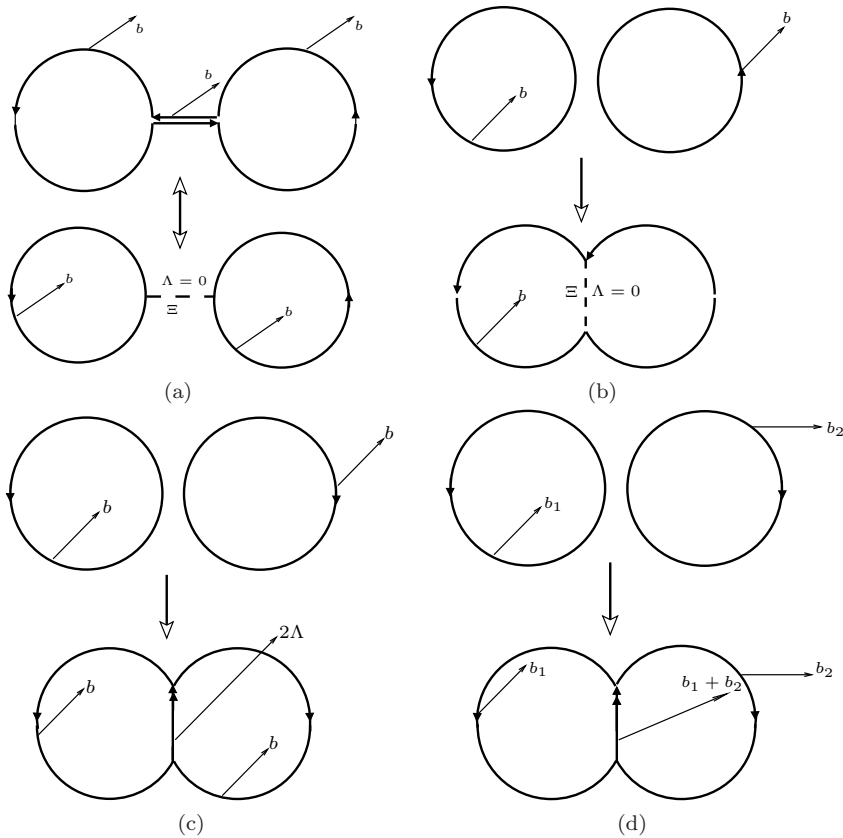


Figure 2: Typical indecomposable dislocation loops and the resulting dislocation currents: in (a), a single b -dislocation loops is equivalently viewed as two indecomposable b -loops with opposite directions and connected by a geometrically unnecessary arc Ξ ; the inverse property is observed in (b) where two identical b -loops give rise to a single connected b -dislocation loops and a geometrically unnecessary arc Ξ where $\Lambda = 0$; in contrast, (c) describes two b -loops with opposite direction which provide a simple cluster showing subarcs with Burgers vectors b and $2b$; the general case is shown in (d) where the cluster is due to the union of two loops with distinct Burgers vectors obeying to Frank rule.

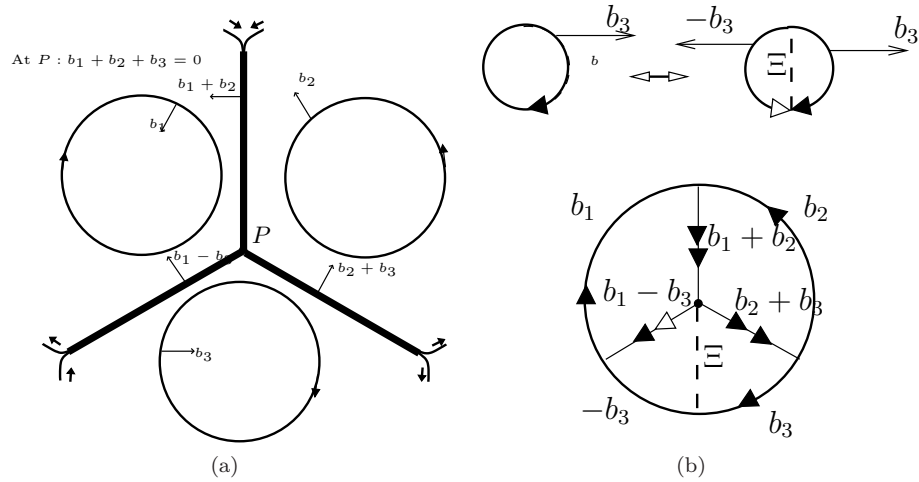


Figure 3: For certain combinations of Burgers vectors, the three separated loops of (a) might intersect and form the cluster element of (b) where the Frank law at the intersection points is satisfied.

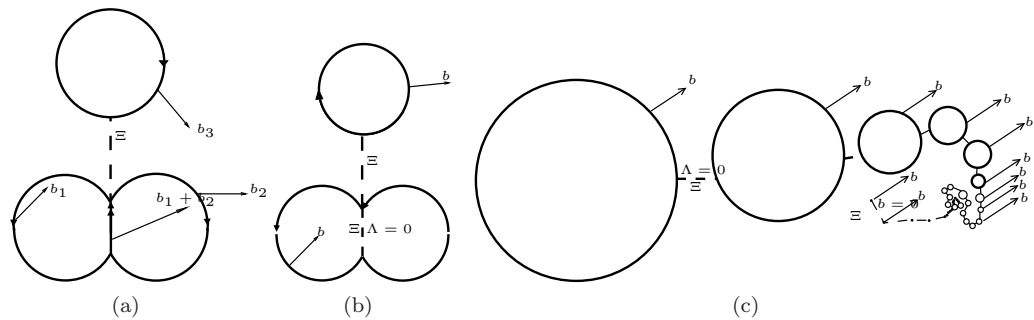


Figure 4: Different kinds of cluster components: in (a) the sum of b -current dislocations $\mathcal{L}^{b_1} + \mathcal{L}^{b_2} + \mathcal{L}^{b_3}$ is depicted, whereas (b) shows a single b -current constituted of three elementary b -loops. In (c) a b -dislocation cluster writing as $\mathcal{L}^b = \varphi_b^{\text{hull}}[[0, T]]$ is shown: it can be viewed as a countable chain of indecomposable b -loops interconnected with geometrically unnecessary arcs.

By definition of rectifiable current, if \mathcal{L}^b is a b -dislocation current then there is a 1-set called *dislocation set* that we denote by L_b , such that

$$\mathcal{L}^b(\omega) = \int_{L^b} \langle \omega(x), \tau^b(x) \rangle \theta^b(x) d\mathcal{H}^1(x) \quad \text{for } \omega \in \mathcal{D}^1(\Omega). \quad (3.6)$$

We can choose

$$L^b := \bigcup_{j=1}^{k_b} \varphi_j^b([0, T_j]), \quad (3.7)$$

for the rectifiable set supporting the current \mathcal{L}^b , and we will also write $\mathcal{L}^b = \{L^b, \tau^b, \theta^b\}$. With such a choice L^b is a compact set. Note that with this choice for the dislocation set, in general L^b does not coincide with the geometrically necessary dislocation set L^* , since somewhere on L^b it may happen that $\theta^b = 0$. Indeed, with this notation, θ^b may also take the value 0 in a set of \mathcal{H}^1 positive measure. If \mathcal{L}_i^b are the indecomposable components of \mathcal{L}^b in (3.5), we write $\mathcal{L}_i^b = \{L_i^b, \tau^b, \theta^b\}$, in such a way that it holds $L^b = (\cup_{i \in \mathcal{I}^b} L_i^b) \cup \Xi^b$, where Ξ^b is defined as the set $\{x \in L^b : \theta^b(x) = 0\}$.

Definition 3.6. *The density of a b -dislocation current \mathcal{L}^b is the measure $\Lambda_{\mathcal{L}^b} \in \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3})$ defined by*

$$\langle \Lambda_{\mathcal{L}^b}, w \rangle := \mathcal{L}^b((wb)^*), \quad (3.8)$$

for every $w \in C_c^\infty(\Omega, \mathbb{R}^{3 \times 3})$, where in the right-hand side $\omega := (wb)^*$ is the covector writing componentwise $(wb)^* := w_{kj} b_j dx_k$.

Since k_b is finite $\Lambda_{\mathcal{L}^b}$ is always a Radon measure. In the sequel we will use the following shortcut notation from (3.6) and (3.8):

$$\Lambda_{\mathcal{L}^b} = \mathcal{L}^b \otimes b = \tau^b \otimes b \theta^b \mathcal{H}^1 \llcorner L^b. \quad (3.9)$$

Definition 3.7 (Regular dislocation). *A regular dislocation is a sequence of b -dislocation currents $\mathcal{L} := \{\mathcal{L}^b\}_{b \in \mathcal{B}}$. We associate to each dislocation a dislocation current, still denoted by \mathcal{L} , and the associated dislocation density $\Lambda_{\mathcal{L}}$,*

$$\mathcal{L} := \sum_{b \in \mathcal{B}} \mathcal{L}^b, \quad \Lambda_{\mathcal{L}} := \sum_{b \in \mathcal{B}} \Lambda_{\mathcal{L}^b}. \quad (3.10)$$

The dislocation set L is defined as

$$L := \bigcup_{b \in \mathcal{B}} L^b, \quad (3.11)$$

so that we can write $\mathcal{L} = \{L, \tau, \theta\}$ with

$$\tau \in \text{Tan}L, \quad \theta = \sum_{b \in \mathcal{B}} \text{sg}(\tau^b) \theta^b, \quad (3.12)$$

where $\text{sg}(\tau^b)$ being 1 or -1 , chosen in such the way that $\tau = \text{sg}(\tau^b) \tau^b$.

