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 cannot be written as the gradient of a one-to-one immersion, and hence that no displacement field can properly be defined as model variable. In fact, the deformation curl equals to the density of dislocations which is a concentrated Radon measure in the dislocation lines. In this paper we consider a countable family of dislocations, discuss the mathematical properties of such constraint deformations and study a variational problem in finite-strain elasticity. It turns out that both the deformation and the dislocation lines may be modelled by means of the mathematical theory of currents. In particular, *Cartesian maps* allow one to consider deformations in L^p with $1 \leq p < 2$, which are appropriate for dislocation-induced strain singularities. Moreover, *integer-multiplicity currents* are perfectly suited to describe either the static or the dynamics of families of dislocations which mutually interact, and possibly form complex structures such as clusters. Though the evolution of dislocations is not considered in this paper, it is the main motivation of our approach. As a matter of fact, this work describes a conservative ground state where dislocations are assumed to obey energy minimization principles, and over which any relevant effect resorting to thermodynamics outside equilibrium might be added in a subsequent step within the proposed mathematical formalism.

Keywords: Cartesian maps, integer-valued currents, dislocations, finite elasticity, minimization

Contents

1 Introduction

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 [13], 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 [16]. 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 constraint motion of dislocation of predefined glide planes only holds for moderate temperature ranges. Overlooking on purpose the specific inter-dislocation dynamics [18,25,29] 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 geometricaly unified way together and accordingly with any single dislocation loop.

Another intrisic difficulty of mesoscopic dislocations is that there is no unambiguous definiton 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 [27,28]. 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 $\phi : \Omega \to \mathbb{R}^3$ such that $\phi(\Omega) = \Omega(t)$ if and only if the Riemannian curvature tensor asssociated to C vanishes identically in $\Omega(t)$ [6]. Let us emphasize that the Riemannian curvature is the finite-elasticity counterpart of the aforementioned incompatibility tensor. By eigendecomposition one has $C = F^TF$ 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 [15, 24, 26], and the same property holds in finite elasticity. The dislocations which generate curvature are called *geometrically necessary* [19,21] and will be given a precise mathematical meaning in this paper, together with their companion *geometrically unnecessary* (called "statistically stored" in the engineering litterature) 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 unconfortable 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 $\mathcal{L}$ and any dividing surface $S_{\mathcal{L}}$ containing $\mathcal{L}$. The set $\Omega(t) \setminus \mathcal{L}$ is not simply connected, but the upper and lower partition of $\Omega(t)$, $\Omega^+(t)$ and $\Omega^-(t)$ divided by $S_{\mathcal{L}}$, are simply connected and in each it holds $\text{inc}\,\mathcal{E} = 0$. Thus there exists a linear-elasticity displacement field $u_{S_{\mathcal{L}}} = u^{\pm}_{S_{\mathcal{L}}}$ such that $\mathcal{E} = \nabla^S u_{S_{\mathcal{L}}}$ in $\Omega^{\pm}(t)$. For any smooth one-to-one φ, the map $\phi^{-1} := \varphi \circ (\text{Id} - u_{S_{\mathcal{L}}})$ defines any reference configuration. It turns out that in the presence of a dislocation there is a mismatch in the reference configuration which we describe at follows. Let $\Omega^{\pm} := \phi^{-1}(\Omega^{\pm}(t))$ define the lower and upper parts of a reference configuration while $F = F^{\pm} = \nabla\phi$ are the associated deformation gradients. Now take two curves $\alpha^{\pm}$ in $\Omega^{\pm}(t)$ with endpoints P and Q, respectively outside and inside $\mathcal{L}$ in $S_{\mathcal{L}}$ and integrate F along $C_L^{\pm} := \phi^{-1}(\alpha^{\pm})$. It results that $b := \int_{C_L^+} F^+ dX + \int_{-C_L^-} F^- dX = (\phi^+)(Q) - (\phi^-)(Q)$ is nonzero and defines the Burgers vector b attached to $\mathcal{L}$. Thus $S_{\mathcal{L}}$ is mapped into two surfaces which match outside $\mathcal{L}$ (i.e., at P) but do not coincide inside (i.e., at Q), where it is denoted by $\tilde{S}_{\mathcal{L}}$ and where by strain compatibility, the Burgers vector b is independent of the choice of Q. The corresponding mapping of the jump set is a curve which will define the dislocation L in the reference configuration. Accordingly, $\tilde{S}_L$ will denote the surface lying inside L in the reference configuration. By this procedure "à la Volterra" it holds

$$b = \int_{C_L} \nabla\phi dC = \int_{C_L} F dC, \tag{1.1}$$

for any $C_L = C_L^+ \cup C_L^-$ with line element dC. On the other hand, since ϕ shows a jump of amplitude b on $\tilde{S}_L$, its distributional derivative writes as $D\phi = F + b \otimes n \mathcal{H}^2_{\llcorner \tilde{S}_L}$ and hence $-$ Curl $F =$ Curl $(b \otimes n \mathcal{H}^2_{\llcorner \tilde{S}_L})$. Thus by Stokes theorem and written in terms of the *dislocation density*

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

as

$$-\,\text{Curl } F = \Lambda^T. \tag{1.2}$$

whereby (1.1) is equivalent to (1.2). The fact that 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.

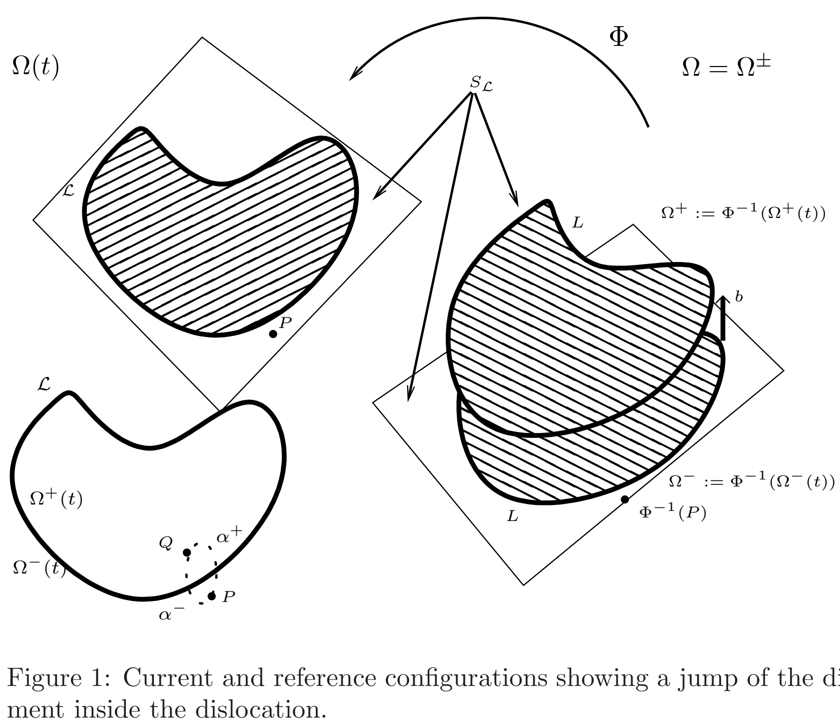

Figure 1: Current and reference configurations showing a jump of the displacement inside the dislocation.

