Currents and dislocations at the continuum scale

Riccardo Scala and Nicolas Van Goethem

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Abstract

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

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

Contents

1 Introduction

1.1 Physical motivation of the problem

Consider one dislocation loop L in a continuum medium $\Omega(t)$ at time t. At the mesoscopic scale it is assumed that $\Omega(t) \setminus L$ is an elastic body, and thus that all dissipative (i.e., including plastic) effects are concentrated in L. It is also assumed that L is a one-dimensional singularity set for the stress and strain fields. Moreover, if a linear elastic constitutive law is chosen, classical examples of screw and edge dislocations show that stress and strain are not square integrable [14], and hence that the strain energy is unbounded near 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. 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* (otherwise named *dislocation networks*). This phenomenon is enhanced if the crystal is considered at high temperature or subjected to high temperature gradients, since the constrained motion of dislocation on predefined glide planes only holds for moderate temperature ranges. Overlooking on purpose the specific inter-dislocation dynamics [26, 29, 30] which causes attraction/repulsion between dislocations and are responsible for their aggregation, in this paper we consider the cluster as a mathematical object which must be described in a geometrically unified way together and accordingly with any single dislocation loop.

1.2 Origin and nature of a dislocation singularity

Another intrisic difficulty of mesoscopic dislocations is that there is no natural definiton of the displacement field (and so for the fictitious reference configuration), whereas the displacement field jump is a physical field attached to $L \subset \Omega(t)$ and called the *Burgers vector* (this is the famous Weingarten's theorem). Consider the current configuration $\Omega(t)$ (a bounded simply connected set) with a single dislocation L and any dividing surface S_L containing L. The set $\Omega(t) \setminus L$ is not simply connected, but the upper and lower subsets of $\Omega(t)$, $\Omega^+(t)$ and $\Omega^-(t)$ divided by S_L, are simply connected and in each (an inverse) displacement field $u_{S_L} : \Omega(t) \to \mathbb{R}^3$ may be defined, which will be discontinuous at S_L, and will define a reference configuration with a mismatch along a surface corresponding to the image of the jump set. This is precisely what characterizes the presence of a dislocation. Now, the map $\Phi := (\mathrm{Id} \ + u_{S_L})$ allows us to define the associated elastic deformation tensor $F = \nabla\phi$ (to be precise, an inverse deformation tensor[1]) which is also discontinuous at S_L. Taking two curves $\alpha^\pm$ in $\Omega^\pm(t)$ with the same startpoint and two distinct endpoints outside and inside L in S_L, one classically has:

$$b = \int_{\alpha^\pm} F dl, \tag{1.1}$$

otherwise said, ϕ shows a jump of amplitude b at the jump set S_L° enclosed by L. Hence its distributional derivative writes as $D\phi = F + b \otimes n\mathcal{H}^2 \llcorner_{S_L^\circ}$ and it holds $-\,\mathrm{Curl}\ F = \ \mathrm{Curl}\ (b \otimes n\mathcal{H}^2 \llcorner_{S_L^\circ})$ (n representing the unit oriented normal to S). Thus by Stokes theorem and written in terms of the *dislocation density*

$$\Lambda := \tau \otimes b\mathcal{H}^1 \llcorner_L$$

(with τ the oriented tangent vector to $L \subset \Omega(t)$) it holds

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

1.3 The variational framework

Coming back to the physics and the mathematical properties of dislocations, we have already mentioned that in linear elasticity $F \in L^p(\Omega(t), \mathbb{M}^3)$ with $1 \leq p < 2$, while specific examples for elastic bodies also show that p cannot be greater or equal to 2 [31]. In fact, this properties originates from relation (1.1) which shows that F behaves asymptotically near L as the inverse of the distance to L. Moreover, with a view to a global model, cavitation solutions cannot be ruled out, since they are at the origin of the nucleation of dislocations from the growth of micro-voids in the bulk [21]. Here, classical examples show that deformation allowing for radial cavitation are such that $\mathrm{cof}F \in L^q(\Omega(t), \mathbb{M}^3)$ with $1 \leq q < 3/2$ [13]. Thus, one cannot restrict to the interval $3/2 \leq p < 2$ where some existence results in finite elaticity exists [20], and must allow F, $\mathrm{cof}F \in L^p(\Omega(t), \mathbb{M}^3)$ in the whole range $1 \leq p < 2$. For this reason, as suggested in [20], *Cartesian maps* will be considered [12]. Moreover, nucleation of a dislocation loop 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

[1] This convention – of considering the inverse deformation gradient, defined in $\Omega(t)$ –, can also be found in [1]. In fact, it is prefered to have a discontinuous reference configuration, while the current configuration is the continuous medium containg the –possible moving– dislocation network. Thus, the energy density of $\Omega(t)$ will also depend on such a F.

only that $\det F$, $\operatorname{cof} F \in L^p(\Omega(t), \mathbb{M}^3)$ but also that their distributional counterpart have no s-dimensional ($0 \leq s \leq 3$) singular parts in $\Omega \setminus L$, that is, $\operatorname{Det} F$, $\operatorname{Cof} F \in L^p(\Omega(t), \mathbb{M}^3)$ locally away from L [19]. Indeed, the dislocation induces a jump set where the distributional Jacobian concentrates. As a consequence, the strain energy density $W_{\mathrm{e}} : \mathbb{M}^3 \to \mathbb{R}$ will depend on F, $\operatorname{cof} F$ and $\det F$ and be assumed polyconvex, i.e., convex in each variable separately, and satisfying the growth

$$W_{\mathrm{e}}(F) \geq C(|F|^p + |\operatorname{cof} F|^p + |\det F|^p) - \beta \tag{1.3}$$

for some $C, \beta > 0$. In our problem, strain gradients play a crucial role and thus a strain-gradient elastic energy involving F and $\operatorname{Curl} F$ will apply. This can be achieved by considering an energy of the form $\tilde{\mathcal{W}}(F, \operatorname{Curl} F) = \int_\Omega W_{\mathrm{e}}(F)dx + \tilde{\mathcal{W}}_{\mathrm{defect}}(\operatorname{Curl} F)$ or equivalently since $-\operatorname{Curl} F = \Lambda_{\mathcal{L}}^{\mathrm{T}}$ (here $\mathcal{L}$ denotes the current associated to L) in terms of the *internal thermodynamic variable* $\Lambda_{\mathcal{L}}$ as $\mathcal{W}(F, \mathcal{L}) = \int_\Omega W_{\mathrm{e}}(F)dx + \mathcal{W}_{\mathrm{defect}}(\Lambda_{\mathcal{L}})$, where

$$\mathcal{W}_{\mathrm{defect}}(\Lambda) \geq C\|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\Omega)}, \tag{1.4}$$

allowing us to control pathological behaviours of dislocation clusters. The defect part of the energy can also be seen as the energy depending on the concentration of the Jacobian of the displacement (see section 6.3).

1.4 Scope and structure of the work

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

$$\min_{\substack{F,\mathcal{L} \\ -\operatorname{Curl} F = \Lambda_{\mathcal{L}}^T}} \mathcal{W}(F, \mathcal{L}). \tag{1.5}$$

To achieve the proof of existence, a series of preliminary results must be proved and in particular we define and carefuly analyze two classes of dislocations, at the *mesoscopic* and at the *continuum* scales. To this respect an important result is Theorem 4.5 which states their equivalence under certain conditions. Let us stress that each of these two classes has a specific interest in terms of modeling, according to choice of the dislocation variable: either the line per se (a current, $\mathcal{L}$, which might be followed with time, though in this work we restrict to statics), or its associated density (i.e., a measure, $\Lambda_{\mathcal{L}}$, while evolution of $\mathcal{L}$ is not known everywhere). Then, the two existence results are Theorems 6.5 and 6.6, respectively for the class of mesoscopic and continuum dislocations.

Let us remark that by solving (1.5) we consider a static problem, whereas dislocations are known to be moving defects inside the crystal by the action of mechanical and thermal forces [1,15]. First, we should precise that by considering an equilibrium problem at fixed time t we indeed define a thermodynamical ground-state on the base of which dynamical effects will be added in a second step, beyond the scope of this paper. Second, such minimization states are reached very fast in actual crystals such as pure copper, where resistence to dislocation motion is negligible [5]. Nonetheless we emphasize that the main objective of this work is not the minimization result *per se*, but rather the mathematical definition of dislocations, achieved by means of *integer-multiplicity currents* with coefficient in a group. A similar approch to continuum dislocations by integral currents was already suggested in [16], [15], and [9], without a sistematic description. 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 [7]), with appropriate laws on their Burgers vectors.

The chosen approach to minimize jointly the deformation and the line location is more physical, since the fields of deformation and dislocation density are bound in essence. To our knowledge, this is the first generalization in that direction. Of course, to achieve this purpose, modeling assumptions on the defect-part of the energy must be made, since otherwise dense clusters might appear as limit of minimizing sequences, and hence the mesoscopicity assumption would be violated. We attempted to also give a physical understanding on the growth assumptions, but our aim was mainly to set a mathematical framework, where the complete problem could be studied. We are certain that better assumptions exist, but left these considerations for a more model-oriented future work. In this respect, thanks to our minimization results, the dynamics of the lines at optimality could be analysed and discussed in a subsequent paper [23].

This paper is self-contained and can be read without previous notions neither on dislocations nor on currrents. After collecting some preliminaries, in Section 3 the general notion of dislocations as described by integral currents is provided, while in Section 4 special emphasis is given on its two subclasses of so-called *mesoscopic* and *continuum* dislocations. In particular the relation between these two notions is discussed in Theorem 4.5. 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. Section 6.3 shows how the concept of deformations in the presence of dislocations is related to the space of functions oh bounded higher variations introduced in [17]. 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

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

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_jA_{ij}.[2] For the remaining of this section, our main references are [11, 12].

2.1 Preliminaries on 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 [4, 6].

Theorem 2.1. *(Blaschke) Let $C \subset \mathbb{R}^n$ be a bounded compact set. Then the space $\mathcal{K}(C)$ endowed with the Gromov-Hausdorff distance d_H is sequentially compact.*

In particular, if K_n is a sequence in $\mathcal{K}(C)$ converging to K, than K is a compact set. Moreover, it holds (for the proof see, e.g., [4, 6]):

Theorem 2.2. (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*

$$\mathcal{H}^1(K) \leq \liminf_{n\to\infty} \mathcal{H}^1(K_n). \tag{2.2}$$

2.2 Currents and graphs of Sobolev functions

Let M, n be integers with $0 \leq M \leq n$. We denote by $\Lambda^M\mathbb{R}^n$ and $\Lambda_M\mathbb{R}^n$ the vector spaces of *M-covectors* and *M-vectors* respectively. A M-vector ξ is said *simple* if it can be written as a single wedge product of vectors, $\xi = v_1 \wedge v_2 \wedge \cdots \wedge v_M$. 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 $|\alpha| + |\beta| = n$, $M_{\bar{\alpha}}^{\beta}(A)$ will denote the determinant of the submatrix of A

[2] In this paper we therefore follow the transpose of Gurtin's notation convention [8] 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 [25]- [27] where it holds Curl $A = -A \times \nabla$).