From Definition 3.5 we have $\partial \mathcal{L} \subseteq \partial \Omega$. Note also that, in general, the multiplicity θ of the dislocation current \mathcal{L} may be also zero in some non-negligible

set. Moreover, the dislocation current $\mathcal{L} = \{L, \tau, \theta\}$ is said connected if L is a connected set. By (3.4), every dislocation current can also be written as

$$\mathcal{L} = \sum_{b \in \mathcal{B}} \mathcal{L}^b = \sum_{b \in \mathcal{B}} \sum_{1 \leq j \leq k_b} \varphi_{j\#}^b \llbracket [0, T_j] \rrbracket, \quad (3.13)$$

and, enumerating the family of generating functions $\{\varphi_j^b\}$, we construct a set of indices $\mathcal{J} = \mathcal{J}(\mathcal{L})$ such that

$$\mathcal{L} = \sum_{j \in \mathcal{J}} \varphi_{j\#} \llbracket [0, T_j] \rrbracket. \quad (3.14)$$

Moreover, setting $S_i := \varphi_i \llbracket [0, T_i] \rrbracket$, from (3.7) and (3.11) we also have

$$L = \bigcup_{j \in \mathcal{J}} S_j. \quad (3.15)$$

Every current of the form $\mathcal{L}' = \sum_{j \in \mathcal{J}'} \varphi_{j\#} \llbracket [0, T_j] \rrbracket$, where $\mathcal{J}' \subset \mathcal{J}$, is said a subcurrent of \mathcal{L} , and we write $\mathcal{L}' \subset \mathcal{L}$. In such a case, setting $L' := \bigcup_{j \in \mathcal{J}'} S_j$, we can write $\mathcal{L}' = \{L', \tau, \theta\}$. Again we say that a subcurrent \mathcal{L}' is connected if the set L' is connected.

Definition 3.8. $\Upsilon \subset \mathcal{L}$ is called a cluster current if it is a maximal connected subset of \mathcal{L} with respect to the inclusion \subset .

3.2 Canonical regular dislocations

Among all geometrically equivalent dislocations there exists one representation which is sharp in the sense that it is expressed in terms of the independent elementary Burgers vectors. In fact the space \mathcal{B} is a vector space and a group generated by the basis $\{\underline{b}_1, \underline{b}_2, \underline{b}_3\}$, where $\underline{b}_i := (\bar{b} \cdot \underline{e}_i) \underline{e}_i$ for $i = 1, 2, 3$, thus since a b -dislocation current \mathcal{L}^b with $b = (\beta_1, \beta_2, \beta_3)$ has integer multiplicity, it can be written by means of projections. Recalling definition (3.1) and notation (2.9), we introduce

$$\mathcal{L}^{b,i} := \{L^b, \tau^b, \beta_i \theta^b\}, \quad (3.16)$$

with the corresponding density $\Lambda_{\mathcal{L}^{b,i}} := \mathcal{L}^{b,i} \otimes \underline{b}_i = \mathcal{L}^b \otimes \beta_i \underline{e}_i$. Hence to any dislocation current we associate univoquely three currents $\{\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3\}$, with

$$\mathcal{L}_i := \sum_{b \in \mathcal{B}} \mathcal{L}^{b,i}, \quad (3.17)$$

with $\mathcal{L}_i = \{L, \tau, \theta_i\}$, θ_i defined by

$$\theta_i := \sum_{b \in \mathcal{B}} \text{sg}(\tau^b) \beta_i \theta^b, \quad \text{with } b = (\beta_1, \beta_2, \beta_3),$$

and $\text{sg}(\tau^b)$ being such that $\tau = \text{sg}(\tau^b) \tau^b$. We then define the *canonical dislocation current equivalent to \mathcal{L}* :

$$\hat{\mathcal{L}} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3. \quad (3.18)$$

A usefull property of the decomposition (3.18) is that the three measures $\{\Lambda_{\mathcal{L}_i}\}_{i=1}^3$ operate on different (pointwise) orthogonal subspaces of $C_c^\infty(\mathbb{R}^3, \mathbb{R}^{3 \times 3})$.

Lemma 3.9. (a) *The dislocation currents \mathcal{L}_i ($i = 1, 2, 3$) are integer-multiplicity currents in $\bar{\Omega}$ provided $\sum_{b \in \mathcal{B}} N(\mathcal{L}^{b,i}) < \infty$.*

(b) *The mass of the current and the total variation of the associated measure are related by*

$$|\mathcal{L}_i|_\Omega \leq B^{-1} \|\Lambda_{\mathcal{L}_i}\|_{\mathcal{M}(\Omega)} \leq B^{-1} \|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\Omega)}, \quad (3.19)$$

for some $B > 0$ independent of \mathcal{L}_i ($i = 1, 2, 3$).

(c) *The geometrically necessary dislocation set reads $L^* := \bigcup_{i=1}^3 \text{spt}(\mathcal{L}_i) \subset \bar{L}$ and coincides with the support of the density $\Lambda_{\mathcal{L}}$.*

Proof. Assertion (a) follows by Theorem 2.1.

To prove (b), observe first that for fixed b it holds

$$\sum_{i=1}^3 \Lambda_{\mathcal{L}^{b,i}} = \sum_{i=1}^3 \mathcal{L}^{b,i} \otimes \underline{b}_i = \sum_{i=1}^3 \tau^b \otimes \beta_i \underline{b}_i \theta^b \mathcal{H}^1 \llcorner L^b = \Lambda_{\mathcal{L}^b}.$$

Thus it also holds

$$\Lambda_{\mathcal{L}} = \sum_{b \in \mathcal{B}} \Lambda_{\mathcal{L}^b} = \sum_{i=1}^3 \Lambda_{\mathcal{L}_i} = \Lambda_{\hat{\mathcal{L}}}, \quad (3.20)$$

and explicitly,

$$\Lambda_{\hat{\mathcal{L}}} = \sum_{i=1}^3 \tau \otimes \underline{b}_i \theta_i \mathcal{H}^1 \llcorner L = \sum_{i=1}^3 \mathcal{L}_i \otimes \underline{b}_i, \quad (3.21)$$

(recall that τ and θ_i are functions of $x \in L$). Note that, $\{\underline{b}_1, \underline{b}_2, \underline{b}_3\}$ being linearly independent,

$$\|\Lambda_{\mathcal{L}}\|_{\mathcal{M}} = \|\Lambda_{\hat{\mathcal{L}}}\|_{\mathcal{M}} \geq \|\Lambda_{\mathcal{L}_i}\|_{\mathcal{M}} \quad \text{for } i = 1, 2, 3. \quad (3.22)$$

Now, since $\Lambda_{\mathcal{L}_i} = \mathcal{L}_i \otimes \underline{b}_i$, it holds $\|\Lambda_{\mathcal{L}_i}\|_{\mathcal{M}(\Omega)} = |\mathcal{L}_i|_\Omega |\bar{\underline{b}}_i \cdot \underline{e}_i| = |\mathcal{L}_i|_\Omega \|\underline{b}_i\|$ so that, setting $B := \min_{i=1,2,3} \{\|\underline{b}_i\|\}$, yields (3.19).

To prove (c), observe first that $\mathcal{L}_i = \{L, \tau, \theta_i\}$ and by definition of \mathcal{L}_i and $\Lambda_{\mathcal{L}_i}$ it easily follows that $\text{spt} \mathcal{L}_i = \text{spt} \Lambda_{\mathcal{L}_i}$. So we only need to prove that $\text{spt} \Lambda_{\mathcal{L}} = \bigcup_{i=1}^3 \text{spt} \Lambda_{\mathcal{L}_i}$. But this is a direct consequence of the fact that $\Lambda_{\mathcal{L}_i}$ acts on orthogonal subspaces of $C_c^\infty(\mathbb{R}^3, \mathbb{R}^{3 \times 3})$. \square

Definition 3.10 (Unnecessary dislocations). *The set of unnecessary dislocations Ξ is defined as $\bar{L} \setminus L^*$.*

Let us remark that L defined in (3.15) depends on the generating loops of Definition 3.5.

4 Classes of admissible dislocations

Two classes of dislocations will now be introduced, the first being useful if one wishes to follow (for instance, with time) each line as it deforms, intersect with others etc., whereas the second will be more appropriate if the model relevant quantity is the dislocation density, and not the single lines. In the latter case dislocations are determined up to the equivalence relation (3.3) and the clusters might exhibit locally dense subsets of unnecessary dislocations.

4.1 The class of dislocations at the mesoscopic scale

At the mesoscopic scale, it is considered that every dislocation \mathcal{L} has been generated by a finite number of b -dislocation currents \mathcal{L}^b .

Assumption 4.1 (Finite generation).

$$k_{\mathcal{L}} := \sum_{b \in \mathcal{B}} k_b < \infty. \quad (4.1)$$

Let us recall that a finite number of generating b -dislocation currents does not imply that the dislocation density $\Lambda_{\mathcal{L}}$ is associated to a finite number of distinct Burgers vectors, since the multiplicity on each arc of L is not limited and since countably intersections of arcs may take place (in other words, the resulting Burgers vector might be very large, provided it is attached to an arc which is small enough). Moreover, the cluster of Fig. 4(c) made of countably many loops whose lengths are summable and interconnected by unnecessary segments, is a mesoscopic dislocation since it can be generated by a single b -loop.

From the definitions above and Assumption 4.1 the following lemma is readily proved.

Lemma 4.2. *The following properties hold for dislocations at the mesoscopic scale:*

(a) *The density of a dislocation $\Lambda_{\mathcal{L}}$ is a bounded Radon measure since*

$$\|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\bar{\Omega})} \leq \sum_{\substack{b \in \bar{\mathcal{B}} \\ i=1, \dots, k_b}} \|b\| l_i^b < \infty. \quad (4.2)$$

with $\bar{\mathcal{B}} := \{b \in \mathcal{B} : k_b \neq 0\}$ (Recall l_i^b is the length of the dislocation loop φ_i^b).

(b) *The dislocation \mathcal{L} is an integer-multiplicity current and it holds $|\mathcal{L}| \leq \sum_{\substack{b \in \bar{\mathcal{B}} \\ i=1, \dots, k_b}} l_i^b < \infty$. Moreover, $\hat{\mathcal{L}}$ is an integer-multiplicity current satisfying*

$$|\hat{\mathcal{L}}| \leq C \sum_{\substack{b \in \bar{\mathcal{B}} \\ i=1, \dots, k_b}} l_i^b < \infty, \quad (4.3)$$

with $\bar{\mathcal{B}} := \{b \in \mathcal{B} : k_b \neq 0\}$, and where $C := 3 \max_{\substack{b \in \bar{\mathcal{B}} \\ j=1,2,3}} |\beta_j|$ with $b =$

$(\beta_1, \beta_2, \beta_3)$. In particular θ and θ_i , for $i = 1, 2, 3$ are all summable functions with respect to $\mathcal{H}^1 \llcorner L$.

(c) The dislocation set L of the current \mathcal{L} (defined in (3.11)) is a closed set with finite \mathcal{H}^1 -measure. In particular $L^* \subseteq L$ and $L = L^* \cup \Xi$.