Coming back to the physics and the mathematical properties of dislocations, we have already mentionned that in linear elasticity $F \in L^p$ with $1 \leq p < 2$, while specific examples for nonlinear 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 [23]. Here, classical examples show that deformation allowing for radial cavitation are such that $\mathrm{cof} F \in L^q$ with $1 \leq q < 3/2$ [12]. Thus one cannot restrict to the interval $3/2 \leq p < 2$ where some existence results in finite elaticity exists [22], and must allow F, $\mathrm{cof} F \in L^p$ in the whole range $1 \leq p < 2$. For this reason, as suggested in [22], *Cartesian maps* will be considered [10]. 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 $J \to 0^+$ 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 $\det F$, $\mathrm{cof} F \in L^p$ but also that their distributional counterpart have no s-dimensional $(0 \leq s \leq 3)$ singular parts in $\Omega \setminus L$, that is, $\mathrm{Det} F$, $\mathrm{Cof} F \in L^p$ locally away from L [17]. As a consequence, the strain energy W_e will depend on F, $\mathrm{cof} F$ 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

$$W_e(F) \geq C(|F|^p + |\,\mathrm{cof} F|^p + |\det F|^p) - \beta$$

for some $C, \beta > 0$. In our problem, strain gradients play a crucial role and thus a strain-gradient elastic energy involving F and $\mathrm{Curl}\ F$ will be considered. This can be written as $W_{\mathrm{deform}}(F, \mathrm{Curl}\ F) = W_e(F) + \tilde{W}_e(\mathrm{Curl}\ F)$ or equivalently since $\mathrm{Curl}\ F = \Lambda$ in terms of the *internal thermodynamic variable* Λ as $W(F, \Lambda) = W_e(F) + W_{\mathrm{defect}}(\Lambda)$, with

$$\int_\Omega W_{\mathrm{defect}}(\Lambda) \geq C \|\Lambda\|_{\mathcal{M}(\Omega)}.$$

With this kind of strain energy, our aim is twofold. In a first step, to define classes of admissible deformations F and admissible dislocations $\mathcal{L}$ satisfying (i) a boundary condition in terms of dislocation density and (ii) the geometric contraint (1.2). In a second step, to prove existence of minimizers of the energy

$$\inf_{-\mathrm{Curl}\ F = \Lambda^T} \mathcal{W} := \int_\Omega W(F, \Lambda) dx. \tag{1.3}$$

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 [1,14]. 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 resistence 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* [9]. 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 vector.

This paper is self-contained and can be read without previous notions neither on dislocations nor on currrents. 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 Section 5, we discuss the admissible deformations satisfying contraint (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 6. Current conclusions and plans to further extend the range of applications of this approach are drawn in Section 7.

2 Preliminary notions and results

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

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

Note that with this convention one has $\mathrm{Div}\ \mathrm{Curl}\ A = 0$ in the sense of distributions, since componentwise the divergence is classicaly defined as $(\,\mathrm{Div}\ A)_i = D_j A_{ij}$.[1] For the remaining of this section, our main references are [9,10].

2.1 Notations

Let M, n be integers with $0 \le M \le n$. 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, $\xi = v_1 \wedge v_2 \wedge \cdots \wedge v_M$. Let α be a multiindex, i.e., an ordered (increasing) subset of $\{1, 2, \ldots, n\}$. 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 $\{1, 2, \ldots, n\} \setminus \alpha$.

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

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

[1] In this paper we therefore follow the transpose of Gurtin's notation convention [20] but care must be payed since the curl and divergence of tensor fields are given alternative definitions in the literature (including the second author references [24]- [28] where the current curl would write $\mathrm{Curl}\ A = -A \times \nabla$).

where $\{e_i, \varepsilon_i\}_{i\leq n}$ is the Euclidean basis of $\mathbb{R}^{2n}$. Accordingly, it holds

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

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

$$M^i_j(A) = A_{ij}, \quad M^I_J(A) = M^I_{\bar{j}}(A) = (\operatorname{cof} A)_{ij} \quad M^{\{1,2,3\}}_{\{1,2,3\}}(A) = \det A, \quad (2.2)$$

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

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

Let also $\mathcal{M}(A) := (A, \operatorname{adj} A, \det A)$ 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, symbol $\mathcal{D}_M(\Omega) := \mathcal{D}'(\Omega; \Lambda^M \mathbb{R}^n)$ denotes 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

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

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

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

$$[\![S]\!](\omega) = \int_S \langle \omega, \vec{S}\rangle d\mathcal{H}^M \qquad \text{for } \omega \in \mathcal{D}^{M-1}(\Omega), \quad (2.4)$$

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

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

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

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 $F : U \to V$ is a smooth map, it is possible to define the *push forward* of a current $T \in \mathcal{D}_M(U)$ through F as

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

where $F^\sharp\omega$ is the standard pull back of ω and ζ is any C^∞ function that is equal to 1 on $\operatorname{spt} T \cap \operatorname{spt} F^\sharp\omega$. 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

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

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

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

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_xS in $\mathbb{R}^n$ such that

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

for all $\varphi \in C_c^0(\mathbb{R}^n)$, where $\eta_{x,\lambda} : \mathbb{R}^n \to \mathbb{R}^n$ 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 $\tau : S \to \Lambda_M(\mathbb{R}^n)$ and $\theta : S \to \mathbb{R}$ are $\mathcal{H}^M$-integrable and such that $\tau(x) \in T_xS$ is a simple unit M-vector for $\mathcal{H}^M$-a.e. $x \in S$, then we can define the current T as

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

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

$$T \equiv \{S, \tau, \theta\} \tag{2.9}$$

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 an integral current and S, τ, and θ in (2.8) satisfies also the property that θ is integer valued. 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*

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

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 $T_{k(i)} \rightharpoonup T$ weakly in Ω as $i \to \infty$.

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 [9, 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*

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

Suppose T is an indecomposable integer multiplicity 1-current on $\mathbb{R}^n$. Then there exists a Lipschitz function $: \mathbb{R} \to \mathbb{R}^n$ with $\mathrm{Lip}(f) \leq 1$ such that

$$f \llcorner [0, |T|] \textit{ is injective and } T = f_\sharp [0, M(T)].$$

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

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 [10, 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 $(\mathrm{Id} \times u) : \Omega \to \Omega \times \mathbb{R}^n$ defined by $(\mathrm{Id} \times u)(x) := (x, u(x))$. 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 $\mathrm{Id} \times u$, i.e.,

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

where

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

This allows us to extend the definition of push-forward of a current T also throughout the map $\mathrm{Id} \times u$, 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 $G_u := (\mathrm{Id} \times u)_\sharp [\![\Omega]\!]$, so that, for all ω satisfying (2.10), we have

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

2.5 Cartesian maps

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

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

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

$$\langle \mathrm{Det} Du, \varphi \rangle := \int_\Omega u_1 (\mathrm{adj} Du)_1 D\varphi dx, \qquad \forall \varphi \in C^\infty_c(\Omega, \mathbb{R}^3),$$

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

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

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 $\mathrm{adj}\ Du,\ \det Du$ 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 rectifiable current with multiplicity 1 and support given by the 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,

$$G_u(\omega) = \int_\Omega \langle \omega, \vec{G}_u \rangle d\mathcal{H}^n \llcorner \mathcal{G}_u, \tag{2.11}$$

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

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

The following closure theorem for Cartesian maps holds (see [10, Section 3.3.3]):

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

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

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

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

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. *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, than 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*

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

3 Dislocations as currents

Let Ω be a bounded and connected open set in $\mathbb{R}^3$, with smooth boundary. Let $\mathcal{L}$ be a integer-multiplicity 1-current in $\bar\Omega$ such that $\partial\mathcal{L} = 0$ in Ω. By Theorem 2.2, it can be rewritten as $\mathcal{L} = \sum_{i\in\mathcal{I}\subset\mathbb{N}} \mathcal{L}_i$ where the $\mathcal{L}_i$'s are indecomposable. For every $i \in \mathcal{I}$, let $b^i \in \mathcal{B}_\mathcal{I}$, where $\mathcal{B}_\mathcal{I}$ is a countable family of vectors indexed by $\mathcal{I}$.