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

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

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

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

For a matrix $A \in \mathbb{M}^3$ 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. Explicitly,

$$M_j^i(A) = A_{ij}, \quad M_J^I(A) = M_{\bar{j}}^{\bar{i}}(A) = (\operatorname{cof} A)_{ij} \quad M_{\{1,2,3\}}^{\{1,2,3\}}(A) = \det A, \tag{2.3}$$

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

$$|M(A)| = \big(1 + \sum_{i,j} A_{ij}^2 + \sum_{i,j} \operatorname{cof}(A)_{ij}^2 + \det(A)^2\big)^{1/2}. \tag{2.4}$$

Let us also define

$$\mathcal{M}(A) := (A, \operatorname{adj} A, \det A), \tag{2.5}$$

and $|\mathcal{M}(A)| := |M(A)|$.

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 and compact support in Ω. Moreover $\mathcal{D}_M(\Omega) := (D(\Omega; \Lambda^M \mathbb{R}^n))'$ is the space of *M-dimensional currents on Ω*, that is, continuous linear functionals on $\mathcal{D}^M(\Omega)$. 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 current obtained by integration on S, i.e.,

$$[\![S]\!](\omega) = \int_S \langle \omega, \vec{S} \rangle d\mathcal{H}^M \qquad \text{for } \omega \in \mathcal{D}^M(\Omega), \tag{2.6}$$

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

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

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

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

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

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

$$\partial F_\sharp T = F_\sharp \partial T. \tag{2.7}$$

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

$$|T| := \sup_{\omega \in \mathcal{D}^M(\Omega), |\omega| \leq 1} T(\omega), \tag{2.8}$$

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

$$|T|_V := \sup_{\substack{\omega \in \mathcal{D}^M(\Omega), |\omega| \leq 1, \\ \mathrm{spt}\omega \subset V}} T(\omega). \tag{2.9}$$

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.

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

$$T(\omega) = \int_S \langle \omega(x), \tau(x) \rangle \theta(x) d\mathcal{H}^M(x) \quad \text{ for } \omega \in \mathcal{D}^M(\Omega). \tag{2.10}$$

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

$$T \equiv \{S, \tau, \theta\} \tag{2.11}$$

will be adopted.

The current $T \in \mathcal{D}_M(\Omega)$ is *rectifiable with integer multiplicity* if it is recifiable with rectifiable boundary, and S, τ, and A integer multiplicity current $\mathcal{T}$ such that $N(\mathcal{T}) < \infty$ is said *integral currents.* The following compactness theorem for integer multiplicity ("i.m.") currents holds:

Theorem 2.3 (Compactness for i.m. currents)**.** *Let $\{\mathcal{T}_i\} \subset \mathcal{D}_k(\Omega)$ be a sequence of integer multiplicity currents such that*

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

with $C > 0$. Then there exist an integer multiplicity current $\mathcal{T} \in \mathcal{D}_k(\Omega)$ and a subsequence, still denoted by $\{\mathcal{T}_i\}_i$, such that $\mathcal{T}_i \rightharpoonup \mathcal{T}$ 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 [11, Section 4.2.25]).

Theorem 2.4. *For every integer-multiplicity current $\mathcal{T}$ there exists a sequence of indecomposable integral currents $\mathcal{T}_i$ such that*

$$\mathcal{T} = \sum_i \mathcal{T}_i \qquad \textit{and} \qquad N(\mathcal{T}) = \sum_i N(\mathcal{T}_i).$$

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

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

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

Approximately differentiability almost everywhere is readily fulfilled if the function u belongs to $W^{1,p}(\Omega, \mathbb{R}^n)$. This will always be the case for the functions considered in the sequel. We refer to [12, Section 3.1.5, Theorem 4] for the proof of this fact and of Theorem 2.5. 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 2.5. *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

$$\omega(x,y) = \sum_{|\alpha|+|\beta|=n} \omega_{\alpha\beta}(x,y))dx^\alpha \wedge dy^\beta. \tag{2.12}$$

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 (2.12), we have

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

2.3 Cartesian maps

Let $u \in W^{1,p}(\Omega;\mathbb{R}^3)$, and suppose $u_i Du_j \in L^1(\Omega,\mathbb{R}^3)$ for all $i \neq j$, we define the *distributional cofactor* of Du, the distribution $\mathrm{Cof}Du$ writing componentwise

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

with indices $i,j \in \{1,2,3\}$ (taken mod 3 when summed and with the derivatives intended in the sense of distributions). Moreover, $\mathrm{Adj}Du$ is the *distributional adjunct* of Du, that is the transpose matrix of the distributional cofactor $\mathrm{Cof}Du$. In general it is not true that the pointwise and distributional adjuncts coincide. Suppose $u_1(\mathrm{adj}Du)^1 \in L^1(\Omega,\mathbb{R}^3)$, with $(\mathrm{adj}Du)^1 := (\mathrm{adj}(Du)_{11}, \mathrm{adj}(Du)_{21}, \mathrm{adj}(Du)_{31})$ being the first column of $\mathrm{adj}Du$. 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.,

$$\langle \mathrm{Det}Du, \varphi\rangle := \int_\Omega u_1(\mathrm{adj}Du)^1 D\varphi dx, \qquad \forall\varphi \in C^\infty_c(\Omega,\mathbb{R}^3).$$

As for the adjunct, in general $\mathrm{Det}Du$ and $\det Du$ differ. Let us define for $p \geq 1$

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

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

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

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

In symbols,

$$G_u(\omega) = \int_\Omega \langle \omega, \frac{M(Du(x))}{|M(Du(x))|}\rangle d\mathcal{H}^n \llcorner_{\mathcal{G}_u}, \tag{2.13}$$

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

$$\mathrm{Cart}^p(\Omega, \mathbb{R}^n) := \{u \in \mathcal{A}^p(\Omega; \mathbb{R}^n) : \partial G_{u \llcorner (\Omega \times \mathbb{R}^n)} = 0\}. \tag{2.14}$$

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

Theorem 2.7. *Let $u_k \in \mathrm{Cart}^p(\Omega, \mathbb{R}^n)$ a sequence such that*

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

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

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

3 Dislocations as currents

A dislocation in an elasto-plastic body arises as a closed arc, or a path connecting two points of the boundary, to which a Burgers vector $b \in \mathbb{R}^3$ and a measure concentrated on the dislocation line (the dislocation density) are associated. Since dislocation densities fullfil linear additivity when dislocation lines overlap, and since to each dislocation 2 preferential directions are associated, which also define its density, we will describe dislocations by the tool of integer-multiplicity 1-currents with coefficients in a group, that in the crystallographic case is assumed isomorphic to $\mathbb{Z}^3$. The coefficient θ represents the Burgers vector with its multiplicity, and the fact that it is constant on any dislocation and that the dislocations are closed correspond to the requirement that such currents are boundaryless (i.e., that the density is divergence free). Moreover, integer-multiplicity 1-currents, thanks to Theorem 3.22, are essentialy Lipschitz curves, and hence a description of dislocations without using the notion of currents is also possi ble. However the notion of currents, as we will see, simplifies some descriptions and provides more direct proofs of some of the following statements. In the sequel, we will introduce and discuss two families of dislocations emphasizing the equivalence between them.

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

Definition 3.1. *A dislocation is a couple $\mathcal{L}_{\mathcal{I}} := (\mathcal{L}_i, b^i)_{i \in \mathcal{I}}$, where $\mathcal{L}_i$ are closed integer-multiplicity 1-currents in Ω, and b^i are vectors of $\mathbb{R}^3$. We define $\mathcal{B}_{\mathcal{I}} = \{b^i\}_{i \in \mathcal{I}}$ the set of* Burgers vectors *of $\mathcal{L}_{\mathcal{I}}$. Each dislocation $\mathcal{L}_{\mathcal{I}}$ can be represented by mean of the quadruple $\{L_i, \tau_i, \theta_i, b^i\}_{i \in \mathcal{I}}$.*

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 basis $\{\bar{b}^1, \bar{b}^2, \bar{b}^3\}$ be fixed, and define the set of *admissible Burgers vectors* as

$$\mathcal{B} := \{b \in \mathbb{R}^3 : \exists \beta \in \mathbb{Z}^3 \text{ such that } b = \sum_{k=1}^{3} \beta_i \bar{b}^i\}. \tag{3.1}$$

Accordingly, if $\mathcal{B}_\mathcal{I} \subset \mathcal{B}$, then $\mathcal{L}_\mathcal{I}$ is called *crystallographic dislocation*. Without loss of generality we will assume that $\bar{b}^i = e_i$, that is $\mathcal{B} := \mathbb{Z}^3$. With this definition we can identify each dislocation with a current with coefficients in the group $\mathbb{Z}^3$. Specifically, given a dislocation $\mathcal{L}_\mathcal{I}$, for all $i \in \mathcal{I}$ we define the current

$$\hat{\mathcal{L}}_i := \{L_i, \tau_i, \theta_i b^i\}, \tag{3.2}$$

which has multiplicity in $\mathbb{Z}^3$. In other words if ω is a 1-form with vector-valued coefficients, i.e. $\omega = (\omega)_j$, $j = 1, 2, 3$, with $\omega_j = \omega_{kj} dx_k$, (with Einstein summation convention on repeated indices), then, for every fixed i,

$$\hat{\mathcal{L}}_i(\omega) := \mathcal{L}_i(\omega b^i),$$

where $\omega b^i = \omega_{kj}(b^i)_j dx_k$. Accordingly, the current associate to the dislocation is defined by

$$\hat{\mathcal{L}}_\mathcal{I} := \sum_{i\in\mathcal{I}} \hat{\mathcal{L}}_i. \tag{3.3}$$

In the sequel the space of 1-forms with vector-valued smooth and compactly supported coefficients will be denoted by $\mathcal{D}^1(\Omega, \mathbb{R}^3)$.

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

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

$$\langle \Lambda_\mathcal{L}, w\rangle := \sum_{i\in\mathcal{I}\subset\mathbb{N}} \mathcal{L}_i((wb^i)^*) = \sum_{i\in\mathcal{I}} \hat{\mathcal{L}}_i(w^T dx), \tag{3.4}$$

for every matrix test function $w := [w_{ij}] \in C^\infty(\bar{\Omega}, \mathbb{M}^3)$, where $(wb^i)^* := w_{kj} b^i_j dx_k$ (with Einstein summation convention on repeated indices) and $dx = (dx_j)_j$.

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

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

$$\Lambda_\mathcal{L} = \Lambda_{\mathcal{L}'}. \tag{3.5}$$

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 Regular dislocations

Definition 3.5 (b-dislocation)**.** *Let $b \in \mathcal{B}$. A b-dislocation $\mathcal{L}^b$ is a dislocation $\mathcal{L}_{\mathcal{I}}$ such that (i) $b^i = b$ for all $i \in \mathcal{B}_{\mathcal{I}}$, (ii) $\mathcal{I}$ is finite with cardinality k_b, (iii) there exist k_b Lipschitz functions $\varphi_i^b : [0, T_i] \to \bar{\Omega}$ with $\mathrm{Lip}(\varphi_i^b) \leq 1$ such that*

$$\mathcal{L}_i = \varphi_{i\sharp}^b [\![[0, T_i]]\!]. \tag{3.6}$$

Moreover, for all $i \leq k_b$ we have either $\varphi_i^b(0) = \varphi_i^b(T_i)$ or $\varphi_i^b(0), \varphi_i^b(T_i) \in \partial\Omega$. We set

$$\mathcal{L}^b = \sum_{i \in \mathcal{I}} \mathcal{L}_i. \tag{3.7}$$

The current $\hat{\mathcal{L}}^b$ defined by

$$\hat{\mathcal{L}}^b(\omega) := \mathcal{L}^b(\omega b), \tag{3.8}$$

for all 1*-form with vector-valued coefficients $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$, is called* b-dislocation current *associate to $\mathcal{L}^b$.*

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

By Theorem 2.4, one can always decompose $\mathcal{L}^b$ as follows

$$\mathcal{L}^b = \sum_{i \in \mathcal{I}^b} \mathcal{L}_i^b, \tag{3.9}$$

with $\mathcal{L}_i^b$ indecomposable 1-current such that $\sum_{i \in \mathcal{I}^b} N(\mathcal{L}_i^b) = N(\mathcal{L}^b)$. The components $\mathcal{L}_i^b$ are called *current loops*. Thanks to the Lipschitzianity of the functions φ_j^b one has $\sum_{j=1}^{k_b} l_j^b := \sum_{j=1}^{k_b} \int_0^{T_j} \|\dot{\varphi}_j^b\| dt < \infty$, meaning that the total length of the supporting set of the current $\mathcal{L}^b$ counted with overlapping is finite. Here 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 path (with endpoints belonging to $\partial\Omega$).