Proof. To prove (a), observe that $\mathcal{L} = \{\mathcal{L}^b\}_{b \in \mathcal{B}}$ and hence $\|\Lambda_{\mathcal{L}}\| \leq \sum_{b \in \mathcal{B}} \|\mathcal{L}^b \otimes b\| \leq$

$$\sum_{\substack{b \in \mathcal{B} \\ i=1, \dots, k_b}} \|\mathcal{L}_i^b \otimes b\| = \sum_{\substack{b \in \mathcal{B} \\ i=1, \dots, k_b}} \|b\| l_i^b, \text{ which is finite since the sum is finite by the}$$

mesoscopicity Assumption 4.1. Statement (b) follows as a direct consequence of the definition of b -dislocation current and from (a) and property (b) of Lemma 3.9. Property (c) is a straightforward consequences of the fact that $\mathcal{H}^1(L) \leq$

$$\sum_{\substack{b \in \mathcal{B} \\ i=1, \dots, k_b}} l_i^b = \sum_{\substack{b \in \mathcal{B} \\ i=1, \dots, k_b}} \int_0^{T_i} \|\dot{\varphi}_i^b\| dt < \infty \text{ by the mesoscopicity Assumption 4.1. } \square$$

From the preceding results, we are ready to define the class of *admissible dislocations at the mesoscale*.

Definition 4.3 (Admissible mesoscopic dislocation).

$$\mathcal{MD} := \{\mathcal{L} = \{\mathcal{L}^b\}_{b \in \mathcal{B}} : \mathcal{L}^b \text{ takes the form (3.4) and satisfies Assumption 4.1.}\}. \quad (4.4)$$

4.2 Dislocations at the continuum scale

A set in \mathbb{R}^n is said a continuum if it is the finite union of connected and compact 1-sets with finite \mathcal{H}^1 measure. Let us recall that the geometric necessary dislocation set L^* is the support of $\Lambda_{\mathcal{L}}$. The space of *admissible dislocations at the continuum scale* is introduced as follows:

Definition 4.4 (Admissible continuum dislocation).

$$\mathcal{CD} := \{\mathcal{L}_{\mathcal{I}}, \mathcal{I} \subset \mathbb{N} : \text{there exists a continuum } \mathcal{K} \text{ such that } L^* \subset \mathcal{K}\}. \quad (4.5)$$

When the context is clear, we will write $\mathcal{L} = \mathcal{L}_{\mathcal{I}}$ and the set of continua \mathcal{K} for which $L^* \subset \mathcal{K}$ will be denoted by $\mathcal{C}_{\mathcal{L}} = \mathcal{C}_{\mathcal{L}_{\mathcal{I}}}$.

In particular every \mathcal{L} such that the support L^* of $\Lambda_{\mathcal{L}}$ consists of finitely many connected sets is an admissible dislocation at the continuum scale. Remark that contrarily to mesoscopic dislocations (cf. Lemma 4.2 (b)), the density of a continuum dislocation must not be finite (this will happen for an unconstrained family of Burgers vectors).

Let $\mathcal{L}' \equiv \mathcal{L}$, where the symbol \equiv refers to the equivalence relation of Definition 3.20, then the support L^* of the density $\Lambda_{\mathcal{L}'}$ is a subset of $\mathcal{C}_{\mathcal{L}}$.

4.3 An equivalence result

In the applications, the notion of continuum dislocations is useful to study the cases in which Assumption 4.1 is not satisfied. Moreover, if one is not interested in the particular dislocation current associated to a given dislocation density, mesoscopic dislocations become a superfluous notion. In fact, crystallographic mesoscopic dislocations turn out to be equivalent to continuum dislocations, in the sense that, for any continuum dislocation \mathcal{L} , there is a mesoscopic dislocation \mathcal{L}' such that $\mathcal{L} \equiv \mathcal{L}'$. The proof of this fact is based on the following theorem

Theorem 4.5. *Let \mathcal{L} be a closed integer-multiplicity current with finite mass and whose support L^* is contained in a connected and compact set K with finite \mathcal{H}^1 -measure. Then there exists a Lipschitz function $\alpha : S^1 \rightarrow K$ such that $\mathcal{L} = \alpha_{\#} \llbracket S^1 \rrbracket$.*

To prove Theorem 4.5 we need some preliminary Lemmas:

Lemma 4.6. *Let K be a compact connected set in \mathbb{R}^n such that $\mathcal{H}^1(K) < \infty$. Then there exists a Lipschitz map $\psi : S^1 \rightarrow K$ that is onto and is homotopic to the constant map.*

Proof. In the following we consider S^1 as a subset of the complex plane \mathbb{C} . Let $P \in K$ and let us consider the set

$$\mathcal{S} := \{ \phi : S^1 \rightarrow K \text{ satisfying the following three properties} \} \quad (4.6)$$

- (i) $\phi(1) = P$.
- (ii) ϕ is homotopic to the constant map $\phi \equiv P$.
- (iii) Letting $C = \phi(S^1)$ and $L_C = \mathcal{H}^1(C)$, the curve ϕ is Lipschitz with constant $\frac{L_C}{\pi}$.

It is easily seen that, since K is a rectifiable set, \mathcal{S} is non-empty. Given a $\phi \in \mathcal{S}$ we want to enlarge its range in order to get an onto map. To this aim we define the following order relation in \mathcal{S} : we say that $\phi < \phi'$ if and only if $\phi(S^1) = C \subseteq C' = \phi'(S^1)$. Let $\{\phi_j\}_{j \in J \subset \mathbb{R}}$ be a chain in \mathcal{S} (assumed ordered by the corresponding ordering of the indices in \mathbb{R}), and set $L_j := \mathcal{H}^1(\phi_j(S^1))$. Then the sequence $\{L_j\}_{j \in J}$ is non-decreasing and bounded by $\mathcal{H}^1(K)$, so that, since the maps $\{\phi_j\}$ are uniformly continuous in j , there is an increasing sequence $j_k \rightarrow \sup J$ and a map ϕ such that $\phi_{j_k} \rightarrow \phi$ uniformly on S^1 . We claim that ϕ is an upper bound for $\{\phi_j\}_{j \in J}$. Indeed, denoting $C_j = \phi_j(S^1)$, the increasing sequence $\{C_j\}$ converges to a compact set $C \subseteq K$ with respect to the Gromov-Hausdorff distance. Since $j_k \rightarrow \sup J$ we see that for each $k \in J$ we have $C_k \subseteq C$, so that we only have to prove that ϕ belongs to the family \mathcal{S} . Setting $L := \mathcal{H}^1(C)$, we have $L \leq \mathcal{H}^1(K)$, and since $L_j \leq L$ the uniform convergence and the uniform bound $\text{Lip}(\phi_j) \leq \frac{L}{\pi}$ implies that $\text{Lip}(\phi) \leq \frac{L}{\pi}$. So (i) and (iii) are readily fulfilled. Also (ii) is easy to see: let Φ_j be the homotopy map between $\Phi_j(\cdot, 1) = \phi_j$ and the constant $\Phi_j(\cdot, 0) \equiv P$, and up to a rescaling, we suppose that for all $x \in S^1$ the map $\Phi_j(x, \cdot)$ is Lipschitz with $\text{Lip}(\Phi_j(x, \cdot)) \leq L$, so that it readily turns out that Φ_j are uniformly continuous in j , and uniformly converge to a map Φ ; now it is straightforward that Φ is a homotopy between ϕ and P , and the claim is proved.

We now are in the hypotheses of the Zorn's Lemma, so that we get a maximal element ψ for the class \mathcal{S} . It remains to show that ψ is onto. Suppose it is not the case. We set $C_\psi := \psi(S^1)$ and suppose $X \in K \setminus C_\psi$. Since C_ψ is closed and K is connected, there is a Lipschitz continuous arc $\alpha : [0, 1] \rightarrow K$ such that $\alpha(0) \in C_\psi$, $\alpha(1) = X$, and $\alpha(y) \in K \setminus C_\psi$ for $y > 0$. Let $x \in \psi^{-1}(\alpha(0))$, and split $S^1 = [1, x] \cup [x, 1]$. Consider the restriction of ψ to this two intervals, ψ_1 and ψ_2 . Then it is readily seen that the arc $\psi_1 \star \alpha \star \alpha^{-1} \star \psi_2$, if suitably rescaled as a function on S^1 , is a map in \mathcal{S} that is strictly greater than ψ , contradicting the maximality of ψ . Hence the thesis follows. \square

Lemma 4.7. *Let K be a compact 1-set and $\psi : S^1 \rightarrow K$ be a Lipschitz continuous map homotopic to a constant map. Then $\psi_{\#}[[S^1]] = 0$.*

Proof. Suppose for simplicity $K \subset \mathbb{R}^2$. Since K is compact, K^c is an open set, with only one unbounded connected component A . If $X \in B := K^c \setminus A$, there exists an open ball centered in X that does not intersect K , so that it follows that any connected component of B has positive Lebesgue measure. As a consequence there are at most countably many connected components in B . Let X_i be a point in the i -th connected component of B . The homotopic group of Lipschitz closed arcs in K coincides with the free group on the generators $\{X_i\}_{i \in \mathbb{N}}$.

Now, if the current carried by ψ is nonzero, the decomposition theorem implies that there exists $T = \alpha_{\#}[[S^1]]$ an undecomposable component of the 1-current $\psi_{\#}[[S^1]]$. If $X = \psi(a) = \psi(b)$, then, since ψ is homotopic to the constant, we can replace ψ with $\hat{\psi}$, setting $\hat{\psi}_{\perp}[a, b] \equiv X$ and $\hat{\psi}_{\perp}[a, b]^c = \psi$, getting a map that is still homotopic to the constant. Moreover the homotopy class of a loop in K does not change under homotopy in the space K , so that the operation above does not change the homotopy class of the current. In this way we find out that α must belong to the same homotopy class of ψ . On the other hand, since α is an injective loop, its homotopy class is $\prod_{X_j \in \Delta} X_j$, with Δ being the bounded connected set with boundary α . Thus the homotopy class of ψ is nonzero, contradicting the hypothesis that ψ was homotopic to a constant map. \square

Now we can prove Theorem (4.5).

Proof of Theorem 4.5. By the decomposition Theorem there are loops β_j such that $\mathcal{L} = \sum_j \beta_{j\#}[[S^1]]$. Consider a function ψ like in Lemma 4.6, so that there are points $x_j \in S^1$ such that $\psi(x_j) = \beta_j(1)$. Suppose for simplicity $x_1 = 1$ and x_j are clockwise ordered on S^1 . Setting $\psi_j := \psi_{\perp}[x_j, x_{j+1}]$, then the chain

$$\varphi := \beta_1 \star \psi_1 \star \beta_2 \star \psi_2 \star \dots \star \beta_j \star \psi_j \dots,$$

suitably rescaled, will match the required conditions, since ψ , being homotopic to the constant, is such that $\psi_{\#}[[S^1]] = 0$ from Lemma 4.7. \square

The precise equivalence theorem is stated as follows.