Definition 3.1. *A dislocation is a couple* $\mathcal{L}_\mathcal{I} := (\mathcal{L}, \mathcal{B}_\mathcal{I})$. *Each* $\mathcal{L}_\mathcal{I}$ *can be represented by means of the quadruple* $\{L, \tau, \theta, \mathcal{B}_\mathcal{I}\}$.

In many applications, the Burgers vector is constraint by crystollagraphic 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

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

Accordingly if $\mathcal{B}_\mathcal{I} \subset \mathcal{B}$ then $\mathcal{L}_\mathcal{I}$ is called an *crystallographic dislocation*.

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 measure* $\Lambda_\mathcal{L} \in \mathcal{M}(\bar{\Omega}, \mathbb{R}^{3\times 3} \cup \infty)$ *defined by*

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

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* $(wb)^* := w_{kj} b_j dx_k$ *(with Einstein summation convention on repeated indices).*

Clearly if $\mathcal{I}$ is finite and $\mathcal{L}$ has finite mass, then $\Lambda_\mathcal{L}$ is a finite Radon measure.

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

$$\Lambda_\mathcal{L} = \Lambda_{\mathcal{L}'}. \tag{3.3}$$

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

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

3.1 Preamble to regular dislocations

So far, dislocations are mathematically represented by currents but it is crucial to keep in mind their physical origin and formation. A dislocation loops 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 dislocation 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, anihilation, 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 in this section. According to the dislocation physics, the basic object will be the loops associated to a given Burgers vector. These simple *generator* loops will then be smootly 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 sigtnificantly as clusters are considered since Frank law applies at dislocation junctions [13]. For this reason, our restriction to finite families of regular loops associated to a finite number of distinct Burgers vectors (the generator loops) does not preclude the formation of complex structures.

From a physical standpoint, the restriction to finitely many generator loops is justified by the nonvanishing energetical cost required for each nucleation. In the following definition, the dislocation is geometrically represented by the image of (non necessarily injective) Lipschitz functions (i.e., allowing for overlapping and self intersections, and permitting cusps) and should be thought of as resulting from the time-evolution of a finite family of generator loops. 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* (denoted with symbol Ξ in the sequel). 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.

All precise mathematical definitions are given in the following section with specific use of calculus with currents.

3.2 Regular dislocations

Definition 3.5 (b-dislocation currents)**.** *We associate to every $b \in \mathcal{B}$ an integer multiplicity* 1*-current $\mathcal{L}^b$ satisfying the following conditions: there exist a non-negative integer k_b and k_b Lipschitz functions $\varphi_j^b : [0, T_j] \to \bar{\Omega}$ with* $\mathrm{Lip}(\varphi_j^b) \leq 1$ *such that*

$$\mathcal{L}^b = \sum_{j=1}^{k_b} \varphi^b_{j\sharp} [\![0, T_j]\!]. \tag{3.4}$$

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.

From Theorem 3.18, one can always decompose $\mathcal{L}^b$ as follows

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

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 $\displaystyle\sum_{j=1}^{k_b} l_j^b := \int_0^{T_j} |\dot{\varphi}_j^b| dt < \infty$, 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 refering to a no-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 $\partial\mathcal{L}^b \subseteq \partial\Omega$.

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

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

We can choose

$$L^b := \bigcup_{j=1}^{k_b} \varphi_j^b(S^1), \tag{3.7}$$

for the rectifiable set supporting the current $\mathcal{L}^b$, and we also write $\mathcal{L}^b = \{L^b, \tau^b, \theta^b\}$. With such a choice L^b is a compact set. Remark also that, 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 component 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*

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

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 $(wb)^* := w_{kj} b_j dx_k$.

In the sequel we will use the following shortcut notation from (3.6) and (3.8):

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

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 *$\Lambda_{\mathcal{L}}$,*

$$\mathcal{L} := \sum_{b\in\mathcal{B}} \mathcal{L}^b, \qquad \Lambda_{\mathcal{L}} := \sum_{b\in\mathcal{B}} \Lambda_{\mathcal{L}^b}. \tag{3.10}$$

The dislocation set *L is defined as*

$$L := \bigcup_{b\in\mathcal{B}} L^b, \tag{3.11}$$

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

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

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

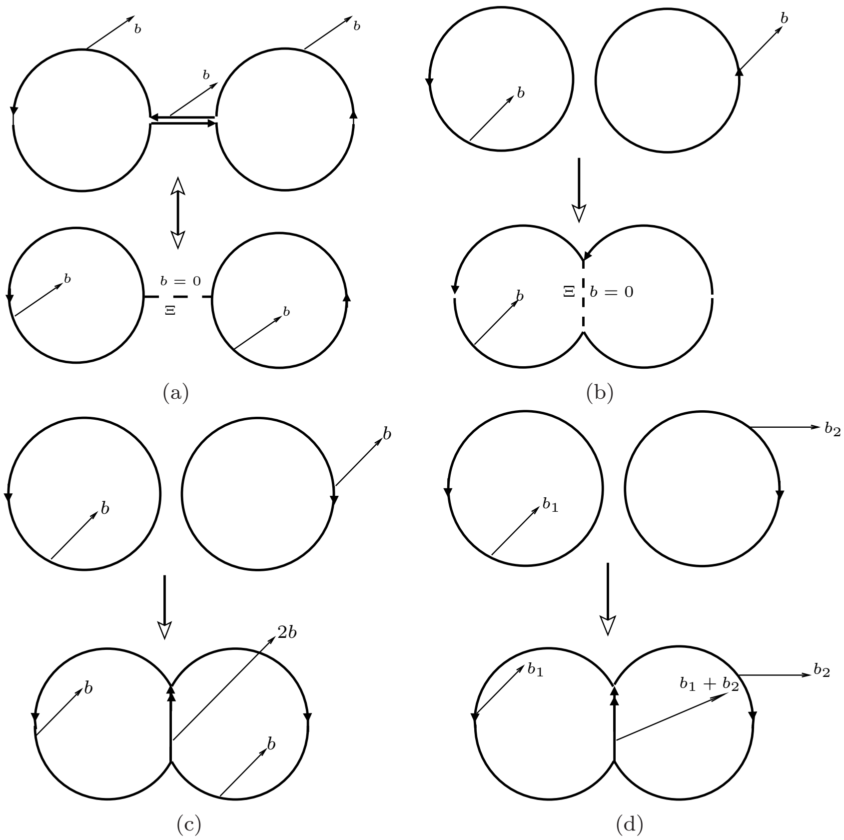

Figure 2: Typical indecomposable dislocation loops and the resulting dislocation currents: in (a), a single b-dislocation loops is equivalently viewed as two indecomposable b-loops with opposite directions and connected by a geometrically unnecessary arc Ξ; the inverse property is observed in (b) where two identical b-loops give rise to a single connected b-dislocation loops and a geometrically unnecessary arc Ξ; 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.