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

$$\mathcal{L}^b(\omega) = \int_{L^b} \langle \omega(x), \tau^b(x) \rangle \theta^b(x) d\mathcal{H}^1(x) \qquad \text{for } \ \omega \in \mathcal{D}^1(\Omega). \tag{3.10}$$

We can choose

$$L^b := \bigcup_{j=1}^{k_b} \varphi_j^b([0, T_j]), \tag{3.11}$$

for the rectifiable set supporting the current $\mathcal{L}^b$, and we will also write $\mathcal{L}^b = \{L^b, \tau^b, \theta^b\}$. With such a choice L^b is a compact set. Note that with this choice for the dislocation set, in general L^b does not coincide with the geometrically necessary dislocation set $L^\star$, since somewhere on L^b it may happen that $\theta^b = 0$. Indeed, with this notation, θ^b may also take the value 0 in a set of $\mathcal{H}^1$ positive measure. If $\mathcal{L}_i^b$ are the indecomposable components of $\mathcal{L}^b$ in (3.9), we write

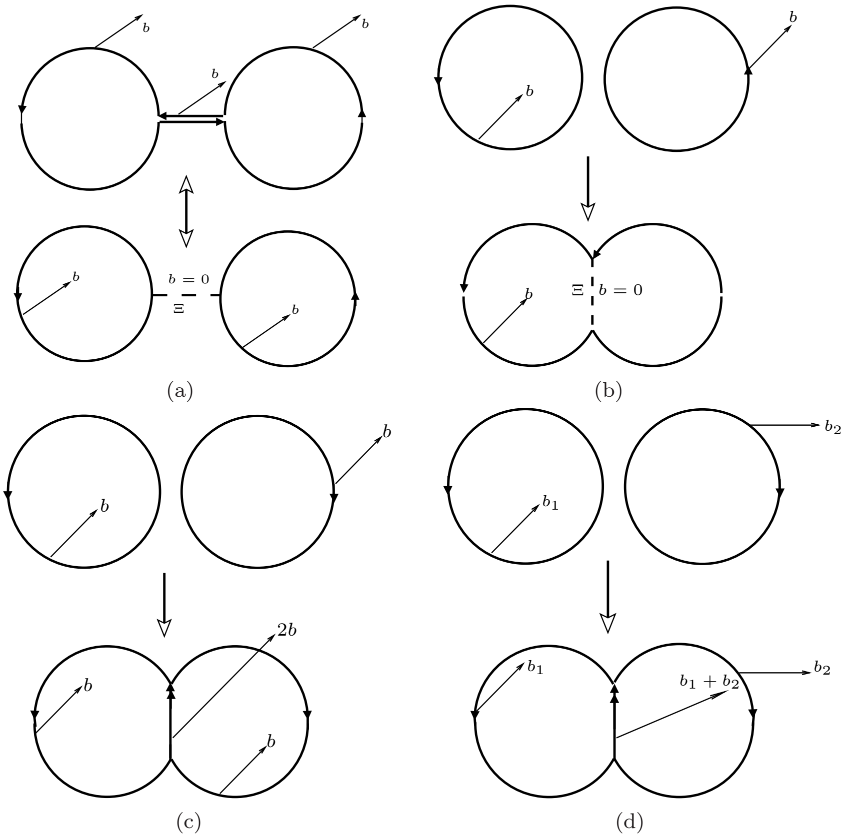

Figure 1: Typical indecomposable dislocation loops and the resulting dislocation currents: in (a), a single b-dislocation loop is equivalently viewed as two indecomposable b-loops with opposite orientations and connected by a geometrically unnecessary arc Ξ; the inverse property is observed in (b) where two identical b-loops give rise to a single connected b-dislocation loop and a geometrically unnecessary arc Ξ where $\Lambda = 0$; in contrast, (c) describes two b-loops with opposite orientation 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.

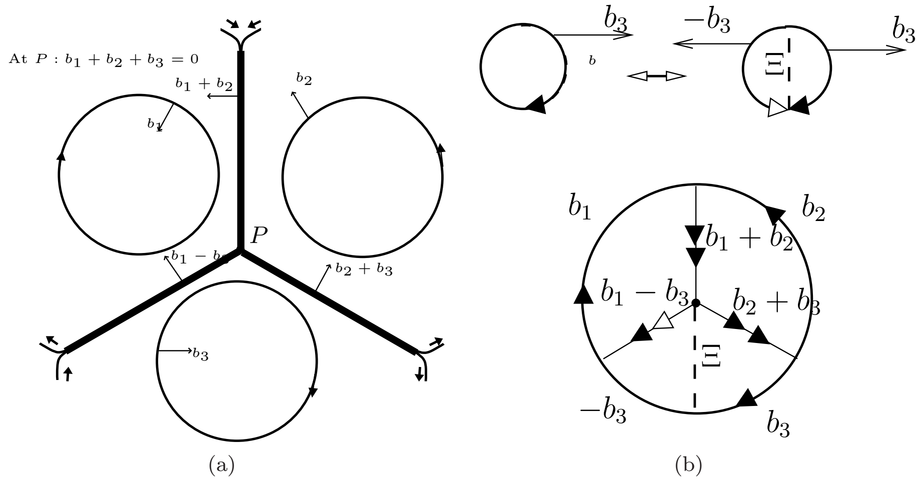

Figure 2: For certain combinations of Burgers vectors, the three separated loops of (a) might intersect and form the cluster element of (b) where the Frank law at the intersection points is satisfied.

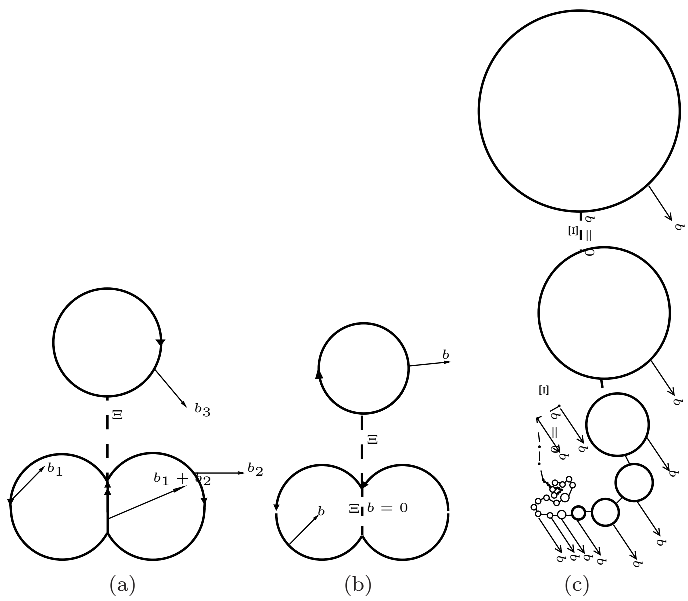

Figure 3: Different kinds of cluster components: in (a) the sum of b-current dislocations $\mathcal{L}^{b_1} + \mathcal{L}^{b_2} + \mathcal{L}^{b_3}$ is depicted, whereas (b) shows a single b-current constituted of three elementary b-loops. In (c) a b-dislocation cluster writing as $\mathcal{L}^b = \varphi^b_\sharp[\![0, T]\!]$ is shown: it can be viewed as a countable chain of indecomposable b-loops interconnected with geometrically unnecessary arcs.

$\mathcal{L}_i^b = \{L_i^b, \tau^b, \theta^b\}$, 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 $\{x \in L^b : \theta^b(x) = 0\}$.

As for general dislocations, to any b-dislocation we associate a *density.*

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

$$\langle \Lambda_{\mathcal{L}^b}, w\rangle := \mathcal{L}^b((wb)^*), \tag{3.12}$$

for every $w := [w_{ij}] \in C_c^\infty(\Omega, \mathbb{M}^3)$, where $(wb)^* := w_{kj} b_j dx_k$.

Note that, by (3.8), if we identify smooth compactly supported tensor-valued fields with smooth 1-forms with vector-valued coefficients, the density and the current associated to a dislocation becomes the same object.

Since k_b is finite $\Lambda_{\mathcal{L}^b}$ is always a Radon measure. In the sequel we will use the following shortcut notation from (3.10) and (3.12):

$$\Lambda_{\mathcal{L}^b} = \mathcal{L}^b \otimes b = \tau^b \otimes b\theta^b\, \mathcal{H}^1 \llcorner_{L^b}. \tag{3.13}$$

Definition 3.7 (Regular dislocation)**.** *A* regular dislocation *is a sequence of b-dislocations $\mathcal{L}_\mathcal{B} := \{\mathcal{L}^b\}_{b\in\mathcal{B}}$ whose total density (or associate current) has finite mass. According to the previous definitions, the dislocation current, still denoted by $\hat{\mathcal{L}}$, and the* dislocation density $\Lambda_\mathcal{L}$*, are given by*

$$\hat{\mathcal{L}} := \sum_{b\in\mathcal{B}} \hat{\mathcal{L}}^b, \qquad \Lambda_\mathcal{L} := \sum_{b\in\mathcal{B}} \Lambda_{\mathcal{L}^b}. \tag{3.14}$$

The dislocation set L *is defined as*

$$L := \bigcup_{b\in\mathcal{B}} L^b, \tag{3.15}$$

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

$$\tau \in \mathrm{Tan}L, \qquad \theta = \sum_{b\in\mathcal{B}} \mathrm{sg}(\tau^b)\theta^b b, \tag{3.16}$$

where $\mathrm{sg}(\tau^b)$ being 1 or -1, chosen in such the way that $\tau = \mathrm{sg}(\tau^b)\tau^b$ (note that $\theta \in \mathbb{Z}^3$, while $\theta^b \in \mathbb{Z}$).

The dislocation current $\mathcal{L} = \{L, \tau, \theta\}$ is said connected if L is a connected set. By (3.7), every dislocation current can also be written as

$$\hat{\mathcal{L}}(\omega) = \sum_{b\in\mathcal{B}} \hat{\mathcal{L}}^b(\omega) = \sum_{b\in\mathcal{B}} \sum_{1\le j\le k_b} \varphi^b_{j\sharp}[\![0, T_j]\!](\omega b), \tag{3.17}$$

for all $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$, and, enumerating the family of generating functions $\{\varphi_j^b\}$, we construct a set of indices $\mathcal{J} = \mathcal{J}(\mathcal{L})$ such that

$$\sum_{b\in\mathcal{B}} \sum_{1\le j\le k_b} \varphi^b_{j\sharp}[\![0, T_j]\!] = \sum_{j\in\mathcal{J}} \varphi_{j\sharp}[\![0, T_j]\!]. \tag{3.18}$$

Moreover, setting $S_i := \varphi_i([0, T_i])$, from (3.11) and (3.15) we also have

$$L = \bigcup_{j\in\mathcal{J}} S_j. \tag{3.19}$$

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* $\subset$.