Theorem 4.8. *Let $\mathcal{L}_{\mathcal{I}}$ be a continuum dislocation such that $\mathcal{B}_{\mathcal{I}} \subset \mathcal{B}$ is countable and $\Lambda_{\mathcal{L}_{\mathcal{I}}}$ is finite. Then $\mathcal{L}_{\mathcal{I}}$ is a mesoscopic dislocation.*

Proof. Considering the canonical dislocation current $\hat{\mathcal{L}}$ equivalent to $\mathcal{L}_{\mathcal{I}}$ (cf. Eq. (3.18)), the thesis follows from Eq. (3.19) and Theorem 4.5. Indeed the latter provides three Lipschitz functions α_i ($i = 1, 2, 3$) such that $\alpha_{i\#}[[S^1]] = \mathcal{L}_i$ so it follows $\Lambda_{\mathcal{L}} = \sum_i \alpha_{i\#}[[S^1]] \otimes \underline{b}_i$. \square

In particular Theorem 4.8 tells us that continuum and mesoscopic dislocation are equivalent if the energy \mathcal{W} of the system does not depend on the particular dislocation current, but only on its dislocation density. We remark that the thesis does not hold true if we do not make the assumption that the set of Burgers vectors \mathcal{B} is crystallographic (i.e., isomorphic to \mathbb{Z}^3).

4.4 Boundary conditions for dislocations

Let U be a bounded open set such that $U \cap \partial\Omega = \partial_D\Omega$. In the sequel we will denote $\bar{\Omega}$ the interior of the set $\bar{U} \cup \bar{\Omega}$.

Definition 4.9 (Boundary conditions). *Let $\partial_D\Omega \subset \partial\Omega$. A boundary condition is a terne $(N, \mathcal{P}, \alpha_D)$ satisfying:*

- (i) $N \geq 0$ is a natural number.
- (ii) \mathcal{P} is a terne $(P_i, Q_i, \mathcal{B}_P)_{0 \leq i \leq N}$ with $\{P_i\}$ and $\{Q_i\}$ sequences of points in $\partial_D\Omega$, and $\mathcal{B}_P = \{b_{P_i}\}_{0 \leq i \leq N}$ a sequence of vectors belonging to \mathcal{B} . We associate to \mathcal{P} the 0-current $T_P := \sum_{0 \leq i \leq N} \delta_{P_i} - \delta_{Q_i}$, with δ_P , the Dirac mass at P .
- (iii) $\alpha_D := \alpha + \hat{\alpha}$ is the sum of two mesoscopic dislocation in \bar{U} . We suppose α is closed in \bar{U} with M loops α_i and Burgers vector b_{α}^i , while $\hat{\alpha}$ consists of the union of N dislocation loops $\hat{\alpha}_i$, such that for all i , $\hat{\alpha}_i$ has boundary $\partial\hat{\alpha}_i = \delta_{Q_i} - \delta_{P_i}$ and associate Burgers vector $b_{P_i} \in \mathcal{B}_D$.

From (iii) we can define $\Lambda_{\alpha_D} = \sum_{0 \leq i \leq M} \alpha_{b_{\alpha}^i} \otimes b_{\alpha}^i + \sum_{0 \leq i \leq N} \alpha_{b_{\hat{\alpha}_i}} \otimes b_{P_i}$ to be the density of the dislocation current α .

Definition 4.10. *We say that the boundary condition $(N_P, \mathcal{P}, \alpha_D)$ is admissible if the following conditions are satisfied: there exist an admissible dislocation \mathcal{L} and an admissible density $\Lambda_{\mathcal{L}}$ such that $\partial\mathcal{L} = T_P$ consisting of N currents $\mathcal{L}_i^{b_{P_i}}$ with boundary $\delta_{P_i} - \delta_{Q_i}$ and associated Burgers vector b_{P_i} , respectively.*

Finally we say that a dislocation \mathcal{L} satisfies the admissible boundary condition (N, \mathcal{P}, α) if it satisfies the property above. As a consequence of the previous definition, it turns out that $\alpha + \mathcal{L}$ is closed in $\bar{U} \cup \bar{\Omega}$.

5 Modeling discussion

So far, dislocations are mathematically represented by currents but it is crucial to keep in mind their physical origin and formation. A dislocation loop in the bulk results from nucleation, that is, the collapse of a void (i.e., a cavitation formed by aggregation of vacancies) which has become unstable. Another source of dislocations is the flux of vacancies or interstitials at the crystal boundary. In each case, the basic dislocation is a loop which is associated to a single Burgers vector that depends on the crystal structure. Submitted to thermal and mechanical forces, to diffusion, annihilation, recombination and any kind of mutual interactions, these loops might in turn deform and move inside the crystal and through its boundary, but also form clusters which themselves will either evolve or behave as fixed obstacle to the motion of other loops, provoking material hardening.

These considerations are at the basis of the notion of *regular dislocation* introduced above. According to the dislocation physics, the basic object will be the loops associated to a given Burgers vector b , i.e., the functions φ_j^b introduced in Definition 3.5. These simple *generator* loops will then be smoothly

deformed and summed (in the sense of currents) in order to form dislocation clusters. Moreover, it should be emphasized that the limited number of Burgers vectors of the generating loops might increase significantly as clusters are considered since Frank law applies at dislocation junctions [14]. For this reason, our restriction to finite families of regular loops associated to a finite number of distinct Burgers vectors (Assumption 4.1) does not preclude the formation of complex structures. As a consequence, a dislocation of this kind might be formed by countably regular loops connected by arcs which are effectless in terms of the intrinsic geometry of the crystal, and therefore referred to as *geometrically unnecessary* Ξ (Definition 3.10). Moreover, though being 1-sets, the clusters might exhibit complex geometries at the countable intersections or at the sets of accumulation points of their generating loops. It should nevertheless be precised that since overlapping of dislocations is not acceptable from a physical viewpoint, it should be equivalently understood as a non-overlapping curve associated to a scalar multiple of the Burgers vector.

Let us describe a pathological case which we must avoid at our scale of matter description. Consider a countable family of loops $L_{i \in \mathcal{I}}$ of lengths $l_{i \in \mathcal{I}}$, with $\sum_{i \in \mathcal{I}} \mathcal{H}^1(l_i)$ finite. If the set $L := \cup L_{i \in \mathcal{I}}$ turns out to be dense locally in Ω , then mesoscopicity assumption will be violated since for some points outside L there is no ball centered at them with empty intersection with L . For this reason we introduced the notion of *continuum dislocations* that corresponds to requiring that the set L will always have finite \mathcal{H}^1 measure.

Let us now describe a dislocation cluster which is not a mesoscopic dislocation. Consider the cluster of Fig. 4(c) but instead of assuming that each loop possesses the same Burgers vector b , suppose that the family $\mathcal{B}_{\mathcal{I}} \not\subseteq \mathcal{B}$ of Burgers vectors is non-crystallographic, that means that if $\mathcal{B}_{\mathcal{I}} = \{b_i\}_{i \in \mathbb{N}}$ then the ratios b_i/b_j is never rational for every $i \neq j$. Thus, it clearly appears that this cluster can not be made of regular dislocations without violating Assumption 4.1. Instead, it turns out that the broader notion of continuum dislocation holds for this kind of pathological cluster, as long as the sum of the length of the loops is finite. We emphasize that from a strictly mesoscopic standpoint allowing the Burgers vectors to take countably many values ($\mathcal{B}_{\mathcal{I}} \not\subseteq \mathcal{B}$ non-crystallographic) is not physical, all the more for bounded crystals. However it can become important to permit this limit case, for instance if one considers homogenization, or from a statistical viewpoint, ensemble averaging of dislocations.

If \mathcal{L} is a regular mesoscopic dislocation, the fact that $\mathcal{L} \in \mathcal{CD}$ does not imply that $\mathcal{H}^1(L) < \infty$, even if $\Lambda_{\mathcal{L}}$ is finite. Indeed *continuum dislocations* in \mathcal{CD} might be quite wild, since they can consist of countable fully disconnected loops and may admit geometrically unnecessary arcs which are locally dense, i.e., $\mathcal{H}^1(\bar{\Xi}) = \infty$. Moreover, since disconnected pieces of a dislocation can be connected by adding geometrically unnecessary arcs Ξ (cf. Fig 4), it might also happen that $\mathcal{H}^1(\Xi) = \infty$.

The introduction of continuum dislocations might be convenient for some other reasons. First, considering time-evolution of dislocations, this latter class, as opposed to the former, allows us to consider an evolution of the unnecessary part $\Xi(t)$ such that $\mathcal{H}^1(\Xi(t)) \rightarrow \infty$ (or $\mathcal{H}^1(\bar{\Xi}(t)) \rightarrow \infty$) as t converges to some limit time. Time-evolution of some subset of \mathcal{K} to a pathological Ξ is also possible within this setting, and it might be taken into account since unnecessary dislocations play an effective role in dynamics (as obstacle to motion, i.e.

hardening), whereas they do not contribute to the dislocation density. Second, continuum dislocations conceptually suits better engineer models of dislocations in which necessary and unnecessary dislocations are treated by distinct, though coupled, equations.

6 The class of admissible deformations

Recall that U be a bounded open set such that $U \cap \partial\Omega = \partial_D\Omega$ and $\hat{\Omega}$ is the interior of $\bar{U} \cup \hat{\Omega}$. Let us fix an admissible boundary condition $(N, \mathcal{P}, \alpha_D)$. In the sequel, whenever we consider an admissible dislocation \mathcal{L} , it is always supposed that such \mathcal{L} satisfies the boundary condition $(N, \mathcal{P}, \alpha_D)$, and hence it will be convenient to still denote the current $\mathcal{L}' := \mathcal{L} + \alpha$ by \mathcal{L} . In other words, when referring to an admissible dislocation current, it is intended that it has been already summed with α . We also fix a map $\bar{F} \in L^p(U, \mathbb{R}^{3 \times 3})$ such that $-\text{Curl } \bar{F} = (\Lambda_\alpha)^T$ on U .