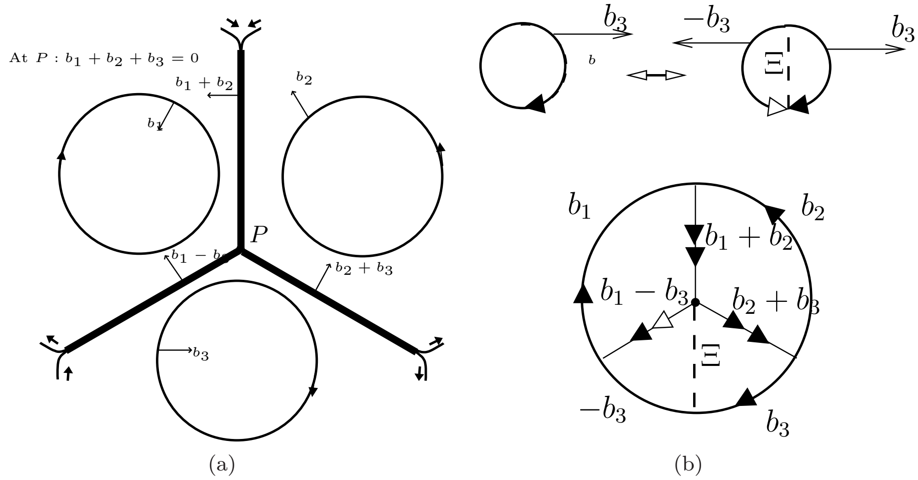

Figure 3: For certain combinations of Burgers vectors, the three separated loops of (a) might intersect and form the cluster element of (b) where the Frank law at the intersection points is satisfied.

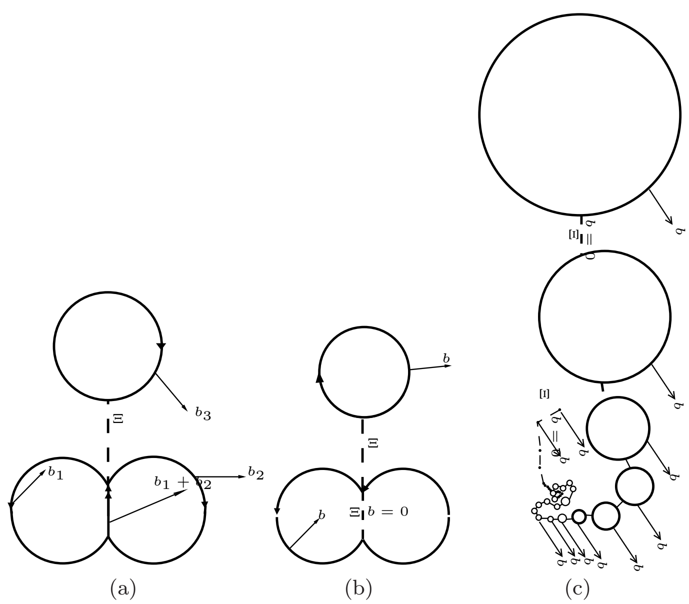

Figure 4: Different kinds of cluster components: in (a) the sum of b-current dislocations $\mathcal{L}^{b_1} + \mathcal{L}^{b_2} + \mathcal{L}^{b_3}$ is depicted, whereas (b) shows a single b-current constituted of three elementary b-loops. In (c) a b-dislocation cluster writing as $\mathcal{L}^b = \varphi^b_\sharp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

From Definition 3.4 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-neglibible set. Therefore the following notion is introduced:

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

$$\mathcal{L} = \sum_{b\in\mathcal{B}} \mathcal{L}^b = \sum_{b\in\mathcal{B}} \sum_{1\le j\le k_b} \varphi^b_{j\sharp}[\![[0,T_j]]\!], \tag{3.13}$$

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

$$\mathcal{L} = \sum_{j\in\mathcal{J}} \varphi_{j\sharp}[\![[0,T_j]]\!]. \tag{3.14}$$

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

$$L = \bigcup_{j\in\mathcal{J}} S_j. \tag{3.15}$$

Every current of the form $\mathcal{L}' = \sum_{j\in\mathcal{J}'} \varphi_{j\sharp}[\![[0,T_j]]\!]$, 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* $\subset$.

3.3 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 $\underline{b}_i := \bar{b} \cdot \underline{e}_i$ 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

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

thus satisfying $\Lambda_{\mathcal{L}^{b,i}} := \mathcal{L}^{b,i} \otimes \underline{b}_i$ and in such a way that to any dislocation current we associate univoquely three currents $\{\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3\}$, with

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

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

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

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

$$\hat{\mathcal{L}} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3. \tag{3.18}$$

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 $C^\infty_c(\mathbb{R}^3, \mathbb{R}^{3\times3})$.

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

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

for some $B > 0$ independent of $\mathcal{L}_i$.

(c) The geometrically necessary dislocation set reads $L^\star := \bigcup_{i=1}^{3} \mathrm{spt}(\mathcal{L}_i) \subset \bar{L}$ 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

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

and explicitely,

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

(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,

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

Now, since $\Lambda_{\mathcal{L}_i} = \mathcal{L}_i \otimes \underline{b}_i$, setting $B := \min_{i=1,2,3}\{\|\underline{b}_i\|\}$, yields (3.19).

To prove (c), oberve 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 $\mathrm{spt}\mathcal{L}_i = \mathrm{spt}\Lambda_{\mathcal{L}_i}$. So we only need to prove that $\mathrm{spt}\Lambda_{\mathcal{L}} = \cup_{i=1}^{3}\mathrm{spt}\Lambda_{\mathcal{L}_i}$. But this is a direct consequence of the fact that $\Lambda_{\mathcal{L}_i}$ acts on orthogonal subspaces of $C_c^\infty(\mathbb{R}^3, \mathbb{R}^{3\times 3})$. □

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

4 Classes of admissible dislocations

Two classes of dislocations will now be introduced, the first being usefull if one wishes to follow (for instance, with time) each line as it deform, 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)**.**

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

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 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 theorem is readily proved.

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

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

$$|\hat{\mathcal{L}}| \leq C \sum_{\substack{b \in \bar{\mathcal{B}} \\ i=1,\dots,k_b}} l_i^b < \infty, \tag{4.2}$$

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 $\mathcal{H}^1 \llcorner L$.

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

$$\|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\bar{\Omega})} \leq \sum_{\substack{b \in \bar{\mathcal{B}} \\ i=1,\dots,k_b}} |b| l_i^b < \infty, \tag{4.3}$$

with $\bar{\mathcal{B}} := \{b \in \mathcal{B} : k_b \neq 0\}$.

(c) The set L supporting the current $\mathcal{L}$ is a closed set with finite $\mathcal{H}^1$-measure. In particular $L^\star \subseteq L$ and $L = L^\star \cup \Xi$.