3.2 Canonical regular dislocations

Among all geometrically equivalent dislocations there exists one representation which is sharp in the sense that it is expressed in terms of the independent elementary Burgers vectors. Let $\mathcal{L}_{\mathcal{B}}$ be a regular dislocation. Since a b-dislocation $\mathcal{L}^b$ 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 (2.11), we introduce

$$\mathcal{L}^{b,i} := \{L^b, \tau^b, \beta_i\theta^b\}, \tag{3.20}$$

with the corresponding density $\Lambda_{\mathcal{L}^{b,i}} := \mathcal{L}^{b,i} \otimes e_i = \mathcal{L}^b \otimes \beta_i e_i$. Observe that for fixed b it holds

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

To any regular dislocation $\mathcal{L}_{\mathcal{B}}$ we associate univoquely three currents $\{\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3\}$, with

$$\mathcal{L}_i := \sum_{b\in\mathcal{B}} \mathcal{L}^{b,i}, \tag{3.21}$$

so that $\mathcal{L}_i = \{L, \tau, \theta_i\}$, 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 associate to* $\mathcal{L}_{\mathcal{B}}$:

$$\hat{\mathcal{L}} = \hat{\mathcal{L}}_1 + \hat{\mathcal{L}}_2 + \hat{\mathcal{L}}_3, \tag{3.22}$$

where $\hat{\mathcal{L}}_i$ is the i-th component of $\hat{\mathcal{L}}$ defined as

$$\hat{\mathcal{L}}_i(\omega) := \mathcal{L}_i(\omega e_i) = \mathcal{L}_i(\omega_i), \tag{3.23}$$

for all $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$, and fixed $i = 1, 2, 3$. In other words $\hat{\mathcal{L}}_i = \{L, \tau, \theta_i e_i\}$.

A usefull property of the decomposition (3.22) is that the three measures $\{\Lambda_{\mathcal{L}_i}\}_{i=1}^3$ operate on different (pointwise) orthogonal subspaces of $C_c^\infty(\mathbb{R}^3, \mathbb{M}^3)$.

Lemma 3.9. *The following assertions hold true:*

(a) The currents $\mathcal{L}_i$ $(i = 1, 2, 3)$ *are integer-multiplicity currents in* Ω. *As a consequence* $\hat{\mathcal{L}}_i$ *are integral currents with coefficients in* $\mathbb{Z}^3$.

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

$$|\mathcal{L}_i|_\Omega = |\hat{\mathcal{L}}_i|_\Omega = \|\Lambda_{\mathcal{L}_i}\|_{\mathcal{M}(\Omega)} \leq \|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\Omega)} = |\hat{\mathcal{L}}|_\Omega, \tag{3.24}$$

for $i = 1, 2, 3$.

(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 2.3 since $\sum_{b\in\mathcal{B}} N(\mathcal{L}^{b,i}) < \infty$ by definition of regular dislocation.

The equalities in (3.24) follows by definitions and identifying forms with smooth functions. Moreover it holds

$$\Lambda_{\mathcal{L}} = \sum_{b\in\mathcal{B}} \Lambda_{\mathcal{L}^b} = \sum_{i=1}^{3} \Lambda_{\mathcal{L}_i}, \tag{3.25}$$

and explicitly,

$$\Lambda_{\mathcal{L}} = \sum_{i=1}^{3} \tau \otimes e_i \theta_i \, \mathcal{H}^1 \llcorner_L = \sum_{i=1}^{3} \mathcal{L}_i \otimes e_i, \tag{3.26}$$

(recall that τ and θ_i are functions of $x \in L$). So that

$$\|\Lambda_{\mathcal{L}}\|_{\mathcal{M}} \geq \|\Lambda_{\mathcal{L}_i}\|_{\mathcal{M}} \qquad \text{for } i = 1, 2, 3. \tag{3.27}$$

To prove (c), observe first that $\mathcal{L}_i = \{L, \tau, \theta_i\}$ and by definition of $\mathcal{L}_i$ and $\Lambda_{\mathcal{L}_i}$ it easily follows that $\mathrm{spt}\mathcal{L}_i = \mathrm{spt}\Lambda_{\mathcal{L}_i}$. 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 $C_c^\infty(\mathbb{R}^3, \mathbb{M}^3)$. □

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

Let us remark that L defined in (3.19) depends on the generating loops of Definition 3.5.

4 Classes of admissible dislocations

In view of studying the dislocations motion, 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 deforms, intersect with others etc., whereas the second will be more appropriate if the model relevant quantity is the dislocation density, and not the single lines. In the latter case dislocations are determined up to the equivalence relation (3.5) 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)**.** *The number of generating loops is finite, i.e.,*

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

with κ_b introduced in Definition 3.5.

Let us recall that a finite number of generating b-dislocation currents does not imply that the dislocation density $\Lambda_{\mathcal{L}}$ is associated to a finite number of distinct Burgers vectors, since the multiplicity on each arc of L is not limited and since countably intersections of arcs may take place (in other words, the resulting Burgers vector might be very large, provided it is attached to an arc which is small enough). Moreover, the cluster of Fig. 3(c) made of countably many loops whose lengths are summable and interconnected by unnecessary segments, is a mesoscopic dislocation since it can be generated by a single b-loop.

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

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

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

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

with $\mathcal{B}^{\mathcal{L}} := \{b \in \mathbb{Z}^3 : k_b \neq 0\}$ (Recall l_i^b is the length of the dislocation loop φ_i^b).

(b) The dislocation current $\hat{\mathcal{L}}$ is an integral current with coefficients in $\mathbb{Z}^3$ satisfying

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

with $\mathcal{B}^{\mathcal{L}} := \{b \in \mathbb{Z}^3 : k_b \neq 0\}$. In particular θ and θ_i, for $i = 1, 2, 3$ are all summable functions with respect to $\mathcal{H}^1 \llcorner_L$.

(c) The dislocation set L of the current $\mathcal{L}$ (defined in (3.15)*) is a closed set with finite $\mathcal{H}^1$-measure. In particular $L^\star \subseteq L$ and $L = L^\star \cup \Xi$.*

Proof. To prove (a), observe that $\mathcal{L} = \{\mathcal{L}^b\}_{b\in\mathcal{B}^{\mathcal{L}}}$ and hence $\|\Lambda_{\mathcal{L}}\| \leq \sum_{b\in\mathcal{B}^{\mathcal{L}}} \|\mathcal{L}^b \otimes b\| \leq \sum_{\substack{b\in\mathcal{B}^{\mathcal{L}}\\ i=1,\ldots,k_b}} \|\mathcal{L}_i^b \otimes b\| \leq \sum_{\substack{b\in\mathcal{B}^{\mathcal{L}}\\ i=1,\ldots,k_b}} |b| l_i^b$, which is finite since the sum is finite by the mesoscopicity Assumption 4.1. Statement (b) follows from (a) and property (b) of Lemma 3.9. Property (c) is a straightforward consequences of the fact that $\mathcal{H}^1(L) \le \sum_{\substack{b\in\mathcal{B}\\ i=1,\dots,k_b}} l_i^b = \sum_{\substack{b\in\mathcal{B}\\ i=1,\dots,k_b}} \int_0^{T_i} \|\dot{\varphi}_i^b\| dt < \infty$ by the mesoscopicity Assumption 4.1. □

We are ready to define the class of *admissible dislocations at the mesoscale*.

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

$$\mathcal{MD} := \{\mathcal{L} = \{\mathcal{L}^b\}_{b\in\mathcal{B}} : \mathcal{L}^b \textit{ takes the form } (3.7) \textit{ and satisfies Assumption 4.1.}\}. \tag{4.4}$$

4.2 Dislocations at the continuum scale

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

Definition 4.4. *[Admissible continuum dislocation]*

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

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 1-sets is an admissible dislocation at the continuum scale. Contrarily to mesoscopic dislocations (cf. Lemma 4.2 (b)), the density of a continuum dislocation must not be finite (this might happen for an unconstraint family of Burgers vectors).

4.3 An equivalence result

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

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

To prove Theorem 4.5 we need some preliminary Lemmas:

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

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

$$\mathcal{S} := \{\phi : S^1 \to K \text{ satisfying the following three properties}\} \tag{4.6}$$

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

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

(iii) Letting $C = \phi(S^1)$ and $L_C = \mathcal{H}^1(C)$, the curve ϕ is Lipschitz with constant $\frac{L_C}{\pi}$.

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

We now are in the hypotheses of the Zorn's Lemma, so that we get a maximal element ψ for the class $\mathcal{S}$. It remains to show that ψ is onto. Suppose it is not the case. We set $C_\psi := \psi(S^1)$ and suppose $X \in K \setminus C_\psi$. Since C_ψ is closed and K is connected, there is a Lipschitz continuous arc $\alpha : [0,1] \to K$ 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 suitably 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 4.7. *Let K be a compact 1-set and $\psi : S^1 \to K$ be a Lipschitz continuous map homotopic to a constant map. 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 nonzero, the decomposition theorem implies that there exists $T = \alpha_\sharp[\![S^1]\!]$ an undecomposable component of the 1-current $\psi_\sharp[\![S^1]\!]$. Let X_α be the homotopy class of T, setting $\hat{T} = \psi_\sharp[\![S^1]\!] - T$, it turns out that the homotopy class of $\hat{T} := \hat{\alpha}_\sharp[\![S^1]\!]$ is $-X_\alpha$. Since K is a compact 1-set, the unique arc (up to adding 0-homotopic branches) with homotopy class X_α is the one passing on ∂X_α. This means that ∂X_α is run (at least) twince, one time by α and another time by $\hat{\alpha}$ with opposite direction. But this contradict the fact that $\alpha_\sharp[\![S^1]\!]$ is an undecomposable component. Thus $\psi_\sharp[\![S^1]\!] = 0$ and the proof is complete. □

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 4.6, so that there are points $x_j \in S^1$ such that $\psi(x_j) = \beta_j(1)$. Suppose for simplicity $x_1 = 1$ and x_j are clockwise ordered on S^1. Setting $\psi_j := \psi\llcorner[x_j, x_{j+1}]$, then the chain

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

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

The precise equivalence theorem is stated as follows.

Theorem 4.8. *Let $\mathcal{L}_\mathcal{I}$ be a continuum dislocation such that $\mathcal{B}_\mathcal{I} \subset \mathbb{Z}^3$ and $\Lambda_{\mathcal{L}_\mathcal{I}}$ is finite. Then $\mathcal{L}_\mathcal{I}$ is a mesoscopic dislocation.*

Proof. Considering the canonical dislocation current $\hat{\mathcal{L}}$ equivalent to $\mathcal{L}_\mathcal{I}$ (cf. Eq. (3.22)), the thesis follows from Eq. (3.24) and Theorem 4.5. Indeed the latter provides three Lipschitz functions α_i $(i = 1, 2, 3)$ such that $\alpha_{i\sharp}[\![S^1]\!] = \mathcal{L}_i$ so it follows $\Lambda_\mathcal{L} = \sum_i \alpha_{i\sharp}[\![S^1]\!] \otimes e_i$. □

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

4.4 Boundary conditions for dislocations

Let U be a bounded open set such that $U \cap \partial\Omega = \partial_D\Omega$.