Definition 6.1.

$$\mathcal{F} := \{(F, \mathcal{L}) \in L^p(\Omega, \mathbb{R}^{3 \times 3}) \times \mathcal{MD} : F \text{ satisfies (i)-(iii) below}\} \quad (6.1)$$

- (i) *The dislocation current $\mathcal{L} = \{L, \tau, \theta\}$ satisfies the boundary condition the function $\hat{F} := \chi_U \bar{F} + \chi_\Omega F \in L^p(\hat{\Omega}, \mathbb{R}^{3 \times 3})$ is such that $-\text{Curl } \hat{F} = (\Lambda_\mathcal{L})^T$ in $\hat{\Omega}$.*
- (ii) *We require that for every point $x \in \Omega \setminus L$ there is a ball $B \subset \Omega \setminus L$ containing x such that there exists a function $\phi \in \text{Cart}^p(B; \mathbb{R}^3)$ with $F = D\phi$ in B .*
- (iii) *$\det F > 0$ almost everywhere in Ω .*

We will show that there exists at least one element in \mathcal{F} with an admissible \mathcal{L} whose generating b -loops have a finite mutual intersection coinciding with α in $\partial\Omega_D$. In the following theorem, we will use the following identity:

$$-\text{Curl } F = b \otimes \tau \mathcal{H}^1 \llcorner L \quad \text{if and only if} \quad \int_{C_L} F \underline{e}_\theta d\mathcal{H}^1 = b. \quad (6.2)$$

for all Lipschitz-continuous closed path C_L in Ω enclosing once L and with unit tangent vector \underline{e}_θ . To check identity (6.2), simply observe that, if \tilde{S}_L is a smooth and closed surface in Ω with boundary L and normal n , $\Omega \setminus \tilde{S}_L$ is simply connected and hence there exists a function $\phi \in W^{1,p}(\Omega \setminus \tilde{S}_L)$ such that $F = \nabla\phi$ in $\Omega \setminus \tilde{S}_L$. By (6.2), ϕ has a constant jump on \tilde{S}_L (i.e., $[[\phi]]_{\tilde{S}_L} = b$). Thus the distributional derivative of ϕ writes as $D\phi = \nabla\phi + b \otimes n \mathcal{H}^2_{\llcorner \tilde{S}_L}$. Multiplying by a test function ψ one has by (2.1) that $\langle \text{Curl } (b \otimes n \mathcal{H}^2_{\llcorner \tilde{S}_L}), \psi \rangle = \langle b \otimes n \mathcal{H}^2_{\llcorner \tilde{S}_L}, \text{Curl } \psi \rangle$. Componentwise it reads by Stokes theorem as

$$\int_{\tilde{S}_L} n_i b_j \epsilon_{ikl} \partial_k \psi_{jl} d\mathcal{H}^2 = b_j \int_L \tau_p \psi_{jp} d\mathcal{H}^1,$$

and hence $\langle \text{Curl } (b \otimes n \mathcal{H}^2_{\llcorner \tilde{S}_L}), \psi \rangle = \langle (b \otimes \tau \mathcal{H}^1_{\llcorner L}), \psi \rangle$.

Theorem 6.2. *The set \mathcal{F} is non-empty for $1 \leq p < 2$.*

Proof. We first construct an admissible function for a simple geometry. Consider the circle $L := \{(x, y, z) \in \mathbb{R}^3 : |x|^2 + |y|^2 = R^2, z = 0\}$ as a dislocation loop with Burgers vector $b = \beta_1 \underline{e}_1 + \beta_2 \underline{e}_2 + \beta_3 \underline{e}_3 = \beta_R \underline{h}_R + \beta_l \underline{h}_l + \beta_z \underline{h}_z$, with the local basis on L , $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\} = Q(l)\{\underline{e}_1, \underline{e}_2, \underline{e}_3\}$ where $Q(l)$ is the matrix of rotation around $\underline{e}_3 = \underline{h}_z$ and with angle l (see Fig. 5(a)). Let V_δ be a tubular neighborhood of L with radius $\delta > 0$, and let $(r, \theta, l) \in [0, 2\delta] \times [0, 2\pi] \times [0, 2\pi R]$ be a system of cylindrical coordinates in V_δ chosen in the following way: the origin of θ is chosen in such a way that all points $(x, y, z) \in V_\delta$ with $z = 0$ and $|x|^2 + |y|^2 < R^2$ satisfy $\theta = a + \pi/4$ for some constant $a > 0$ which fix the orientation of the solid angle of amplitude $\pi/2$ constructed on L (cf. the black triangle on the box below right of Fig. 5(a) denoted as S or V in the sequel), while the coordinate r is the distance from the set L , and l , as before, R times the angle around z axis. In V_δ we denote by $\underline{g} := (\underline{g}_r, \underline{g}_\theta, \underline{g}_l)$, with $\underline{g}_l = \underline{h}_l$, the local cylindrical basis defined on the normal sections ∂V_δ , corresponding to such coordinates. We then consider the function F inside V_δ whose components in the basis $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\}$ read

$$F(r, \theta, l) = \zeta(\theta) \begin{pmatrix} -\frac{\sin \theta}{r} \beta_R & +\frac{\cos \theta}{r} \beta_R & 0 \\ -\frac{\sin \theta}{r} \beta_l & +\frac{\cos \theta}{r} \beta_l & 0 \\ -\frac{\sin \theta}{r} \beta_z & +\frac{\cos \theta}{r} \beta_z & 0 \end{pmatrix}, \quad (6.3)$$

where (r, θ, l) are the coordinates associated to the basis system \underline{g} , and ζ is a smooth function on $[0, 2\pi]$ which is non-negative in $(a, a + \pi/2)$, zero outside, and has integral equal to 1. It is readily checked that $\text{curl } F = 0$ in $V_\delta \setminus \gamma$. It is known that there exists a solution to equation $F = \nabla \phi_\delta$ in the simply connected domain $S := \{(r, \theta, l) : a < \theta < a + \pi/2, 0 < r < \delta\}$ with $0 \leq l \leq 2\pi$, and in order to fix the arbitrary constant, set $\phi_\delta = 0$ on $S \cap \{\theta = a\}$ and $\phi_\delta = b$ on $S \cap \{\theta = a + \pi/2\}$. Let V be the solid of revolution around the z -axis generated by S . Considering the axisymmetry we then extend ϕ_δ over the whole V and note that U is constant on the sets $C_{\bar{\theta}} := \{(\delta, \bar{\theta}, l) : 0 \leq l \leq 2\pi R\}$ for every $a < \bar{\theta} < a + \pi/2$. Let $D_{\bar{\theta}}$ be the disk with boundary $C_{\bar{\theta}}$ where for every $x \in D_{\bar{\theta}}$, $\phi_\delta(x)$ is defined as $\phi_\delta(x) = \phi_\delta(y)$ with $y \in C_{\bar{\theta}}$; define also $D := \bigcup_{\theta \in (a, a + \pi/2)} D_\theta$. We set $\phi_\delta = 0$ in $\Omega \setminus V \setminus D$ and observe that it is smooth everywhere except at the interface I between V and D and on $J := \bar{D}_{a + \pi/2} \cup (V \cap \{\theta = a + \pi/2\})$ where it has a constant jump of magnitude b (cf. Fig. 5(b) above). Therefore we introduce $\tilde{\phi}_\delta$, a C^∞ -regularization of ϕ_δ in a set $D \cap \mathcal{V}$, with \mathcal{V} a neighborhood of I , in such a way that $\|\nabla \tilde{\phi}_\delta\|_{L^\infty(D \cap \mathcal{V})} \leq 2\|\nabla \phi_\delta\|_{L^\infty(D \cap \mathcal{V})}$ and define $F := \nabla \tilde{\phi}_\delta$, the absolutely continuous part of the distributional gradient $D\tilde{\phi}_\delta$ (i.e., the pointwise gradient of $\tilde{\phi}_\delta$), while in the jump set J , the jump part of $D\tilde{\phi}_\delta$ reads $b \otimes \nu \mathcal{H}^2 \llcorner J$. Moreover, (6.2) and (6.3) together entail that $-\text{Curl } F = b \otimes \tau \mathcal{H}^1$ on L . As a consequence, we have constructed a function F which is smooth outside L and vanishes outside $T := V \cup D$, while from expression (6.3), $F \in L^p(\Omega)$ for $p \in [1, 2)$, since

$$\|F\|_{L^p(\Omega)}^p \leq C|b|(R\delta^{2-p} + \delta^{1-p}R^2), \quad (6.4)$$

for some positive constant C independent of R and δ . Moreover, by adding to F an appropriate multiple of the identity it is readily seen that $\det(F + cI) > 0$ for some $c > 0$, while $\det(F + cI)$, $\text{adj}(F + cI)$ also belong to $L^p(\Omega)$ for $p \in [1, 2)$.

Finally, fix a ball $B \subseteq \Omega \setminus L$: in such a ball the function F is smooth and has null rotation and hence there exists a $\phi \in C^\infty(B)$ such that $D\phi = F$. In

particular we can take $\phi = \tilde{\phi}_\delta$ when the ball does not intersect the jump set J , otherwise, if it does, we sum to $\tilde{\phi}_\delta$ the constant b at all points of B which are below J , thereby nullifying the discontinuity due to the jump. Thus ϕ is smooth, and hence, is a cartesian map.