Proof. Statement (a) follows as a direct consequence of the definition of b-dislocation current and from Assumption 4.1. Formula (4.2) follows from (3.16). Statements (b) and (c) are straightforward consequences of the definitions. □

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

Definition 4.3 (Admissible mesoscopic dislocation)**.**

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

4.2 Preamble to continuum dislocations

Let us first describe a pathological case which we must avoid at our scale of matter description. Consider a countable set of points $P_{i\in\mathcal{I}}$ in a surface S, each of which being the center of a segment l_i such that $\sum_{i\in\mathcal{I}}\mathcal{H}^1(l_i)$ is finite. One can view l_i as the the intersection with S of a countable family of dislocation loops $L := L_{i\in\mathcal{I}}$ such that it also holds $\sum_{i\in\mathcal{I}}\mathcal{H}^1(L_i)$ is finite. Then $\bar{L}$ will have a infinite $\mathcal{H}^1$-measure if the set of P's consists of a locally dense set of S. In this case the mesoscopicity assumption is violated since there is no ball centered at those points with empty intersection with L. The mesoscopicity assumption will be weakened by introducing the notion of *continuum*, understood here as a finite union of compact and connected 1-sets of $\bar{\Omega}$ (that is, set which are of Hausdorff dimension 1 and have finite one-dimensional Hausdorff 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, assume that each can be taken in a countable but not finite family $\mathcal{B}_{\mathcal{I}} \nsubseteq \mathcal{B}$ of vectors (that is, a non-crystallographic family). 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. Moreover, with this notion, the countable loops might always be connected by rather wild segments of unnecessary dislocation.

Let us emphasize that from a strictly mesoscopic standpoint allowing the Burgers vectors to take countably many values ($\mathcal{B}_{\mathcal{I}} \nsubseteq \mathcal{B}$ 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.

4.3 Dislocations at the continuum scale

The space of *admissible dislocations at the continuum scale* is introduced as follows:

Definition 4.4 (Admissible continuum dislocation)**.**

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

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

In particular every $\mathcal{L}$ such that the support $L^\star$ 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. Theorem 4.2 (b)), the density of a continuum dislocation must not be finite.

Let $\mathcal{L}' \equiv \mathcal{L}$, where the symbol $\equiv$ refers to the equivalence relation of Definition 3.20, then the support $L^\star$ of the density $\Lambda_{\mathcal{L}'}$ is a subset of $\mathcal{C}_{\mathcal{L}}$. Remark that $\mathcal{L} \in \mathcal{CD}$ does not imply that $\mathcal{H}^1(L) < \infty$, even if $\Lambda_{\mathcal{L}}$ is finite. Remark also that *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 $\mathcal{H}^1(\Xi) = \infty$.

Let us further motivate the introduction of continuum dislocations. 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 $\mathcal{H}^1(\Xi(t)) \to \infty$ (or $\mathcal{H}^1(\bar{\Xi}(t)) \to \infty$) as t converges to some limit time. Note that time- evolution of some subset of $\mathcal{K}$ to a pathological Ξ is also possible within this setting. Recall in fact that 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, an existence result considering $\mathcal{CD}$ will be more general since it does not require the a priori Lipschitzianity of the functions nor to prescribe a bound for number of the generator loops, while permitting optimal curves with the aforementioned pathological behaviour or with non-crystallographic Burgers vectors. Remark also that continuum dislocations conceptually suits beter engineer models of dislocations in which necessary and unnecessary dislocations are treated by distinct, though coupled, equations.

In the applications, the notion of continuum dislocations is usefull to study the cases in which Assumption 4.1 is not satisfied. However, 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 dislocatis 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, whose proof is rather technical and can be found in the Appendix.

Theorem 4.5. *Let $\mathcal{L}$ be a closed current with finite mass whose support $L^\star$ is contained in a compact 1-set $\mathcal{K}$. Then there exists a Lipschitz function $\alpha : S^1 \to \mathcal{K}$ such that $\mathcal{L} = \alpha_\sharp[\![S^1]\!]$.*

Now, we can state the precise equivalence theorem.

Theorem 4.6. *Let $\mathcal{L}_\mathcal{I}$ be a continuum dislocation such that $\mathcal{B}_\mathcal{I}$ is finite. Then $\mathcal{L}_\mathcal{I}$ is a mesoscopic dislocation. The thesis holds if $\mathcal{B}_\mathcal{I} \subset \mathcal{B}$ is countable and if $\Lambda_{\mathcal{L}_\mathcal{I}}$ is finite.*

Proof. By Theorem 4.5 a finite number of Lipschitz curves, each made of a subset associated to a certain Burgers vector of $\mathcal{B}_\mathcal{I}$ and another subset of unnecessary curves, can be summed in such a way to contain the support of $\mathcal{L}$, achieving the proof of the first statement.

Now, if $\mathcal{B}_\mathcal{I} \subset \mathcal{B}$ is not finite but $\Lambda_{\mathcal{L}_\mathcal{I}}$ is finite then 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. □

In particular Theorem 4.6 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.

4.4 Boundary conditions for dislocations

Definition 4.7 (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* $\mathcal{B}_P = \{b_{Pi}\}_{0<i\leq N}$ *a sequence of vectors belonging to* $\mathcal{B}$*. We associate to* $\mathcal{P}$ *the* 0*-current* $T_P := \sum_{0<i\leq N} \delta_{P_i} - \delta_{Q_i}$*, with* δ_P*, the Dirac mass at* P*.*

(iii) α_D *is a couple* $(\alpha, \mathcal{B}_D)$*, where* α *is a dislocation current with* $\mathrm{spt}(\alpha_D) \subset \partial_D\Omega$ *consisting of a finite union of* b^i_α*-dislocation currents with* $\{b^i_\alpha\}_{0\leq i\leq N} \in \mathcal{B}_D$*.*

From (iii) we can define $\Lambda_\alpha = \sum_{0\leq i\leq N} \alpha_{b^i_\alpha} \otimes b^i_\alpha$ to be the density of the dislocation current α_D.

Definition 4.8. *We say that the boundary condition* $(N_P, \mathcal{P}, \alpha_D)$ *is* admissible *if the following conditions are satisfied:*

(I) there exist an admissible dislocation $\mathcal{L}$ *and an admissible density* $\Lambda_{\mathcal{L}}$ *such that* $\partial\mathcal{L} = T_P$ *and, for any* i *there is a loop* $L_i^{b_{P_i}}$ *with boundary* $\delta_{P_i} - \delta_{Q_i}$ *and associated Burgers vector* b_{P_i}*.*

(II) $\alpha + \mathcal{L}$ *is still an admissible dislocation (either mesoscopic or continuum).*

Finally we say that a dislocation $\mathcal{L}$ satisfies the admissible boundary condition $(N, \mathcal{P}, \alpha)$ if it satisfies properties (I) and (II).

5 The class of admissible deformations

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

Definition 5.1.

$$\mathcal{F} := \{(F, \mathcal{L}) \in L^p(\Omega, \mathbb{R}^{3\times 3}) \times \mathcal{MD} : F \text{ satisfies (i)-(iii) below}\} \tag{5.1}$$

(i) The dislocation current $\mathcal{L} = \{L, \tau, \theta\}$ *satisfies 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* $-\mathrm{Curl}\, \hat{F} = \Lambda_{\mathcal{L}}$ *in* $\hat{\Omega}$*.*

(ii) We require that for every point $x \in \Omega \setminus L$ *there is a ball* $B \subset \Omega \setminus L$ *containig* x *such that there exists a function* $\phi \in \mathrm{cart}^p(B; \mathbb{R}^3)$ *with* $F = D\phi$ *in* B*.*

(iii) $\det F > 0$ *almost everywhere in* Ω*.*

We will show that there exists at leat 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:

$$-\operatorname{Curl} F = b \otimes \tau\, \mathcal{H}^1 \llcorner L \quad \text{if and only if} \quad \int_{C_L} F\, \underline{e}_\theta d\mathcal{H}^1 = b. \tag{5.2}$$

for all Lipschitz-continuous closed path C_L in Ω enclosing once L and with unit tangent vector $\underline{e}_\theta$. To check identity (5.2), 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 (5.2), 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 $\langle \operatorname{Curl}\,(b \otimes n\mathcal{H}^2_{\llcorner \tilde{S}_L}), \psi\rangle = \langle b \otimes n\mathcal{H}^2_{\llcorner \tilde{S}_L}, \operatorname{Curl}\,\psi\rangle$. 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 $\langle \operatorname{Curl}\,(b \otimes n\mathcal{H}^2_{\llcorner \tilde{S}_L}), \psi\rangle = \langle (b \otimes \tau\mathcal{H}^1_{\llcorner L}), \psi\rangle$.