Definition 4.9 (Boundary conditions)**.** *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 $(P_i, Q_i, \mathcal{B}_D)_{0\leq i\leq N}$ with $\{P_i\}$ and $\{Q_i\}$ sequences of points in $\partial_D\Omega$, and $\mathcal{B}_D = \{b_D^i\}_{0<i\leq N}$ a sequence of vectors belonging to $\mathcal{B}$. We associate to $\mathcal{P}$ the 0-current with coefficients in $\mathbb{Z}^3$ as* $\hat{T}_D := \sum_{0<i\leq N} \delta_{P_i} b_D^i - \delta_{Q_i} b_D^i$*, with δ_P the Dirac mass at P.*

(iii) $\alpha_D := \alpha + \alpha'$ *is the sum of two mesoscopic dislocations in* U. *We suppose that* α *is a closed current with support in* $\partial_D\Omega$ *consisting of* $M < \infty$ *loops* α_i *and Burgers vector* b^i_α, *while* α' *consists of the union of* N *dislocation loops* α_i *with support in* $\bar{U} \setminus \Omega$, *such that for all* i, α_i *has boundary* $\partial\alpha_i = \delta_{Q_i} - \delta_{P_i}$ *and associated Burgers vector* $b^i_D \in \mathcal{B}_D$.

From (iii) we can define $\Lambda_{\alpha_D} = \sum_{0\le i\le M} \alpha_{b^i_\alpha} \otimes b^i_\alpha + \sum_{0\le i\le N} \alpha_{b_{\hat{\alpha}^i}} \otimes b^i_D$ to be the density of the dislocation current α. According to the definitions of dislocation currents given above we denote by $\hat{\alpha}_D$, $\hat{\alpha}$, and $\hat{\alpha}'$ the corresponding currents with coefficient in $\mathbb{Z}^3$.

Definition 4.10. *We say that the boundary condition* $(N, \mathcal{P}, \alpha_D)$ *is* admissible *if the following condition is satisfied: there exists a regular dislocation* $\mathcal{L}$ *such that* $\partial\hat{\mathcal{L}} = \hat{T}_D$. *We say that a dislocation* $\mathcal{L}$ *satisfies the admissible boundary condition* $(N, \mathcal{P}, \alpha_D)$ *if it satisfies the previous property.*

As a consequence of the previous definition, it turns out that $\hat{\alpha}_D + \hat{\mathcal{L}}$ is closed in $\bar{U} \cup \bar{\Omega}$.

5 The class of admissible deformations

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 dislocation $\mathcal{L}' := \mathcal{L} + \alpha$ by $\mathcal{L}$. In other words, when referring to an admissible dislocation current, it is intended that it has been already summed with $\hat{\alpha}$. We also fix a map $\bar{F} \in L^p(\hat{\Omega}, \mathbb{M}^3)$ such that $-\operatorname{Curl} \bar{F} = (\Lambda_\alpha)^{\mathrm{T}}$ on U.

Definition 5.1.

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

(i) *The dislocation current* $\hat{\mathcal{L}} = \{L, \tau, \theta\}$ *satisfies the boundary condition and the function* $\hat{F} := \chi_{\hat{\Omega}\setminus\Omega}\bar{F} + \chi_\Omega F \in L^p(\hat{\Omega}, \mathbb{M}^3)$ *is such that* $-\operatorname{Curl} \hat{F} = (\Lambda_{\mathcal{L}})^{\mathrm{T}}$ *in* $\hat{\Omega}$ *(*χ_A *denoting the characteristic function of* A*).*

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

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

Let us recall that if $F = Du$ is the gradient of a Cartesian map, then it is readily satisfied that the distributional determinant $\operatorname{Det}(F)$ and adjoint $\operatorname{Adj}(F)$ of F are elements of $L^1(U, \mathbb{M}^3)$ and coincide with $\det(Du)$ and $\operatorname{adj}(Du)$ respectively. It is also straightforward that smooth functions $u \in C^1(U, \mathbb{R}^3)$ are Cartesian.

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

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

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 S_L is a Lipschitz and closed surface in Ω with boundary L and normal ν, $\Omega \setminus S_L$ is simply connected and hence there exists a function $\phi \in W^{1,p}(\Omega \setminus S_L)$ such that $F = \nabla\phi$ in $\Omega \setminus S_L$. By (5.2), ϕ has a constant jump on S_L (i.e., $[\![\phi]\!]_{S_L} = b$). Thus the distributional derivative of ϕ writes as $D\phi = \nabla\phi + b \otimes \nu\mathcal{H}^2 \llcorner_{S_L}$. Multiplying by a test function ψ one has by (2.1) that $\langle \operatorname{Curl}(b \otimes \nu\mathcal{H}^2 \llcorner_{S_L}), \psi\rangle = \langle b \otimes \nu\mathcal{H}^2 \llcorner_{S_L}, \operatorname{Curl}\psi\rangle$. Componentwise, by Stokes theorem, it reads as

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

and hence $\langle \operatorname{Curl}(b \otimes \nu\mathcal{H}^2 \llcorner_{S_L}), \psi\rangle = \langle (b \otimes \tau\mathcal{H}^1 \llcorner_L), \psi\rangle$.

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

Proof. We first construct an admissible function for a simple geometry. Consider the circle $L := \{(x, y, z) \in \mathbb{R}^3 : |x|^2 + |y|^2 = R^2,\ z = 0\}$ as a dislocation loop with Burgers vector $b = \beta_1\underline{e}_1 + \beta_2\underline{e}_2 + \beta_3\underline{e}_3 = \beta_R\underline{h}_R + \beta_l\underline{h}_l + \beta_z\underline{h}_z$, with the local basis on L, $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\} = Q(l)\{\underline{e}_1, \underline{e}_2, \underline{e}_3\}$ where $Q(l)$ is the matrix of rotation around $\underline{e}_3 = \underline{h}_z$ and with angle l (see Fig. 4(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 left of Fig. 4(a) denoted as S or V in the sequel), while the coordinate r is the distance from the set L, and l, as before, R times the angle around z axis. In V_δ we denote by $\underline{g} := (\underline{g}_r, \underline{g}_\theta, \underline{g}_l)$, with $\underline{g}_l = \underline{h}_l$, the local cylindrical basis defined on the normal sections ∂V_δ, corresponding to such coordinates. We then consider the function F inside V_δ whose components in the basis $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\}$ read

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

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 $0 \leq l \leq 2\pi$, and in order to fix the arbitrary constant, set $\phi_\delta = 0$ on $S \cap \{\theta = a\}$ and $\phi_\delta = b$ on $\bar{S} \cap \{\theta = a + \pi/2\}$. 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 $C_{\bar\theta} := \{(\delta, \bar\theta, l) : 0 \leq l \leq 2\pi R\}$ for every $a < \bar\theta < a + \pi/2$. Let $D_{\bar\theta}$ be the disk with boundary $C_{\bar\theta}$ where for every $x \in D_{\bar\theta}$, $\phi_\delta(x)$ is defined as $\phi_\delta(x) = \phi_\delta(y)$ with $y \in C_{\bar\theta}$; define also $D := \bigcup_{\theta \in (a, a+\pi/2)} D_\theta$. We set $\phi_\delta = 0$ in $\Omega \setminus V \setminus D$ and observe that it is smooth everywhere except at the interface I between V and D and on $J := \bar{D}_{a+\pi/2} \cup (V \cap \{\theta = a + \pi/2\})$ where it has a constant jump of magnitude b (cf. Fig. 4(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.

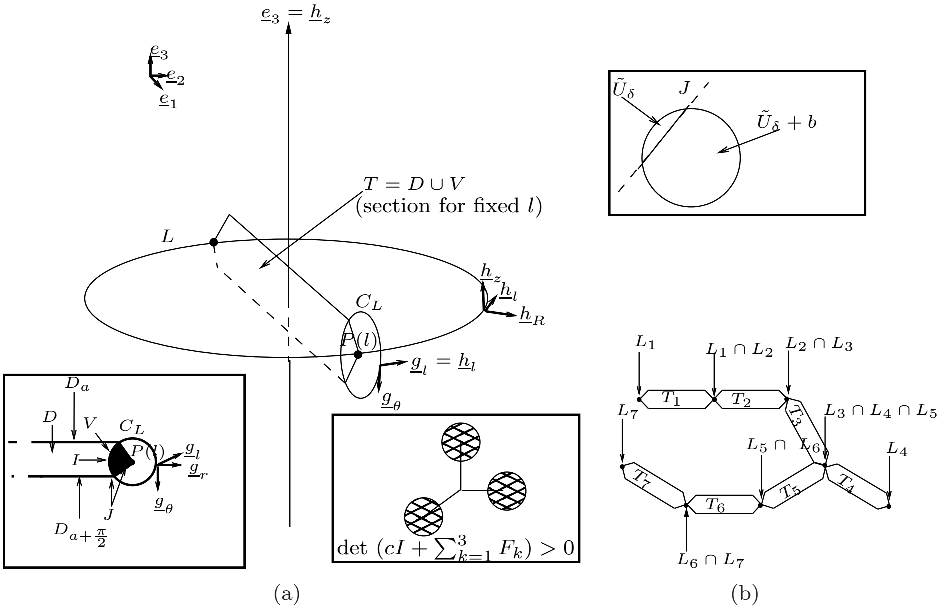

Figure 4: Picture of the tube construction for the proof (a); the case of finitely many boundary dislocation segments (b)

Let us now reproduce this argument for a finite number of circles with possible mutual intersection in $\partial\Omega$, and show that the constant $c > 0$ can be chosen in such a way that the determinant of the resulting deformation still remains non-negative. Let us consider a finite number of loops L_k with $1 \leq k \leq K$ with the associated $T_k := V_k \cup D_k$ constructed as described above, and observe that (by possibly adapting the amplitude of the solid angle S_k, i.e., replacing $\pi/2$ by π/N) the T_k's only intersect at points in L_k for some k's, while keeping the V_k's with empty mutual intersection (cf. Fig 4(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 $f_k(\theta,l) := \beta_l^k(l)\cos\theta - \beta_R^k(l)\sin\theta = \beta_2^k\cos(\theta + \frac{l}{R}) - \beta_1^k \sin(\theta + \frac{l}{R}) \geq 0$ (for instance, if $\beta_1, \beta_2 > 0$ then $a_k := \frac{3\pi}{2} - \frac{l}{R}$). Defining $F := \sum_{k=1}^{K} F_k + cI$, (5.4) entails that F, $\det F$, $\operatorname{adj} F$ belong to L^p and also that

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

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. 4a).