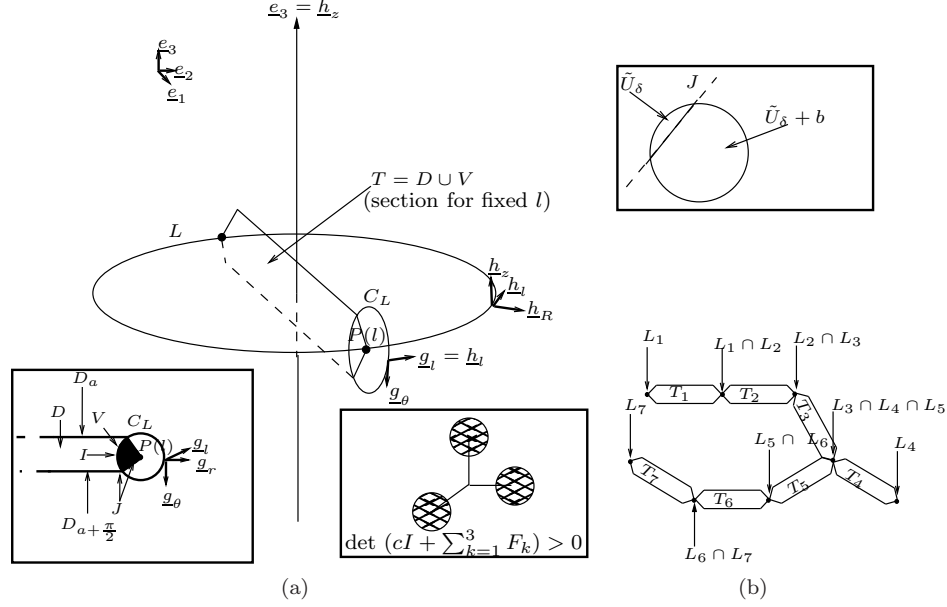


Figure 5: Picture of the tube construction for the proof (a); the case of finitely many boundary dislocation segments (b)

Let us now reproduce this argument for a finite number of circles with possible mutual intersection in $\partial\Omega$, and show that the constant $c > 0$ can be chosen in such a way that the determinant of the resulting deformation still remains non-negative. Let us consider a finite number of loops L_k with $1 \leq k \leq K$ with the associated $T_k := V_k \cup D_k$ constructed as described above, and observe that (by possibly adapting the amplitude of the solid angle S_k , i.e., replacing $\pi/2$ by π/N) the T_k 's only intersect at points in L_k for some k 's, while keeping the V_k 's with empty mutual intersection (cf. Fig 5(b) below left). Let F_k be defined as (6.3) with β_k in place of β and $a_k = \hat{a}_k(l)$ in place of a such that $f_k(\theta, l) := \beta_l^k(l) \cos \theta - \beta_R^k(l) \sin \theta = \beta_2^k \cos(\theta + \frac{l}{R}) - \beta_1^k \sin(\theta + \frac{l}{R}) \geq 0$ (for instance, if $\beta_1, \beta_2 > 0$ then $a_k := \frac{3\pi}{2} - \frac{l}{R}$). Defining $F := \sum_{k=1}^K F_k + cI$, (6.4) entails that $F, \det F, \text{adj} F$ belong to L^p and also that

$$\det F = \frac{c^2}{r} f_k(\theta, l) \zeta(\theta) + c^3 \geq 0 \quad \text{in } V_k, \quad (6.5)$$

while in D_k , one has $\det F > 0$ provided $c > 3 \max_k \{\|F_k\|_{L^\infty(D_k)}\}$ (cf. box below right in Fig. 5a).

Since the arguments presented above for a finite family of circular loops remain valid for a finite family of Lipschitz deformation of such loops, with appropriate Lipschitz deformations of the T_k s. In particular, it holds for the

boundary current α and for any finite family of curves joining P_i 's to the Q_i 's without self-intersections and prolonged by a geometrically unnecessary arc in $\partial\Omega$ (an admissible F can be constructed as above in $\hat{\Omega} \supset \Omega$ and then restricted to Ω with its curl restricted to $\hat{\Omega}$). Thus the proof is achieved. \square

7 Existence of minimizers

Let us recall that U is a bounded open set such that $U \cap \partial\Omega = \partial_D\Omega$, $\hat{\Omega} := U \cup \Omega$. We propose two models in which the energy does not depend on the particular currents generating the dislocations but only on the density. However, we remark that in general, energies depending on the loops per se may also be considered (this was considered beyond the scope of this paper). In the first existence result the model variables are the deformation and the family of mesoscopic dislocations. In the second existence result, the model variable is the sole deformation, while the dislocations are sought at the continuum scale and hence are only found in an equivalence class.

7.1 Existence result in $\mathcal{F} \times \mathcal{MD}$

We are given a potential $\mathcal{W} : \mathcal{F} \times \mathcal{MD} \rightarrow \bar{\mathbb{R}}$ such that there are positive constants C and β for which

$$\begin{aligned} \mathcal{W}(F, \Lambda_{\mathcal{L}}) := & \int_{\Omega} W_e(F) dx + W_{\text{defect}}(\Lambda_{\mathcal{L}}) \geq \\ & C(\|\mathcal{M}(F)\|_{L^p} + \sum_{j \leq k_{\mathcal{L}}} b^j \|\dot{\varphi}_j\|_{L^1} + k_{\mathcal{L}}) - \beta, \end{aligned} \quad (7.1)$$

where we recall that $k_{\mathcal{L}}$ is defined in (4.1), and $\{\varphi_j\}_{j \leq k_{\mathcal{L}}}$ are the generating loops defined in 3.4. Here, W_e is an integrable function and W_{defect} a functional defined on Radon measures. It is also assumed that

- (W1) $W_e(F) \geq h(\det F)$, for a continuous real function h such that $h(t) \rightarrow \infty$ as $t \rightarrow 0$,
- (W2) W_e is polyconvex, i.e., there exists a convex function $g : \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \times \mathbb{R}^+ \rightarrow \bar{\mathbb{R}}$ s.t. $W_e(F) = g(\mathcal{M}(F))$, $\forall F \in \mathcal{F}$,
- (W3) $W_{\text{defect}}(\Lambda_{\mathcal{L}}) \geq \kappa_1 k_{\mathcal{L}} + \kappa_2 \sum_{1 \leq j \leq k_{\mathcal{L}}} b^j \|\dot{\varphi}_j\|_{L^1}$ convex, for some constitutive material parameters κ_1 and κ_2 .
- (W4) g and W_{defect} are weakly lower semicontinuous, i.e., $\liminf_{k \rightarrow \infty} g(\mathcal{M}(F^k)) \geq W_e(F)$ as $\mathcal{M}(F^k) \rightarrow \mathcal{M}(F)$ weakly in $L^p(\Omega, \mathbb{R}^{3 \times 3}) \times L^p(\Omega, \mathbb{R}^{3 \times 3}) \times L^p(\Omega)$ and $\liminf_{k \rightarrow \infty} W_{\text{defect}}(\Lambda^k) \geq W_{\text{defect}}(\Lambda)$ as $\Lambda^k \rightharpoonup \Lambda$ weakly* in $\mathcal{M}(\hat{\Omega}, \mathbb{R}^{3 \times 3})$.

Remark 7.1. *The term involving $\|\dot{\varphi}_j\|_{L^1}$ in the energy bound is mandatory for mesoscopic dislocations, since it controls the length of the lines. In fact, minimizing sequences of Lipschitz maps (describing minimizing sequences of lines) might become locally dense, a phenomenon which should be prohibited to*

get existence. For a physical viewpoint this term is questionable since dense arcs of the dislocation cluster might be nonnecessary, and hence admissible from an energetical standpoint. This drawback is addressed in the second existence result for continuum dislocations in Section 7.2. Moreover, recalling (4.2), this term implies a bound on the densities.

Remark 7.2. The semicontinuity required in (W6) might only hold for the relaxation of W_{defect} , see [8].

Before stating the existence of minimizers of the problem

$$\inf_{\substack{(F, \Lambda_{\mathcal{L}}) \in \mathcal{F} \times \mathcal{MD} \\ -\text{Curl } F = \Lambda_{\mathcal{L}}^T}} \mathcal{W}(F, \Lambda_{\mathcal{L}}), \quad (7.2)$$

some technical results should be stated and proven.

Lemma 7.3. Let (F_k, \mathcal{L}_k) be a minimizing sequence for the problem (7.2), and suppose $\det F_k \rightharpoonup D$ in $L^p(\Omega)$. Then $D > 0$ a.e. in Ω .

Proof. Let $A := \{D = 0\}$ and suppose A has positive Lebesgue measure. We have $\det F_k \rightharpoonup 0$ in $L^1(A)$, which since $\det F_k \geq 0$ on A is equivalent to $\det F_k \rightarrow 0$ in $L^1(A)$ and hence, up to a subsequence, almost everywhere in A . So from condition (W1) we must have $\mathcal{W}(F_k, \Lambda_{\mathcal{L}_k}) \geq \int_A W(F_k, \Lambda_{\mathcal{L}_k}) dx \geq \int_A h(\det F_k) dx$. By Fatou's lemma and the fact that (F_k, \mathcal{L}_k) is a minimizing sequence, the contradiction follows, and hence A must be negligible, achieving the proof. \square

Lemma 7.4. Let γ_n be a sequence of 1-currents inside $\bar{\Omega}$ such that $\gamma_n = \varphi_{n\sharp} \llbracket [0, M] \rrbracket$ for Lipschitz functions φ_n with $\text{Lip}(\varphi_n) \leq 1$ for all n . Then, there is 1-current γ such that, up to subsequence, $\gamma_n \rightharpoonup \gamma$, and $\gamma = \varphi_{\sharp} \llbracket [0, M] \rrbracket$ for a Lipschitz function φ with $\text{Lip}(\varphi) \leq 1$.

Proof. The functions φ_n are equibounded and equicontinuous on $[0, M]$, and by the Ascoli-Arzelà Theorem there is a map $\varphi : [0, M] \rightarrow \mathbb{R}^3$ with $\text{Lip}(\varphi) \leq 1$ such that, up to subsequence, $\varphi_n \rightarrow \varphi$ uniformly. So it easily follows that $\gamma_n \rightharpoonup \gamma := \varphi_{\sharp} \llbracket [0, M] \rrbracket$, and the proof is complete. \square

Lemma 7.5. Let $\mathcal{L}_n = \{S_n, \tau_n, \theta_n\}$ be a sequence of dislocation currents of the form (3.18) all satisfying the same boundary condition. Assume that the sequence \mathcal{L}_n weakly converges to an integer multiplicity current \mathcal{L} and that $\Lambda_n := \Lambda_{\mathcal{L}_n}$, the sequence of density of \mathcal{L}_n , weakly* converges to $\Lambda \in \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3})$. Then \mathcal{L} satisfies the boundary condition and has density equal to $\Lambda = \Lambda_{\mathcal{L}}$.