Theorem 5.2. *The set $\mathcal{F}$ is non-empty for $1 \le p < 2$.*

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), and in V_δ we choose $\underline{e}_3 = \underline{g}_\theta$, where $\underline{g} := (\underline{g}_r, \underline{g}_\theta, \underline{g}_l)$ with $\underline{g}_l = \underline{h}_l$ is the local cylindrical basis defined on the normal sections ∂V_δ, andWe then consider the function F inside V_δ whose components in the basis $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\}$ read

$$F(r, \theta, l) = \zeta(\theta) \begin{pmatrix} -\frac{\sin\theta}{r}\beta_R & +\frac{\cos\theta}{r}\beta_R & 0 \\ -\frac{\sin\theta}{r}\beta_l & +\frac{\cos\theta}{r}\beta_l & 0 \\ -\frac{\sin\theta}{r}\beta_z & +\frac{\cos\theta}{r}\beta_z & 0 \end{pmatrix}, \tag{5.3}$$

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 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 $0 \le l \le 2\pi$, and in order to fix the arbitrary constant, set $\phi_\delta = 0$ on $S \cap \{\theta = a\}$ and $\phi_\delta = b$ on $\bar{S} \cap \{\theta = a+\pi/2\}$. 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 $C_{\bar{\theta}} := \{(\delta, \bar{\theta}, l) : 0 \le l \le 2\pi R\}$ 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, (5.2) and (5.3) together entail that $-\operatorname{Curl} F = b \otimes \tau\ \mathcal{H}^1$ 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 (5.3), $F \in L^p(\Omega)$ for $p \in [1, 2)$, since

$$\|F\|^p_{L^p(\Omega)} \leq C|b|(R\delta^{2-p} + \delta^{1-p}R^2), \tag{5.4}$$

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 $\det(F + cI)$, $\operatorname{adj}(F + cI)$ 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.

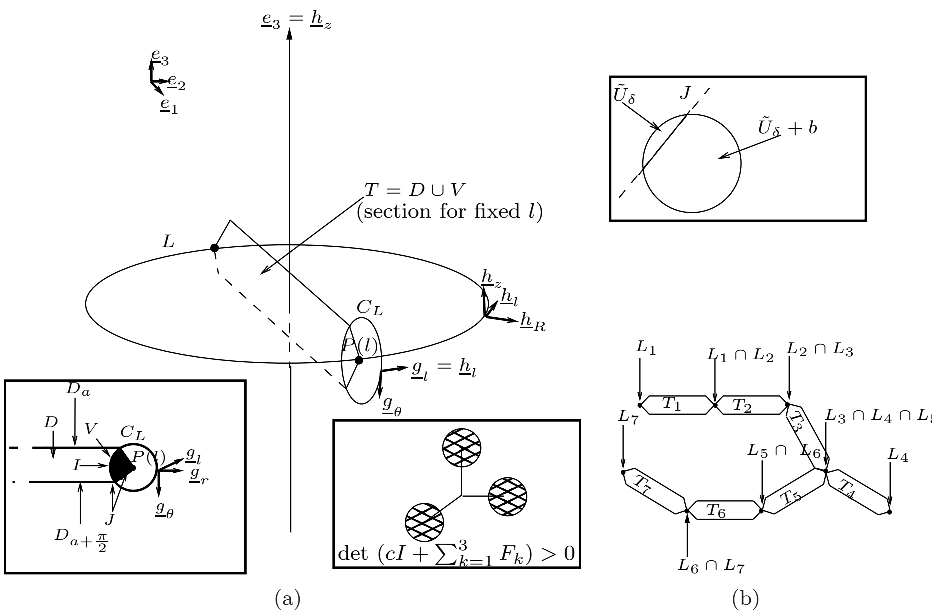

Figure 5: Picture of the tube construction for the proof (a); the case of finitely many boundary dislocation segments (b)

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 is still remains non-negative. Let us consider a finite number of loops L_k with $1 \le k \le K$ 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 keeeping the V_k's with empty mutual intersection (cf. Fig 5(b) below left). Let F_k be defined as (5.3) with β_k in place of β and $a_k = \hat{a}_k(l)$ in place of a such that $f_k(\theta, l) := \beta_l^k(l)\cos\theta - \beta_R^k(l)\sin\theta = \beta_2^k \cos(\theta + \frac{l}{R}) - \beta_1^k \sin(\theta + \frac{l}{R}) \ge 0$ (for instance, if $\beta_1, \beta_2 > 0$ then $a_k := \frac{3\pi}{2} - \frac{l}{R}$). Defining $F := \sum_{k=1}^{K} F_k + cI$, (5.4) entails that F, $\det F$, $\operatorname{adj} F$ belong to L^p and also that

$$\det F = \frac{c^2}{r} f_k(\theta, l)\zeta(\theta) + c^3 \ge 0 \quad \text{in } V_k, \tag{5.5}$$

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_ks. In particular, it holds for the boundary current α and for any finite family of curve 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 $\bar{\Omega}$). Thus the proof is achieved.

□

6 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.

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

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

$$\begin{aligned}\mathcal{W}(F, \Lambda_{\mathcal{L}}) := \int_\Omega W_e(F)dx + W_{\text{defect}}(\Lambda_{\mathcal{L}}) \ge \\ C\big(\||\mathcal{M}(F)|\|_{L^p} + \|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\bar{\Omega})} + k(\mathcal{L})\big) - \beta,\end{aligned} \tag{6.1}$$

where we recall that $k(\mathcal{L})$ is defined in (4.1). It is also assumed that

(W1) $W_e(F) \ge h(\det F)$, for a continuous real function h such that $h(t) \to \infty$ as $t \to 0$, (W2) W_e is polyconvex, i.e., there exists a convex function $g : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R}_* \to \bar{\mathbb{R}}$ s.t. $W_e(F) = g(\mathcal{M}(F))$, $\forall F \in \mathcal{F}$,

(W3) $W_{\text{defect}} := W^1_{\text{defect}} + W^2_{\text{defect}}$, with $W^1_{\text{defect}}(\Lambda_{\mathcal{L}}) := \int_{\bar{\Omega}} H(\frac{\Lambda_{\mathcal{L}}}{|\Lambda_{\mathcal{L}}|}) d|\Lambda_{\mathcal{L}}|$ is convex in the sense of [11], where H is a 1-homogeneous positive and convex map (see also [8]), and $W^2_{\text{defect}}(\Lambda_{\mathcal{L}}) \geq \kappa k(\mathcal{L})$ convex, for some constitutive material parameter κ.