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 curves joining P_i's to the Q_i's without self-intersections and prolonged by a geometrically unnecessary arc in $\partial\Omega$ (an admissible F can be constructed as above in $\hat{\Omega} \supset \Omega$ and then restricted to Ω with its curl restricted to $\bar{\Omega}$). 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 $\mathcal{W} : \mathcal{F}\times\mathcal{MD} \to \bar{\mathbb{R}}$ such that there are positive constants C and β for which

$$\begin{aligned}\mathcal{W}(F,\mathcal{L}) &:= \int_\Omega \mathrm{W_e}(F)dx + \mathcal{W}_{\mathrm{defect}}(\Lambda_{\mathcal{L}}) \geq \\ &\quad C\big(\|\mathcal{M}(F)\|_p + \sum_{j\leq k_{\mathcal{L}}} b^j \|\dot{\varphi}_j\|_{L^1} + k_{\mathcal{L}}\big) - \beta.\end{aligned} \tag{6.1}$$

with the notation

$$\|\mathcal{M}(F)\|_p = \|F\|^p_{L^p} + \|\operatorname{cof} F\|^p_{L^p} + \|\det F\|^p_{L^p}.$$

Let us recall that $k_{\mathcal{L}}$ is defined in (4.1), $\{\varphi_j\}_{j\leq k_{\mathcal{L}}}$ are the generating loops defined in 3.7, and $\mathcal{M}(F)$ is the vector defined in (2.5). Here, W_e is an integrable function and $\mathcal{W}_{\mathrm{defect}}$ a functional defined on Radon measures. It is also assumed that

(W1) $W_{\mathrm{e}}(F) \geq h(\det F)$, 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 $g : \mathbb{M}^3 \times \mathbb{M}^3 \times \mathbb{R}^+ \to \bar{\mathbb{R}}$ s.t. $W_{\mathrm{e}}(F) = g(\mathcal{M}(F))$, $\forall F \in \mathcal{F}$,

(W3) $\mathcal{W}_{\mathrm{defect}} := \mathcal{W}^1_{\mathrm{defect}} + \mathcal{W}^2_{\mathrm{defect}}$, with $\mathcal{W}^1_{\mathrm{defect}}(\Lambda_{\mathcal{L}}) \geq \kappa_1 k_{\mathcal{L}}$ and $W^2_{\mathrm{defect}}(\Lambda_{\mathcal{L}}) \geq \kappa_2 \sum_{1 \leq j \leq k_{\mathcal{L}}} b^j \|\dot{\varphi}_j\|_{L^1}$, for some constitutive material parameters κ_1 and κ_2.

(W4) W^1_{defect} is weakly* lower semicontinuous, that is $\liminf_{k \rightharpoonup \infty} \mathcal{W}^1_{\mathrm{defect}}(\Lambda^k) \geq \mathcal{W}^1_{\mathrm{defect}}(\Lambda)$ as $\Lambda^k \rightharpoonup \Lambda$ weakly* in $\mathcal{M}_b(\bar{\Omega}, \mathbb{M}^3)$.

Note that assumption $(W2)$ implies that $\mathcal{W}_{\mathrm{e}}(F) := \int_\Omega W_e(F)dx$ is weakly lower semicontinuous, i.e., $\liminf_{k\to\infty} \mathcal{W}_{\mathrm{e}}(F^k) \geq \mathcal{W}_e(F)$ as $\mathcal{M}(F^k) \to \mathcal{M}(F)$ weakly in $L^p(\Omega, \mathbb{M}^3) \times L^p(\Omega, \mathbb{M}^3) \times L^p(\Omega)$.

Remark 6.1. *The term involving $\|\dot{\varphi}_j\|_{L^1}$ in the energy bound is mandatory for mesoscopic dislocations, since it controls the length of the lines. In fact, minimizing sequences of Lipschitz maps (describing minimizing sequences of lines) might become locally dense, a phenomenon which should be prohibited to get existence. For a physical viewpoint this term is questionnable since dense arcs of the dislocation cluster might be nonnecessary, and hence admissible from an energetical standpoint. This drawback is addressed in the second existence result for continuum dislocations in Section 6.1. Moreover, recalling* (4.2)*, this term implies a bound on the densities.*

Before stating the existence of minimizers of the problem

$$\inf_{\substack{(F,\Lambda_{\mathcal{L}}) \in \mathcal{F} \times \mathcal{MD} \\ -\operatorname{Curl} F = \Lambda^{\mathrm{T}}_{\mathcal{L}}}} \mathcal{W}(F, \Lambda_{\mathcal{L}}), \tag{6.2}$$

some technical results should be stated and proven.

Lemma 6.2. *Let $(F_k, \mathcal{L}_k)$ be a minimizing sequence for the problem* (6.2)*, and suppose* $\det F_k \rightharpoonup D$ *weakly 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 $\det F_k \rightharpoonup 0$ weakly in $L^p(A)$, which since $\det F_k \geq 0$ on A implies that $\liminf \det F_k = 0$ almost everywhere in A. Indeed, if $B := \{x \in A : \liminf \det F_k(x) > 0\}$ has positive measure, then $\liminf \int_A \det F_k > 0$ since $\chi_A \in L^q(A)$, a contradiction.

Hence from condition $(W1)$ we must have $\mathcal{W}(F_k, \Lambda_{\mathcal{L}_k}) \geq \int_A W_{\mathrm{e}}(F_k, \Lambda_{\mathcal{L}_k})dx \geq \int_A h(\det F_k)dx$. By Fatou's Lemma and the fact that $(F_k, \mathcal{L}_k)$ is a minimizing sequence, the contradiction follows, so A must be negligible, achieving the proof. ☐

Lemma 6.3. *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* $\mathrm{Lip}(\varphi_n) \leq 1$ *for all n. Then, there is a 1-current γ such that, up to subsequence, $\gamma_n \rightharpoonup \gamma$, and $\gamma = \varphi_\sharp[\![0, M]\!]$ for a Lipschitz function φ with* $\mathrm{Lip}(\varphi) \leq 1$.

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 $\mathrm{Lip}(\varphi) \leq 1$ such that, up to subsequence, $\varphi_n \to \varphi$ uniformly. So it easily follows that $\gamma_n \rightharpoonup \gamma := \varphi_\sharp [\![[0, M]]\!]$. ☐

Lemma 6.4. *Let $\hat{\mathcal{L}}_n = \{S_n, \tau_n, \theta_n\}$ be a sequence of equibounded dislocation currents of the form* (3.22) *satisfying the same boundary condition. Then there is a dislocation current $\hat{\mathcal{L}}$ such that $\hat{\mathcal{L}}_n$ weakly converges to $\hat{\mathcal{L}}$ in the sense of currents and that $\Lambda_n := \Lambda_{\mathcal{L}_n}$, the sequence of densities of $\mathcal{L}_n$, weakly* converges to $\Lambda \in \mathcal{M}(\bar{\Omega}, \mathbb{M}^3)$. Moreover $\hat{\mathcal{L}}$ satisfies the boundary condition, it has density equal to $\Lambda = \Lambda_{\mathcal{L}}$, and for all $i = 1, 2, 3$, $\mathcal{L}_i^n \rightharpoonup \mathcal{L}_i$, $\Lambda_i^n \rightharpoonup \Lambda_i$, and $\Lambda_i = \mathcal{L}_i \otimes e_i$ (with the notation* (3.13)*).*

Proof. As in (3.22) we write $\hat{\mathcal{L}}_n = \hat{\mathcal{L}}_n^1 + \hat{\mathcal{L}}_n^2 + \hat{\mathcal{L}}_n^3$, and $\Lambda_n = \Lambda_n^1 + \Lambda_n^2 + \Lambda_n^3$, with $\Lambda_n^i = \mathcal{L}_n \otimes e_i$. By the assumption we have that also $\mathcal{L}_n^i$ are boundaryless in Ω and, thanks to (3.24), we have that $N(\mathcal{L}_n^i)$ are uniformly bounded, so that, by Theorem 2.3, we deduce the existence of three closed integer multiplicity currents $\{\mathcal{L}^i\}_{i=1}^3$ such that $\mathcal{L}_n^i \rightharpoonup \mathcal{L}^i$. Since

$$\hat{\mathcal{L}}_n(\omega) = \sum_{i=1}^{3} \mathcal{L}_n^i(\omega_i) \to \sum_{i=1}^{3} \mathcal{L}^i(\omega_i), \tag{6.3}$$

for all $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$, we get $\hat{\mathcal{L}}_n \rightharpoonup \hat{\mathcal{L}} := \sum_{i=1}^3 \hat{\mathcal{L}}^i$. The fact that $\hat{\mathcal{L}}$ satisfies the boundary condition follows from the fact that $\partial\hat{\mathcal{L}}_n \rightharpoonup \partial\hat{\mathcal{L}}$. Identifying $\mathcal{D}^1(\Omega, \mathbb{R}^3)$ with $C_c^\infty(\Omega, \mathbb{M}^3)$ it is straightforward that $\Lambda_n \rightharpoonup \Lambda = \Lambda^1 + \Lambda^2 + \Lambda^3$ weakly* in $\mathcal{M}(\bar{\Omega}, \mathbb{M}^3)$, with $\Lambda_n^i \rightharpoonup \Lambda^i$ weakly* in $\mathcal{M}(\bar{\Omega}, \mathbb{M}^3)$, and that $\Lambda^i = \mathcal{L}^i \otimes e_i$ for all $i = 1, 2, 3$, achieving the proof. ☐

Now we are ready to solve Problem (6.2).

Theorem 6.5 (Existence in $\mathcal{F} \times \mathcal{MD}$)**.** *Under assumptions $(W1) - (W4)$ and assuming that there exists an admissible $(F, \mathcal{L}) \in \mathcal{F} \times \mathcal{MD}$ such that $\mathcal{W}(F, \Lambda_{\mathcal{L}}) < \infty$, there is at least a $(F, \mathcal{L})$ solution of the minimum problem* (6.2).

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

$$F_n \rightharpoonup F \quad \text{weakly in } L^p(\Omega, \mathbb{M}^3), \tag{6.4a}$$

$$\mathrm{adj}\ F_n \rightharpoonup A \quad \text{weakly in } L^p(\Omega, \mathbb{M}^3), \tag{6.4b}$$

$$\det F_n \rightharpoonup D \quad \text{weakly in } L^p(\Omega). \tag{6.4c}$$

Since we consider extensions $\hat{F}_n$ of F on $\hat{\Omega}$, it is straightforward that we can suppose the same boundedness for $\hat{F}_n$ on $\hat{\Omega}$ as for F_n on Ω, so that $\hat{F}$, $\hat{A}$, and $\hat{D}$ are such that (6.4a)-(6.4c) hold for $\hat{F}_n$, $\hat{F}$, $\hat{A}$, and $\hat{D}$. Moreover, since F_n satisfy the same boundary condition, it is obvious that $\hat{F}_n = \hat{F} = \bar{F}$ on $\hat{\Omega} \setminus \Omega$, so $\hat{F}$ satisfies the boundary condition.

By the uniform bound on $\sum_{j \leq k_{\mathcal{L}}} b^j \|\dot{\varphi}_j\|_{L^1}$ in (6.1) and by (4.2), it holds a uniform bound on $\Lambda_n^T := -\,\mathrm{Curl}\ \hat{F}_n$, and there is a measure $\Lambda \in \mathcal{M}(\bar{\Omega}, \mathbb{M}^3)$ such that

$$\Lambda_n \rightharpoonup \Lambda \quad \text{weakly* in } \mathcal{M}(\bar{\Omega}, \mathbb{M}^3). \tag{6.4d}$$

The result will follow by the direct method of the calculus of variations and classical semicontinuity results for convex functionals, since conditions $(W1)$ – $(W4)$ hold, provided the found minimizer is admissible.