Proof. As in (3.18) we write $\mathcal{L}_n = \mathcal{L}_n^1 + \mathcal{L}_n^2 + \mathcal{L}_n^3$, and $\Lambda_n = \Lambda_n^1 + \Lambda_n^2 + \Lambda_n^3$, with, using notation (3.9), $\Lambda_n^i = \mathcal{L}_n \otimes \underline{b}_i$. Let $w = (w_1, w_2, w_3)$ be a smooth vector field in Ω and let ω be the smooth 1-form given by $\omega := \sum_{j=1}^3 w_j dx_j$. By the assumption of the preceding section we have that also \mathcal{L}_n^j are boundaryless in Ω and thanks to inequalities (3.22) and (3.19), we have that $N(\mathcal{L}_n^j)$ are uniformly bounded, so that by Theorem 2.1 we deduce the existence of three integer multiplicity currents $\{\mathcal{L}^j\}_{j=1}^3$ such that $\mathcal{L}_n^j \rightharpoonup \mathcal{L}^j$. Since

$$\langle \mathcal{L}_n, \omega \rangle \rightarrow \langle \mathcal{L}, \omega \rangle, \quad \text{and at the same time} \quad (7.3)$$

$$\langle \mathcal{L}_n, \omega \rangle = \langle \sum_{j=1}^3 \mathcal{L}_n^j, \omega \rangle \rightarrow \langle \sum_{j=1}^3 \mathcal{L}^j, \omega \rangle, \quad (7.4)$$

we get $\mathcal{L} = \sum_{j=1}^3 \mathcal{L}^j$. The fact that \mathcal{L} satisfies the boundary condition follows from the fact that $\partial \mathcal{L}_n \rightharpoonup \partial \mathcal{L}$. A similar argument shows that $\Lambda = \Lambda^1 + \Lambda^2 + \Lambda^3$, where $\Lambda^i \in \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3})$ such that $\Lambda_n^i \rightharpoonup \Lambda^i$ weakly*. Now for $i = 1, 2, 3$, it holds

$$\langle \Lambda_n^j, w \otimes e_i \rangle = \langle \mathcal{L}^j \otimes \underline{b}_i, w \otimes e_i \rangle = (\underline{b}_j \cdot e_i) \langle \mathcal{L}_n^j, w \rangle \rightarrow \bar{b}_j \delta_{ij} \langle \mathcal{L}^j, w \rangle.$$

Since the left-hand side of the last expression tends to $\langle \Lambda^j, w \otimes e_i \rangle$, thanks to the fact that $\{w \otimes e_i\}_{1 \leq i \leq 3, w \in C_c^\infty}$ is a basis for the space $C_c^\infty(\Omega, \mathbb{R}^{3 \times 3})$, we also get $\Lambda^i = \mathcal{L}^i \otimes \bar{b}_i$ for $i = 1, 2, 3$, and the thesis follows. \square

Now we are ready to solve Problem (7.2).

Theorem 7.6 (Existence in $\mathcal{F} \times \mathcal{MD}$). *Under assumptions (W1) – (W5) and assuming that there exists an admissible $(F, \mathcal{L}) \in \mathcal{F} \times \mathcal{MD}$ such that $\mathcal{W}(F, \Lambda_{\mathcal{L}}) < \infty$, there is at least a (F, \mathcal{L}) solution of the minimum problem (7.2).*

Proof. Let (F_n, \mathcal{L}_n) be a minimizing sequence in \mathcal{F} . Then $\|F_n\|_{L^p}$, $\|\text{adj} F_n\|_{L^p}$, $\|\det F_n\|_{L^p}$ are uniformly bounded, so that there exist F , $A \in L^p(\Omega, \mathbb{R}^{3 \times 3})$, $D \in L^p(\Omega)$ such that

$$F_n \rightharpoonup F \quad \text{weakly in } L^p(\Omega, \mathbb{R}^{3 \times 3}), \quad (7.5a)$$

$$\text{adj } F_n \rightharpoonup A \quad \text{weakly in } L^p(\Omega, \mathbb{R}^{3 \times 3}), \quad (7.5b)$$

$$\det F_n \rightharpoonup D \quad \text{weakly in } L^p(\Omega). \quad (7.5c)$$

Since we consider extensions \hat{F}_n of F on $\hat{\Omega}$, it is straightforward that we can suppose the same boundedness for \hat{F}_n on $\hat{\Omega}$ as for F_n on Ω , so that \hat{F} , \hat{A} , and \hat{D} are such that (7.5a)-(7.5c) hold for \hat{F}_n , \hat{F} , \hat{A} , and \hat{D} .

Moreover, by the uniform bound on $\sum_{j \leq k_{\mathcal{L}}} b^j \|\varphi_j\|_{L^1}$ in (7.1) and by (4.2), it holds a uniform bound on $\Lambda_n := \text{Curl } \hat{F}_n$, and in the limit a measure $\Lambda \in \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3})$ such that

$$\Lambda_n \rightharpoonup \Lambda \quad \text{weakly* in } \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3}). \quad (7.5d)$$

The result will follow by the direct method of the calculus of variations and classical semicontinuity results for convex functionals, since conditions (W1) – (W5) hold. It remains to check admissibility of the minimizer.

Since their length is uniformly bounded by (7.1), we can suppose that the dislocation currents \mathcal{L}_n are generated by the same number k of 1-Lipschitz functions $\{\varphi_n^j\}_{j=1}^k$, i.e.,

$$\mathcal{L}_n = \sum_{j=1}^k \varphi_n^j \llbracket [0, M] \rrbracket \quad \text{and} \quad \Lambda_n = \sum_{j=1}^k \varphi_n^j \llbracket [0, M] \rrbracket \otimes b^j. \quad (7.6)$$

So by Lemma 7.4 we can suppose that for every j we have

$$\varphi_n^j \llbracket [0, M] \rrbracket \rightharpoonup \varphi^j \llbracket [0, M] \rrbracket,$$

for some 1-Lipschitz functions $\{\varphi^j\}_{j=1}^k$. If we set $\mathcal{L} := \sum_j \varphi^j \llbracket [0, M] \rrbracket$ we then also have $\mathcal{L}_n \rightharpoonup \mathcal{L}$ and, by Lemma 7.5, $\Lambda_n \rightharpoonup \sum_j \varphi^j \llbracket [0, M] \rrbracket \otimes b^j$ weakly* in $\mathcal{M}(\bar{\Omega}, \mathbb{R}^{3 \times 3})$, so from (7.5d) we get

$$\Lambda = \sum_j \varphi^j \llbracket [0, M] \rrbracket \otimes b^j. \quad (7.7)$$

Writing, for a test function $w \in C_c^\infty(\mathbb{R}^3, \mathbb{R}^{3 \times 3})$,

$$\langle \text{Curl } \hat{F}_n, w \rangle = -\langle \hat{F}_n, \text{Curl } w \rangle \rightarrow -\langle \hat{F}, \text{Curl } w \rangle = \langle \text{Curl } \hat{F}, w \rangle. \quad (7.8)$$

Since the first term in the left-hand side of (7.8) also tends to $\langle -\Lambda^T, w \rangle$, we finally get

$$-\text{Curl } \hat{F} = \sum_j b^j \otimes \varphi_{\#}^j[[0, M]]. \quad (7.9)$$

Let us set $L_n := \cup_{j=1}^k \varphi_n^j([0, M])$ and $L := \cup_{j=1}^k \varphi^j([0, M])$. We now want to show that for every point $x \in \Omega \setminus L$ there is a ball $B \subset \Omega \setminus L$ containing x and a map $u \in \text{Cart}^p(B, \mathbb{R}^n)$ such that $Du = F$ in B . Let x be such a point, since $\varphi_n^j \rightarrow \varphi^j$ uniformly, it follows that L_n tends to L in the Gromov-Hausdorff topology, so that we have $B \cap L_n = \emptyset$ for n sufficiently large. In such a ball, by hypotheses, there are maps $u_n \in \text{Cart}^p(B, \mathbb{R}^n)$ satisfying $Du_n = F_n$, and, up to summing suitable constants to u_n , we can also suppose u_n have all zero average in B . So that the Poincaré's inequality provides u such that $u_n \rightharpoonup u$ weakly in $W^{1,p}$. Now the thesis follows from Theorem 2.5, (7.5a)-(7.5c), and Lemma 7.3. \square

We remark that with the formulation (7.1) the potential $W(F, \Lambda_{\mathcal{L}})$ depends explicitly on the dislocation density. Yet it is beyond the scope of this paper to discuss the nature and the possible expressions of the defect energy.

7.2 Second existence result

We now prove an existence result with \mathcal{W} a function of F only, and where the dislocations associated to the optimal F are *geometrically equivalent* to a 1-set. This means that the dislocation itself can be locally dense and of infinite length. We redefine the set of admissible functions:

$$\mathcal{F}' := \{F \in L^p(\Omega, \mathbb{R}^{3 \times 3}) : F \text{ satisfies (i)-(iii) below}\} \quad (7.10)$$

- (i) There exists a continuum dislocation $\mathcal{L} := \mathcal{L}_{\mathcal{I}} \in \mathcal{CD}$ satisfying the boundary condition and there exists $\hat{F} \in L^p(\hat{\Omega}, \mathbb{R}^{3 \times 3})$ with $\hat{F} \llcorner \Omega = F$ such that $-\text{Curl } \hat{F} = (\Lambda_{\mathcal{L}})^T$ in $\hat{\Omega}$.
- (ii) There is a continuum \mathcal{C} such that $L^* \subset \mathcal{C}$ and such that for every $x \in \Omega \setminus \mathcal{C}$ there is a ball $B \subset \Omega \setminus \mathcal{C}$ centered at x and a function $\phi \in \text{Cart}^p(B; \mathbb{R}^3)$ satisfying $F = D\phi$ in B .
- (iii) $\det F > 0$ almost everywhere in Ω .

We consider a slightly different set of assumptions on $\mathcal{W} : \mathcal{F}' \rightarrow \bar{\mathbb{R}}$:

- (W5) there is a positive constant C such that $\mathcal{W}(F) \geq C(\|\mathcal{M}(F)\|_{L^p} + \|\text{Curl } \hat{F}\|_{\mathcal{M}(\hat{\Omega})} + G(\mathcal{L})) - \beta$, with

$$G(\mathcal{L}) := \inf_{\mathcal{K} \in \mathcal{C}_{\mathcal{L}}} (\mathcal{H}^1(\mathcal{K}) + \kappa \#\mathcal{K}), \quad (7.11)$$

where $\#\mathcal{K}$ represents the number of connected components of the embedding continuum \mathcal{K} . Note that by Golab theorem G is also lower semi-continuous.

(W6) there exists a convex and weakly lower semicontinuous function g and a weakly lower semicontinuous functional W_{defect} s.t. $\mathcal{W}(F) = \int_{\Omega} g(\mathcal{M}(DF)) dx + W_{\text{defect}}(-(\text{Curl } \hat{F})^T)$. It is also assumed that $g(\mathcal{M}(DF)) \geq h(\det F)$, for some continuous real function h such that $h(t) \rightarrow \infty$ as $t \rightarrow 0$.

Since \mathcal{F}' is not empty, we now solve the minimum problem with these new assumptions.