(W4) g and W_{defect} are weakly lower semicontinuous, i.e., $\liminf_{k\to\infty} g(\mathcal{M}(F^k)) \geq W_e(F)$ as $\mathcal{M}(F^k) \to \mathcal{M}(F)$ weakly in $L^p(\Omega, \mathbb{R}^{3\times 3}) \times L^p(\Omega, \mathbb{R}^{3\times 3}) \times L^p(\Omega)$ and $\liminf_{k\rightharpoonup\infty} W_{\text{defect}}(\Lambda^k) \geq W_{\text{defect}}(\Lambda)$ as $\Lambda^k \rightharpoonup \Lambda$ weakly* in $\mathcal{M}(\bar{\Omega}, \mathbb{R}^{3\times 3})$.

Before stating the existence of minimizers of the problem

$$\inf_{\mathcal{F}\times\mathcal{MD}} \mathcal{W}(F, \Lambda_{\mathcal{L}}), \tag{6.2}$$

some technical results should be stated and proven.

Lemma 6.1. *Let $(F_k, \mathcal{L}_k)$ be a minimizing sequence for the problem (6.2), 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 $\det F_k \to 0$ 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. □

Lemma 6.2. *Let γ_n be a sequence of 1-currents inside $\bar{\Omega}$ such that $\gamma_n = \varphi_{n\sharp}[\![0, M]\!]$ 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 $\gamma = \varphi_\sharp[\![0, M]\!]$ 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 $\varphi : [0, M] \to \mathbb{R}^3$ with $\text{Lip}(\varphi) \leq 1$ such that, up to subsequence, $\varphi_n \to \varphi$ uniformly. So it easily follows that $\gamma_n \rightharpoonup \gamma := \varphi_\sharp[\![0, M]\!]$, and the proof is complete. □

Lemma 6.3. *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 $\mathcal{L}_n = \mathcal{L}^1_n + \mathcal{L}^2_n + \mathcal{L}^3_n$, and $\Lambda_n = \Lambda^1_n + \Lambda^2_n + \Lambda^3_n$, with, using notation (3.9), $\Lambda^i_n = \mathcal{L}_n \otimes \underline{b}_i$. 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 $\mathcal{L}^j_n$ are boundaryless in Ω and thanks to inequalities (3.22) and (3.19), we have that $N(\mathcal{L}^j_n)$ 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

$$\langle \mathcal{L}_n, \omega\rangle \to \langle \mathcal{L}, \omega\rangle, \quad \text{and at the same time} \tag{6.3}$$

$$\langle \mathcal{L}_n, \omega\rangle = \langle \textstyle\sum_{j=1}^3 \mathcal{L}_n^j, \omega\rangle \to \langle \textstyle\sum_{j=1}^3 \mathcal{L}^j, \omega\rangle, \tag{6.4}$$

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

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

Since the left-hand side of the last expression tends to $\langle \Lambda^j, w\otimes e_i\rangle$, thanks to the fact that $\{w\otimes e_i\}_{1\le i\le 3, w\in C_c^\infty}$ 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. □

Now we are ready to solve Problem (6.2).

Theorem 6.4 (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* $\mathcal{W}(F, \Lambda_{\mathcal{L}})dx < \infty$*, there is at least a* $(F, \mathcal{L})$ *solution of the minimum problem* (6.2)*.*

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

$$F_n \rightharpoonup F \quad \text{weakly in } L^p(\Omega, \mathbb{R}^{3\times 3}), \tag{6.5a}$$

$$\text{adj } F_n \rightharpoonup A \quad \text{weakly in } L^p(\Omega, \mathbb{R}^{3\times 3}), \tag{6.5b}$$

$$\det F_n \rightharpoonup D \quad \text{weakly in } L^p(\Omega). \tag{6.5c}$$

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 we get $\hat{F}$, $\hat{A}$, and $\hat{D}$ such that (6.5a)-(6.5c) hold for $\hat{F}_n$, $\hat{F}$, $\hat{A}$, and $\hat{D}$.

Moreover, thanks to the uniform boundedness of the sequence of measures $\Lambda_n :=$ Curl $\hat{F}_n$, we get a measure $\Lambda \in \mathcal{M}(\bar\Omega, \mathbb{R}^{3\times 3})$ such that

$$\Lambda_n \rightharpoonup \Lambda \quad \text{weakly* in } \mathcal{M}(\bar\Omega, \mathbb{R}^{3\times 3}). \tag{6.5d}$$

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.

We can suppose that every dislocation current $\mathcal{L}_n$ is generated by the same number k of 1-Lipschitz functions $\{\varphi_n^j\}_{j=1}^k$, i.e.,

$$\mathcal{L}_n = \sum_{j=1}^k \varphi^j_{n\sharp}[\![0, M]\!] \qquad \text{and} \qquad \Lambda_n = \sum_{j=1}^k \varphi^j_{n\sharp}[\![0, M]\!] \otimes b^j. \tag{6.6}$$

So by Lemma 6.2 we can suppose that for every j we have

$$\varphi^j_{n\sharp}[\![0, M]\!] \rightharpoonup \varphi^j_{\sharp}[\![0, M]\!],$$

for some 1-Lipschitz functions $\{\varphi^j\}_{j=1}^k$. If we set $\mathcal{L} := \sum_j \varphi^j_\sharp[\![0,M]\!]$ we then also have $\mathcal{L}_n \rightharpoonup \mathcal{L}$ and $\Lambda_n \rightharpoonup \sum_j \varphi^j_\sharp[\![0,M]\!] \otimes b^j$ weakly* in $\mathcal{M}(\bar{\Omega}, \mathbb{R}^{3\times 3})$, so from (6.5d) we get

$$\Lambda = \sum_j \varphi^j_\sharp[\![0,M]\!] \otimes b^j. \tag{6.7}$$

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

$$\langle \operatorname{Curl} \hat{F}_n, w\rangle = -\langle \hat{F}_n, \operatorname{Curl} w\rangle \to -\langle \hat{F}, \operatorname{Curl} w\rangle = \langle \operatorname{Curl} \hat{F}, w\rangle. \tag{6.8}$$

Since the first term in the left-hand side of (6.8) also tends to $\langle -\Lambda^T, w\rangle$, we finally get

$$-\operatorname{Curl} \hat{F} = \sum_j b^j \otimes \varphi^j_\sharp[\![0,M]\!]. \tag{6.9}$$

Let us set $L_n := \cup_{j=1}^k \varphi^j_n([0,M])$ 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 $u \in \operatorname{cart}^p(B, \mathbb{R}^n)$ such that $Du = F$ in B. Let x be such a point, since $\varphi^j_n \to \varphi^j$ uniformly, it follows that L_n tends to L in the Gromov-Hausdorff topology, so that we have $B \cap L_n = \varnothing$ for n sufficently large. In such a ball, by hypotheses, there are maps $u_n \in \operatorname{cart}^p(B, \mathbb{R}^n)$ satisying $Du_n = F_n$, and, up to summing suitable constants to u_n, we can also suppose u_n have all mean zero 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, (6.5a)-(6.5c), and Lemma 6.1. □

We remark that with the formulation (6.1) the potential $W(F, \Lambda_{\mathcal{L}})$ depends explicitely on the dislocation density. Yet it beyond the scope of this paper to discuss the nature and the possible expressions of the defect energy. Moreover the optimal dislocations are here assumed regular.