Since the energies at $(F_n, \mathcal{L}_n)$ are uniformly bounded by $k_{\mathcal{L}}$ in (6.1), we can suppose that the dislocation currents $\hat{\mathcal{L}}_n$ are generated by the same number k of 1-Lipschitz functions $\{\varphi_n^j\}_{j=1}^k$, i.e.,

$$\hat{\mathcal{L}}_n(\omega) = \sum_{j=1}^{k} \varphi^j_{n\sharp}[\![[0,M]]\!](\omega b^j) \qquad \text{and} \qquad \Lambda_n = \sum_{j=1}^{k} \varphi^j_{n\sharp}[\![[0,M]]\!] \otimes e_i. \tag{6.5}$$

for all $\omega \in \mathcal{D}^1(\hat{\Omega}, \mathbb{R}^3)$. So by Lemma 6.3 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 $\hat{\mathcal{L}}(\omega) := \sum_j \varphi^j_\sharp[\![[0,M]]\!](\omega b^j)$ for all $\omega \in \mathcal{D}^1(\hat{\Omega}, \mathbb{R}^3)$, by Lemma 6.4 we have $\hat{\mathcal{L}}_n \rightharpoonup \hat{\mathcal{L}}$, $\Lambda_n \rightharpoonup \sum_j \varphi^j_\sharp[\![[0,M]]\!] \otimes b^j$ weakly* in $\mathcal{M}(\hat{\Omega}, \mathbb{M}^3)$, so from (6.4d) we get

$$\Lambda = \sum_j \varphi^j_\sharp[\![[0,M]]\!] \otimes b^j. \tag{6.6}$$

Now, for a test function $w \in C_c^\infty(\hat{\Omega}, \mathbb{M}^3)$, it holds

$$\langle \operatorname{Curl} \hat{F}_n, w\rangle = \langle \hat{F}_n, \operatorname{Curl} w\rangle \to \langle \hat{F}, \operatorname{Curl} w\rangle = \langle \operatorname{Curl} \hat{F}, w\rangle. \tag{6.7}$$

Since the first term in the left-hand side of (6.7) also tends to $\langle -\Lambda^T, w\rangle$, we finally get

$$-\operatorname{Curl} \hat{F} = \sum_j b^j \otimes \varphi^j_\sharp[\![[0,M]]\!]. \tag{6.8}$$

Let us set $L_n := \cup_{j=1}^k \varphi_n^j([0,M])$ and $L := \cup_{j=1}^k \varphi^j([0,M])$. We now want to show that for every point $x \in \Omega \setminus L$ there is a ball $B \subset \Omega \setminus L$ centered at 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 $\varphi_n^j \to \varphi^j$ 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 zero average in B. So that the Poincaré's inequality provides u such that $u_n \rightharpoonup u$ weakly in $W^{1,p}$. Now Theorem 2.6 implies that $A = \operatorname{adj} F$ and $D = \det F$, so the thesis follows from (6.4a)-(6.4c) and Lemma 6.2. $\square$

We remark that with the formulation (6.1) the potential $W(F, \Lambda_{\mathcal{L}})$ depends explicitly on the dislocation current.

6.2 Second existence result

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

As for the first result, we fix a boundary condition α and a map $\bar{F} \in L^p(\hat{\Omega}, \mathbb{M}^3)$ such that $-\operatorname{Curl} \bar{F} = (\Lambda_\alpha)^{\mathrm{T}}$ on U. We redefine the set of admissible functions:

$$\mathcal{F}' := \{F \in L^p(\Omega, \mathbb{M}^3) : F \text{ satisfies (i)-(iii) below}\} \tag{6.9}$$

(i) There exists a continuum dislocation $\mathcal{L} := \mathcal{L}_{\mathcal{I}} \in \mathcal{CD}$ satisfying the boundary condition such that $\hat{F} := \bar{F}\chi_{\hat{\Omega}\setminus\Omega} + F\chi_\Omega \in L^p(\hat{\Omega}, \mathbb{M}^3)$ satisfies $-\operatorname{Curl} \hat{F} = (\Lambda_{\mathcal{L}})^{\mathrm{T}}$ 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 $\mathcal{W} : \mathcal{F}' \to \bar{\mathbb{R}}$:

(W5) there is a positive constant C such that

$$\mathcal{W}(F) \geq C\big(\|\mathcal{M}(F)\|_p + \|\operatorname{Curl} \hat{F}\|_{\mathcal{M}(\bar{\Omega})} + G(\mathcal{L})\big) - \beta,$$

with

$$G(\mathcal{L}) := \inf_{\mathcal{K} \in \mathcal{C}_{\mathcal{L}}} \left(\mathcal{H}^1(\mathcal{K}) + \kappa \#\mathcal{K}\right), \tag{6.10}$$

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

(W6) there exists a weakly lower semicontinuous functional $\mathcal{W}_{\text{defect}}$ such that

$$\mathcal{W}(F) = \mathcal{W}_{\mathrm{e}}(F) + \mathcal{W}_{\text{defect}}(-(\operatorname{Curl} \hat{F})^{\mathrm{T}}).$$

It is also assumed that $\mathcal{W}_{\mathrm{e}}(F) = \int_\Omega g(\mathcal{M}(DF))dx$ with g as in (W2) above and $g(\mathcal{M}(DF)) \geq h(\det F)$, for some continuous real function h such that $h(t) \to \infty$ as $t \to 0$.

As mentioned for the first minimum problem, again we can assume $\mathcal{W}_{\text{defect}} = \mathcal{W}^1_{\text{defect}} + \mathcal{W}^2_{\text{defect}}$, with, for instance, $\mathcal{W}^2_{\text{defect}} = \kappa G$ for some $\kappa > 0$, whereas a typical example for $\mathcal{W}^1_{\text{defect}}$ is the form

$$\mathcal{W}^1_{\text{defect}}(\Lambda) = \int_L \psi(\theta b, \tau) d\mathcal{H}^1, \tag{6.11}$$

where b, θ, and τ represent the Burgers vector, its multiplicity, and the tangent vector to the dislocation loop L, respectively. Under suitable hypotheses on the function ψ, this is proved to be lower semicontinuous in the sense of $(W6)$ (see [9]). As for the function g, hypothesis $(W2)$ fulfills the requirements.

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

Theorem 6.6 (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 $\hat{\mathcal{L}}_n$, and their densities by $\Lambda_n = \Lambda_{\mathcal{L}_n}$. Without loss of generality, if we deal as in the proof of Theorem 6.5, we can assume F_n and $\hat{\mathcal{L}}_n$ be defined on the whole $\hat{\Omega}$. By $(W5)$, F_n converges weakly to F in L^p and Λ_n converges weakly-* to a Radon measure Λ. Thanks to (3.24) $\{\hat{\mathcal{L}}_n\}$ is equibounded, so that one has by Theorem 2.3 the existence of an integer multiplicity current $\hat{\mathcal{L}}$ such that $\hat{\mathcal{L}}_n \rightarrow \hat{\mathcal{L}}$, while by Lemma 6.4, $\Lambda = \Lambda_{\hat{\mathcal{L}}} = -\operatorname{Curl} \hat{F}$ in the distribution sense. Moreover, by admissibility, one can associate to every $\hat{\mathcal{L}}_n$ a continuum $\mathcal{K}_n \subset \hat{\Omega}$ such that $G(\hat{\mathcal{L}}_n) = \big(\mathcal{H}^1(\mathcal{K}_n) + k(\mathcal{K}_n)\big)$. By $(W5)$, Blaschke and Golab theorems, there is convergence in the Gromov-Hausdorff sense to a continuum $\mathcal{K}$. Now we see that the support $L^\star$ of $\hat{\mathcal{L}}$ is a subset of $\mathcal{K}$. Indeed, for all forms $\omega \in \mathcal{D}^1(\hat{\Omega}, \mathbb{R}^3)$ whose support is contained in $\hat{\Omega} \setminus \mathcal{K}$, it holds $\lim_{n\to\infty} \hat{\mathcal{L}_n}(\omega) = 0$, thanks to the fact that $\hat{\mathcal{L}_n}$ has support in $\mathcal{K}_n$ which converges to $\mathcal{K}$ in the Gromov-Hausdorff topology. So we find out that $\hat{\mathcal{L}} = (\hat{L}, \tau, \theta)$ is admissible since $L^\star :=$ supp $\Lambda \subset \mathcal{K}$. Taking now any ball in $\Omega \setminus \mathcal{K}$, we conclude as in the proof of Theorem 6.5. □

The physical interpretation of $G(\mathcal{L})$ is the following. To create a new loop at some finite distance d from the current dislocation $\mathcal{L}$, it is worth to nucleate (i.e., add a connected component) rather than deforming the existent dislocation, as soon as $d > \kappa$. However it should be recognized that (6.10) is at this stage a mathematical assumption whose physical meaning remains to be elucidated. It basicaly 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.

6.3 A weak notion of Jacobian for displacements in the presence of dislocations

Let us firstly introduce some conventions.

Definition 6.7. *For every 1-form $\omega \in \mathcal{D}^1(\mathbb{R}^3)$ we identify $\omega = \omega_i dx_i$, with the vector field $w = w_i \in C_c^\infty(\mathbb{R}^3, \mathbb{R}^3)$ by setting $w_i := \omega_i$ for all $i = 1, 2, 3$. Moreover we identify every 2-form $\omega = \omega_{ij} dx_i \wedge dx_j \in \mathcal{D}^2(\mathbb{R}^3)$ with another vector field $w \in C_c^\infty(\mathbb{R}^3, \mathbb{R}^3)$ by setting $w_i := (-1)^i \omega_{\bar{i}}$. In particular we introduce the* curl *operator on $C_c^\infty(\mathbb{R}^3, \mathbb{R}^3)$ into itself by mean of these identifications, i.e.,*

$$\operatorname{curl} w := d\omega, \tag{6.12}$$

where in the right-hand side we first identificate w with the 1-form ω, then we compute the external derivative, and identificate the resulting 2-form with the corrensponding vector field in $\mathbb{R}^3$.

Definition 6.8. *We can also identify elements $v \in \mathbb{R}^3$ with 2-vectors $v \in \Lambda_2(\mathbb{R}^3)$ by $\Lambda_2(\mathbb{R}^3) \ni v = (-1)^i v_i e_{\bar{i}}$. Similarly, elements $v \in \mathbb{R}^3$ are seen as 1-vectors, as $v = v_i e_i$, $i = 1, 2, 3$. From this correspondence it is possible to identify a distribution $T \in \mathcal{D}'(\mathbb{R}^3, \mathbb{R}^3)$ with a 2-current in $\mathcal{D}_2(\mathbb{R}^3)$, or with a 1-current in $\mathcal{D}_1(\mathbb{R}^3)$, respectively. In particular we can define che* Curl *operator for distributions,* Curl $: \mathcal{D}'(\mathbb{R}^3, \mathbb{R}^3) \rightarrow \mathcal{D}'(\mathbb{R}^3, \mathbb{R}^3)$*, by*

$$\langle \operatorname{Curl} T, \varphi \rangle := \langle T, \operatorname{curl} \varphi \rangle, \tag{6.13}$$

for all $\varphi \in C_c^\infty(\mathbb{R}^3, \mathbb{R}^3)$, where curl *in the right-hand side has been defined in Definition 6.7.*

With this convention we can see the Curl operator defined so far, if applied to $\mathbb{R}^3$-fields, turns out to coincide with the classical definition of curl. For instance, if curl denotes the classical operator and F is a vector field in $\mathbb{R}^3$, then $(\operatorname{Curl} F)_i = (\operatorname{curl} F)_i$, where in the right-hand side we make use of the previous identification.

As a consequence of this identification, if $\mathcal{L}$ is a 1-current with finite mass, then it is a measure in $\mathcal{M}_b(\Omega, \mathbb{R}^3)$. The same holds true for 1-dimensional currents $\mathcal{S}$, that are measures in $\mathcal{M}_b(\Omega, \mathbb{R}^3)$. In particular the boundary of a current corresponds to the Curl of the correspondent measure, since

$$\partial\mathcal{S}(\omega) = \mathcal{S}(d\omega) = \langle \mathcal{S}, \operatorname{curl} w\rangle = \langle \operatorname{Curl} \mathcal{S}, w\rangle. \tag{6.14}$$

We now collect two classic results.