Theorem 7.7 (Existence in \mathcal{F}'). *Under assumption (W5) and (W6) and assuming that there exists an admissible $F \in \mathcal{F}'$ such that $\mathcal{W} := \int_{\Omega} W(F) < \infty$, there exists a minimizer of problem $\inf_{\mathcal{F}'} \mathcal{W}$.*

Proof. Let F_n be a minimizing sequence in \mathcal{F}' . We denote the dislocation currents associated to F_n by \mathcal{L}_n , and their densities by $\Lambda_n = \Lambda_{\mathcal{L}_n}$. By (W6), F_n converges weakly to F in L^p and Λ_n converges weakly- \star to a Radon measure Λ . Consider the same extensions \hat{F}_n, \hat{F} as in the proof of Theorem 7.6. By (3.18), we can take $\hat{\mathcal{L}}_n \equiv \mathcal{L}_n$ satisfying $\Lambda_n = \Lambda_{\hat{\mathcal{L}}_n}$ and thanks to (3.19) $\{\hat{\mathcal{L}}_n\}$ is equibounded, so that one has by Theorem 2.1 the existence of an integer multiplicity current $\hat{\mathcal{L}}$ such that $\hat{\mathcal{L}}_n \rightarrow \hat{\mathcal{L}}$, while by Lemma 7.5, $\Lambda = \Lambda_{\hat{\mathcal{L}}} = -\text{Curl } \hat{F}$ in the distribution sense. Moreover, by admissibility, one can associate to every \mathcal{L}_n and hence to every $\hat{\mathcal{L}}_n$ a continuum \mathcal{K}_n such that $G(\mathcal{L}_n) = (\mathcal{H}^1(\mathcal{K}_n) + k(\mathcal{K}_n))$. By (W5), Blaschke and Golab theorems, there is convergence in the Gromov-Hausdorff sense to a continuum \mathcal{K} . Moreover, $\hat{\mathcal{L}} = (\hat{L}, \tau, \theta)$ is admissible since $L^* := \text{supp } \Lambda \subset \mathcal{K}$ and $\hat{\mathcal{L}} \equiv \hat{\mathcal{L}}^* := (L^*, \tau, \theta)$. Since $\mathcal{K} = \text{argmin}_{\mathcal{C}_{\hat{\mathcal{L}}}} G$ admits a tangent vector almost everywhere and letting $\theta = 0$ on $\mathcal{K} \setminus L^*$, it is readily seen that $(\mathcal{K}, \tau, \theta) \equiv \hat{\mathcal{L}}$. Taking any ball in $\Omega \setminus \mathcal{K}$, we conclude as in the proof of Theorem 7.6. \square

The physical interpretation of $G(\mathcal{L})$ is the following. To create a new loop at some finite distance d from the current dislocation \mathcal{L} , it is worth to nucleate (i.e., add a connected component) rather than deforming the existent dislocation, as soon as $d > \kappa$. However it should be recognized that (7.11) is at this stage a mathematical assumption whose physical meaning remains to be elucidated. It basically means that the continuum dislocation lies in a compact 1-set which keeps as minimal the balance between the number of its connected subsets (of the continuum, not of the dislocation cluster) and its length.

7.3 An example

Let $\Omega \subset \mathbb{R}^3$ be the open set defined, in cylindrical coordinates, by

$$\Omega := \{0 < \rho < R, z \in (-h, h)\}.$$

Let Ω_{ϵ} be a ϵ -neighborhood of Ω and set $U := \Omega_{\epsilon} \setminus \Omega$.

With this example we would like to show that provided a boundary condition for the dislocation density, the dislocation of the minimizers will not be in U but will stay inside Ω .

Then we consider the map $\bar{F} : U \rightarrow \mathbb{R}^{3 \times 3}$ defined as

$$\bar{F}(\rho, \theta, z) = \zeta(\theta) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{\sin \theta}{\rho} \beta & \frac{\cos \theta}{\rho} \beta & 1 \end{pmatrix}, \quad (7.12)$$

so that it turns out that

$$-\text{Curl } \bar{F} = b \otimes e_z \mathcal{H}^1 \llcorner_{\hat{z} \cap U},$$

that is \bar{F} shows a screw dislocation on the z -axis \hat{z} with Burgers vector $b = (0, 0, \beta)$. We want to minimize the energy (7.1) satisfying (W1)-(W4)

$$\mathcal{W}(F, \Lambda_{\mathcal{L}}) := \int_{\Omega} W_e(F) dx + W_{\text{defect}}(\Lambda_{\mathcal{L}}),$$

among all the deformations F belonging to the class (6.1) with \bar{F} as boundary condition. Let us suppose that the defect part of the energy takes the form

$$W_{\text{defect}}(\Lambda_{\mathcal{L}}) = \gamma \int_0^1 \|\dot{\varphi}(s)\| ds + \sum_{i < k} \gamma \int_{S^1} \|\dot{\varphi}_i(s)\| ds + \mu |\Lambda_{\mathcal{L}}(\Omega)|, \quad (7.13)$$

where the mesoscopic dislocation \mathcal{L} is the image of $k - 1$ closed loops φ_i with Burgers vector b_i and of φ which is a dislocation with endpoints $P := (0, 0, h)$ and $Q := (0, 0, -h)$ and Burgers vector b . Then let us consider an admissible deformation which shows only one dislocation path φ^0 coinciding with the segment \overline{PQ} . In this case $k = 1$ and the energy is

$$\begin{aligned} \mathcal{W}(F^0) &= \int_{\Omega} W_e(F^0) dx + \gamma \int_0^1 \|\dot{\varphi}^0(s)\| ds + \mu |\Lambda_{\mathcal{L}^0}(\Omega)| = \\ &= \int_{\Omega} W_e(F^0) dx + 2h\gamma + 2h\mu\beta. \end{aligned} \quad (7.14)$$

Let us now take another admissible deformation F^1 which has the dislocation path φ^1 connecting P and Q which has an intermediate point at $\varphi(t) = (x_t, y_t, z_t) \in \Omega$ with $R_t := (x_t^2 + y_t^2)^{1/2} > 0$. In this case we have

$$\begin{aligned} W_{\text{defect}}(\mathcal{L}^1) &\geq \gamma \int_0^1 \|\dot{\varphi}^1(s)\| ds + \mu |\Lambda_{\mathcal{L}^1}(\Omega)| \\ &\geq 2\gamma(R_t^2 + h^2)^{1/2} + 2h\mu\beta, \end{aligned} \quad (7.15)$$

so that, if $2\gamma(R_t^2 + h^2)^{1/2} > \int_{\Omega} W_e(F^0) dx + 2h\gamma$ it turns out that $\mathcal{W}(F^0) < \mathcal{W}(F^1)$. This may happen if

$$R > R_t > \bar{R} := \frac{1}{2\gamma} \left(\left(\int_{\Omega} W_e(F^0) dx + 2h\gamma \right)^2 - h^2 \right)^{1/2}$$

so that in this case we see that the minimizer of the energy must have the dislocation path connecting P and Q inside the cylinder $\{x^2 + y^2 < \bar{R}, z \in (-h, h)\} \subsetneq \Omega$. In the contrary, if $R < \bar{R}$ then the dislocation of the minimizer could lie outside Ω . In particular we see that with our choice of boundary datum dislocations tends to remain inside the body Ω and not to escape from the boundary.

8 Concluding remarks

In this paper we have shown that the theory of currents is rather well suited to describe elastic deformations induced by the presence of dislocation loops and

clusters. Let us emphasize that dislocations in *single* crystals can form complex structures since there are no internal boundaries known to be preferential regions of concentration. After a detailed description of the dislocations as currents, a variational problem is studied with two optimization variables, namely the deformation gradient F and the dislocation density Λ , together bound by relation $-\text{Curl } F = \Lambda^T$. The data is here the boundary dislocation density, while deformation boundary conditions could have also been prescribed within this framework.

Two approaches coexist in this paper. On the one hand there is the theory of integer-multiplicity 1-currents which is a sharp tool to describe a single dislocation together with complex geometries such as dislocation clusters, including their possible evolution in time. Thus it would allow one to model mesoscopic plasticity, which is due to the motion of dislocations and their mutual interaction. On the other hand there is a variational setting where the model variables are *deformation* internal variable F and the *defect* internal variable Λ . From this point of view the individuality of the lines is replaced by a measure and hence all geometrically unnecessary dislocation are effectless in the model. These two approaches are connected since the mass of a current is finite as soon as the density is bounded, at least as long as the Burgers vectors are crystallographic, that is, when canonical dislocation are chosen to represent dislocation currents.

Since Cartesian maps are considered to represent the deformation F , its adjunct and determinant are only locally defined away from a continuum, that is $\text{Cof}F = \text{cof}F \in L^p_{loc}(\Omega \setminus \mathcal{K})$ and $\text{Det}F = \det F \in L^p_{loc}(\Omega \setminus \mathcal{K})$. Moreover, the fact that the adjunct and the determinant might be concentrated *distributions* on \mathcal{K} means that the continuum (thus not only the support of the density but also the geometrically unnecessary parts) represents a singular set where spurious effects might take place, such as cavitation, and hence nucleation of elementary dislocation loops. This makes sense from a physical standpoint, since dislocations at the mesoscale are by essence the location of field singularities. From a mathematical point of view it is due to the fact that the currents of the minimizing sequence might have a dense limit, though of bounded length, whereas this pathological behaviour is precluded by the presence of the embedding continuum.

It is yet an open question to elucidate the structure of the distributional determinant, which one would like for physical reasons to be a Radon measure (i.e., an extensive field) on \mathcal{K} . To the knowledge of the authors few results exist about this issue, without the too restrictive assumptions of field boundedness, high space dimension and with the current range of p between 1 and 2.

The described mathematical framework will be considered for future work in order to describe evolution problems involving the dissipation due to dislocation motion. Here a preliminary step before the complete dynamics will be the quasi-static problem, that is, dynamics under the assumption that optimality (i.e., global minimization) is reached within any time step. The role of higher-order strains acting as constrain reactions to the geometrical condition $-\text{Curl } F = \Lambda^T$ will also be studied in forthcoming publications.

Two other extensions of this work are the analysis of the distributional determinant at the continuum \mathcal{K} , in particular to address the open question wether it is a measure, and homogenization of a countable family to the continuum

to the macroscale where Γ -convergence tools may be considered (see, eg., [9]). About the latter problem let us mention that our setting at the continuum scale, allowing for countable many dislocations was thought with a view to homogenization, since limit passage from finite to countable families must unavoidably be faced.

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