6.2 Second existence result

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

$$\mathcal{F}' := \{F \in L^p(\Omega, \mathbb{R}^{3\times 3}) : F \text{ satisfies (i)-(iii) below}\} \tag{6.10}$$

(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 $-\operatorname{Curl} \hat{F} = \Lambda_{\mathcal{L}}$ in $\hat{\Omega}$.

(ii) There is a continuum $\mathcal{C}$ such that $L^\star \subset C$ 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 $\phi \in \operatorname{cart}^p(B; \mathbb{R}^3)$ satisfying $F = D\phi$ in B.

(iii) $\det F > 0$ almost everywhere in Ω.

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

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

$$G(\mathcal{L}) := \inf_{\mathcal{K}\in\mathcal{C}_{\mathcal{L}}} \left(\mathcal{H}^1(\mathcal{K}) + \kappa k(\mathcal{K})\right), \tag{6.11}$$

where $k(\mathcal{K})$ represents the number of connected components of $\mathcal{K}$. Note that by Golab's theoremstyle G is also lower semi continuous.

(W6) there exists a weakly lower semicontinuous convex function $\tilde{g}$ s.t. $W(F) = \tilde{g}(\mathcal{M}(DF), \operatorname{Curl} F)$.

Since $\mathcal{F}'$ is non empty, we now solve the minimum problem with these new assumptions.

Theorem 6.5 (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 6.4. 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 $\hat{\mathcal{L}}_n \to \hat{\mathcal{L}}$, while by Lemma 6.3, $\Lambda = \Lambda_{\hat{\mathcal{L}}} = -\operatorname{Curl}\hat{F}$ in the distribution sense. Moreover, by admissiblity, one can associate to every $\mathcal{L}_n$ and hence to every $\hat{\mathcal{L}}_n$ a continuum $\mathcal{K}_n$ such that $G(\mathcal{L}_n) = \big(\mathcal{H}^1(\mathcal{K}_n) + k(\mathcal{K}_n)\big)$. By $(W6)$, Blaschke and Golab's 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 $L^\star := \operatorname{supp}\Lambda \subset \mathcal{K}$ and $\hat{\mathcal{L}} \equiv \hat{\mathcal{L}}^\star := (L^\star, \tau, \theta)$. Since $\mathcal{K} = \operatorname{argmin}_{\mathcal{C}_{\hat{\mathcal{L}}}} G$ admits a tangent vector almost everywhere and letting $\theta = 0$ on $\mathcal{K} \setminus L^\star$, 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 6.4. □

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 that deform the existent dislocation, as soon as $d > \kappa$. However it should be recognized that (6.11) is at this stage a mathematical assumption whose physical meaning remains to be elucidated. It basicly 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 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 detail 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 constraint by relation $-\operatorname{Curl} F = \Lambda^T$. The data is here the boundary dislocation density, while deformation boundary conditions could have also been prescibed 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 $\operatorname{Cof}F = \operatorname{cof}F \in L^p_{loc}(\Omega\backslash\mathcal{K})$ and $\operatorname{Det}F = \det F \in L^p_{loc}(\Omega\backslash\mathcal{K})$. 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 dislocation 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 quasistatic 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 $-\operatorname{Curl} F = \Lambda^T$ will also be studied in forthcomming publications.

Two others extension 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., [7]). 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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A Appendix

In this section we prove Theorem 4.5. The proof follows from the following Lemmas:

Lemma A.1. *Let K be a compact connected set in $\mathbb{R}^n$ such that $\mathcal{H}^1(K) < \infty$. Then there exists a map $\psi : S^1 \to K$ that is onto, is homotopic to the constant map, and satisfies $\mathcal{H}^1\{X : \mathrm{card}\psi^{-1}(X) > 2\} = 0$.*

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

$$\mathcal{S} := \{\phi : S^1 \to K \text{ satisfying the following three properties}\} \tag{A.1}$$

(i) $\phi(1) = P$.

(ii) ϕ is homotopic to the constant map $\phi \equiv P$.

(iii) $\mathcal{H}^1\{X : \mathrm{card}\phi^{-1}(X) > 2\} = 0$. In particular, letting $C = \phi(S^1)$ and $L_C = \mathcal{H}^1(C)$, the curve ϕ is parametrized with respect to a multiple of $\frac{2\pi}{L_C}$ the arc length scale, so that it 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 $\mathbb{R}$). Then the sequence $\{L_j\}_{j\in J}$ is non-decreasing and bounded by $2\mathcal{H}^1(K)$, so that, since the maps $\{\phi_j\}$ are uniformly continuous in j, there is an increasing sequence $j_k \to \sup J$ and a map ϕ such that $\phi_{j_k} \to \phi$ 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 $j_k \to \sup J$ 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 $\mathrm{Lip}(\phi_j) \leq \frac{L}{\pi}$ implies that $\mathrm{Lip}(\phi) \leq \frac{L}{\pi}$. Now (i) is 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 $\mathrm{Lip}(\Phi_j(x, \cdot)) \leq L$, 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. To see (iii) we employ the coarea formula

$$\int_{S^1} |\dot\phi(s)|ds = \int_C \mathrm{card}\{\phi^{-1}(X)\} d\mathcal{H}^1(X). \tag{A.2}$$

From this and $\mathrm{Lip}(\phi) \le \frac{L}{\pi}$ it follows

$$\int_C \mathrm{card}\{\phi^{-1}(X)\} d\mathcal{H}^1(X) \le 2L,$$

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 $\alpha : [0,1] \to K$ 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 readly seen that the arc $\psi_1 \star \alpha \star \alpha_{-1} \star \psi_2$, if suitable rescaled as a function on S^1, is a map in $\mathcal{S}$ that is strictly greater than ψ, contraddicting the maximality of ψ. Hence the thesis follows. $\square$

Lemma A.2. *Let $\psi : S^1 \to K$ Lipschitz continuous, with K a compact 1-set, that is homotopic to the identity. Then $\psi_\sharp[\![S^1]\!] = 0$.*

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 lebesque 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 non-zero, the decomposition theorem implies that there exists $T = \alpha_\sharp[\![S^1]\!]$ an undecomposable component of the 1-current $\psi_\sharp[\![S^1]\!]$. If $X = \psi(a) = \psi(b)$, then, since ψ is homotopic to the constant, we can replace ψ with $\hat\psi$, setting $\hat\psi \llcorner [a,b] \equiv X$ and $\hat\psi \llcorner [a,b]^c = \psi$, getting a map that is still homotopic to the constant. In such a way we find out that α must belong to the same homotopy class of ψ. On the other side, since α is an iniective loops, its homotopy class is $\prod_{X_j \in \Delta} X_j$, with Δ being the bounded connected set with boundary α. In particular α is not trivial, contraddicting the hypothesis. $\square$

Now we can prove Theorem (4.5).

Proof of Theorem 4.5. By the decomposition Theorem there are loops β_j such that $\mathcal{L} = \sum_j \beta_{j\sharp}[\![S^1]\!]$. Consider a function ψ like in Lemma A.1, 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 $\psi_j := \psi \llcorner [x_j, x_{j+1}]$, then the chain

$$\beta_1 \star \psi_1 \star \beta_2 \star \psi_2 \star \ldots \beta_j \star \psi_j \ldots$$

will match the required conditions, thanks to the property that ψ is homotopic to the constant, so that Lemma A.1 implies $\psi_\sharp[\![S^1]\!] = 0$. $\square$

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