Theorem 6.9. *Let Ω be a bounded and simply connected open set. Let $\lambda \in \mathcal{M}_b(\Omega, \mathbb{R}^3)$ be a Radon measure such that* Curl $\lambda = 0$ *as a distribution. Then there exists a function with bounded variation $u \in BV(\Omega)$ such that $Du = \lambda$.*

This Theorem can be found in [18]. The following one provides a chain rule to compute the derivative of the composition of a smooth function with a function with bounded variation (see [3] or [28]).

Theorem 6.10. *Let $u \in BV(\Omega)$ with $\Omega \subset \mathbb{R}^3$ a bounded open set, and let $f \in C^1(\Omega)$. Then the distributional derivative of $f \circ u$ is given by*

$$D(f\circ u) = Df(u)D^a u\mathcal{L}^n + Df(\tilde{u})D^c u + (f(u^+) - f(u^-))\nu_{J_u}\mathcal{H}^2\llcorner_{J_u}, \tag{6.15}$$

where $\tilde{u}$ is the Lebesgue representative of u, i.e., $\tilde{u}(x)$ is the Lebesgue value of u at x.

We can now prove the following result. This states that each strain F in the presence of dislocations can be written by mean of the gradient of a Sobolev map with value in $(S^1)^3$.

Theorem 6.11. *Let Ω be a bounded and simply-connected open set. Let $\mathcal{L} \in \mathcal{D}_1(\Omega)$ be a closed 1-integer multiplicity current and suppose $F \in L^1(\Omega, \mathbb{R}^3)$ is such that* Curl $F = \mathcal{L}$ *(with the identification* (6.14)*). Then there exists $u \in W^{1,1}(\Omega, S^1)$ such that $-u_2 Du_1 + u_1 Du_2 = F$ on Ω.*

Proof. Since $\mathcal{L}$ is a closed 1-integer multiplicity current, there exists a 2-integer multiplicity current $\mathcal{S}$ with finite mass and such that $-\partial\mathcal{S} = \mathcal{L}$. Let us now define the distribution $\mu \in \mathcal{D}'(\Omega, \mathbb{R}^3)$ as follows

$$\lambda(\varphi) := \mathcal{S}(\varphi) + \langle F, \varphi\rangle,$$

for all $\varphi \in C_c^\infty(\Omega, \mathbb{R}^3)$, where we have identified the map φ with the 2-form $\sum_{i=1}^n \varphi_i dx_{\bar{i}}$ as in Definition 6.7. The distribution λ is easily seen to be a Radon measure with finite mass. We compute the curl of λ, that is

$$\langle \operatorname{Curl} \lambda, \varphi\rangle = \mathcal{S}(\operatorname{curl} \varphi) + \langle F, \operatorname{curl} \varphi\rangle = \partial\mathcal{S}(\varphi) + \mathcal{L}(\varphi) = 0,$$

for all $\varphi \in C_c^\infty(\Omega, \mathbb{R}^3)$, by definition of $\mathcal{S}$. Then Theorem 6.9 implies that then exists $v \in SBV(\Omega)$ such that $Dv = \mu = \mathcal{S} + F$. Since $\mathcal{S}$ is an integer multiplicity current, there exist a 2-rectifiable set S with unit normal the vector ν and an integer-valued function $\theta \in L^1(S, \mathcal{H}^2)$ such that $\mathcal{S} = (S, \nu, \theta)$. In particular we see that the jump of v is given by the measure $\theta\nu \cdot \mathcal{H}^2 \llcorner_S$, while the absolutely continuous part of the gradient Dv is F. We then set

$$u(x) = (u_1(x), u_2(x)) := (\cos(2\pi v(x)), \sin(2\pi v(x))).$$

The map $t \to 2\pi t$ is of class C^1 on $\mathbb{R}$, so formula (6.15) applies and we obtain $D^j u_1 = (\cos(2\pi v^+(x)) - \cos(2\pi v^-(x)))\nu\mathcal{H}^{n-1}\llcorner_S = 0$, since $v^+ - v^- = \theta \in \mathbb{Z}$, and we conclude that u_1 has not jump part, and then it belongs to $W^{1,1}(\Omega)$. The same being true for u_2, we get $u \in W^{1,1}(\Omega, S^1)$. Moreover $Du_1 = -\sin(2\pi v)F$ and $Du_2 = \cos(2\pi v)F$ so that $-u_2 Du_1 + u_1 Du_2 = F$ and we have concluded. $\square$

This result shows that if $F \in L^p(\Omega, \mathbb{M}^3)$ is a map such that $-\operatorname{Curl} F = \hat{\mathcal{L}}$ for some integral closed current $\hat{\mathcal{L}}$ with coefficients in $\mathbb{Z}^3$, then there is a map $u := (u^1, u^2, u^3) \in W^{1,1}(\Omega, (S^1)^3)$ such that $-u_2^i D_j u_1^i + u_1^i D_j u_2^i = F_{ij}$ on Ω, for $i = 1, 2, 3$. The statement and the proof is in the simpler one dimensional case, but it can be generalized since it can be apply for every row of F.

In some sense, also the opposite of Theorem 6.11 holds true.

Theorem 6.12. *Let $u \in W^{1,1}(\Omega, S^1)$ and assume that u satisfies*

$$\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) \in \mathcal{M}_b(\Omega, \mathbb{R}^3). \tag{6.16}$$

Then there exists a closed integral 1-current $\mathcal{L}$ such that $\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) = 2\pi\mathcal{L}$.

This Theorem is a particular case of [2, Theorem 3.8]. In general, without hipothesis (6.16), $\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) = 2\pi\mathcal{L}$ is a closed 1-current $\mathcal{L}$, possibly with nonfinite mass. A constructive proof of Theorem 6.12 can be found in [22, Theorem 2.3.9].

In the theory of functions of bounded higher variation, introduced by Jerrard and Soner ([17]), the distributional jacobian $[Ju]$ of a sobolev map $u \in W^{1,1}(\Omega, S^1)$ is defined as the external derivative of the pull-back by u of the standard volume form ω_0 on S^1, that is $\omega_0 = x_1 dx_2 - x_2 dx_1$. Noting $j(u) := u^\sharp \omega_0$, then

$$[J(u)] := dj(u), \tag{6.17}$$

that is a 2-form on Ω. Using identification 6.7 and 6.8, it turns out that $[Ju]$ is exactly $\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2)$. Hence, standing to the notations of [17], condition (6.16) is equivalent to require that the map u has bounded higher variation, and we write $u \in B2V(\Omega, S^1)$.

As a consequence we see that the class of admissible displacements in the presence of dislocations, defined as

$$\begin{aligned}\mathcal{U} := \{u \in W^{1,1}(\Omega, (S^1)^3) : \ &\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) \text{ is an integral} \\ &\text{1-current with coefficients in } \mathbb{Z}^3\},\end{aligned} \tag{6.18}$$

is exactly the space $B2V(\Omega,(S^1))^3$.

Let

$$\mathcal{U}_c := \{u \in B2V(\Omega,(S^1))^3 : [Ju] \text{ belongs to } \mathcal{CD}, \\ \text{and } u \in \mathrm{Cart}^p(B,(S^1)^3) \text{ whenever } B \cap L = \emptyset\}, \tag{6.19}$$

where we recall $L := \mathrm{spt}[Ju]$. We can therefore restate our existence result in the following form.

Theorem 6.13. *Let $\mathcal{W}$ satisfies (W6) with $\mathcal{W}_{\mathrm{defect}} = \mathcal{W}^1_{\mathrm{defect}} + \mathcal{W}^2_{\mathrm{defect}}$, $\mathcal{W}^2_{\mathrm{defect}} = \kappa_1 G$, and*

$$\mathcal{W}^1_{\mathrm{defect}}([Ju]) = \kappa_2|[Ju]|(\Omega), \tag{6.20}$$

for some $\kappa_1, \kappa_2 > 0$. Then there exists a minimizer $u \in \mathcal{U}_c$ of $\mathcal{W}(F)$, where $F_{ij} = u_1^i D_j u_2^i - u_2^i D_j u_1^i$.

In the previous result, it can be tacitely assumed that also a boundary condition is fixed.

6.4 An example

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

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

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

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

Then we consider the map $\bar{F} : \hat{\Omega} \to \mathbb{M}^3$ defined as

$$\bar{F}(\rho,\theta,z) = \zeta(\theta)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{\sin\theta}{\rho}\beta & \frac{\cos\theta}{\rho}\beta & 1 \end{pmatrix}, \tag{6.21}$$

for some suitable smooth functions ζ, so that it turns out that

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

that is $\bar{F}$ shows a screw dislocation on the z-axis $\hat{z}$ with Burgers vector $b = (0,0,\beta)$. We want to minimize the energy (6.1) satisfying (W1)-(W4)

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

among all the deformations F belonging to the class (5.1) with $\bar{F}$ as boundary condition. Let us suppose that the defect part of the energy takes the form

$$W_{\mathrm{defect}}(\Lambda_{\mathcal{L}}) = \gamma\int_0^1 \|\dot{\varphi}(s)\|ds + \sum_{1\le i<k_{\mathcal{L}}} \gamma\int_{S^1}\|\dot{\varphi}_i(s)\|ds + \mu|\Lambda_{\mathcal{L}}(\Omega)|, \tag{6.22}$$

where the mesoscopic dislocation $\mathcal{L}$ is the image of $k_{\mathcal{L}}$ closed loops φ_i with Burgers vector b^i and of φ which is a dislocation with endpoints $P := (0,0,h)$

and $Q := (0, 0, -h)$ and Burgers vector b. Then let us consider an admissible deformation which shows only one dislocation path φ^0 coinciding with the segment $\overline{PQ}$. In this case $k_{\mathcal{L}} = 1$ and the energy is

$$\begin{aligned} \mathcal{W}(F^0) &= \int_\Omega \mathrm{W_e}(F^0)dx + \gamma \int_0^1 \|\dot{\varphi}^0(s)\|ds + \mu|\Lambda_{\mathcal{L}^0}(\Omega)| = \\ &= \int_\Omega \mathrm{W_e}(F^0)dx + 2h\gamma + 2h\mu\beta. \end{aligned} \tag{6.23}$$

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

$$\begin{aligned} W_{\mathrm{defect}}(\mathcal{L}^1) &\geq \gamma \int_0^1 \|\dot{\varphi}^1(s)\|ds + \mu|\Lambda_{\mathcal{L}^1}(\Omega)| \\ &\geq 2\gamma(R_t^2 + h^2)^{1/2} + 2h\mu\beta, \end{aligned} \tag{6.24}$$

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

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

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

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 detailed description of the dislocations as currents, a variational problem is studied with two optimization variables, namely the deformation gradient F and the dislocation density Λ, together bound by relation $-\operatorname{Curl} F = \Lambda^T$.

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

It is yet an open question to elucidate the structure of the distributional determinant, which one would like for physical reasons to be a Radon measure (i.e., an extensive field) on $\mathcal{K}$. To the knowledge of the authors few results exist about this issue, without the too restrictive assumptions of field boundedness, high space dimension and with the current range of p between 1 and 2. Let us mention a partial answer in a companion paper [24].

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 $-\,\mathrm{Curl}\ F = \Lambda^T$ will also be studied in forthcomming publications.

Two other extensions of this work are the analysis of the distributional determinant at the continuum $\mathcal{K}$, in particular to address the open question wether it is a measure, and homogenization of a countable family to the continuum to the macroscale (see, eg., [10]). 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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