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CURRENTS AND DISLOCATIONS AT THE CONTINUUM SCALE*

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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, its curl being nonzero and equal to the density of the dislocations, a measure concentrated 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. Firstly, we address the problem of mathematical modeling of dislocations. It is a key purpose of the paper to 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.

Key words. Cartesian maps, integer-multiplicity currents, dislocations, finite elasticity, modeling, variational problem.

AMS subject classifications. 74G65, 74B20, 74N05, 58A25, 49J45, 46E40, 32C30, 49Q15, 53C65.

1. Introduction.

Physical motivation of the problem. In single crystals, dislocations naturally arise as closed lines where microscopic defects of the atomic structure of the material are concentrated. At the macroscale, their presence is responsible for plastic behavior and dissipative phenomena linked to the deformation of the medium and to the forces exerted in the bulk or at the boundary. Consider one dislocation loop L in a continuous medium Ω. At the mesoscopic scale it is assumed that $\Omega \setminus L$ 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 the stress and strain are not square integrable [15], 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 Ω 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 dislocations on predefined glide planes only holds for moderate temperature ranges. In this paper, overlooking on purpose

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the specific inter-dislocation dynamics [31, 32, 28] which causes attraction/repulsion between dislocations and are responsible for their aggregation, 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.

Origin and nature of a dislocation singularity. One intrinsic difficulty of mesoscopic dislocations is that there is no natural definition of the displacement field (note that this also holds for the fictitious reference configuration), whereas the displacement field jump is a physical field attached to $L \subset \Omega$ and called *Burgers vector* (this is the famous Weingarten's theorem). Consider the current configuration Ω (taken as a bounded simply-connected set) with a single dislocation L and any separating surface S_L containing L. The set $\Omega \setminus L$ is not simply-connected, but the upper and lower subsets of Ω, Ω^+ and Ω^- separated by S_L, are simply-connected and in each of them (an inverse) displacement field $u_{S_L} : \Omega \to \mathbb{R}^3$ may be defined, which will be discontinuous at S_L. This field 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 $F = \nabla\phi$ which is also discontinuous at S_L (to be precise, an inverse deformation tensor[1]). Now, taking two curves $\alpha^\pm$ in $\Omega^\pm$ with the same endpoints A and B in S_L, respectively outside and inside L, one has:

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

where α denotes the loop from B to itself, obtained by running first α^- and then α^+ in the opposite direction. Otherwise said, ϕ shows a discontinuity of amplitude b at the jump set S_L° enclosed by L. Hence the distributional derivative of ϕ writes as $D\phi = F + b \otimes n\mathcal{H}^2 \llcorner S_L^\circ$ and it holds $-\operatorname{Curl} F = \operatorname{Curl}(b \otimes n\mathcal{H}^2 \llcorner S_L^\circ)$ (where n stands for 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 $L \subset \Omega$), it holds

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

which is the key geometric/kinematic constraint relating deformation and dislocations.

The variational framework. Coming back to the physics and the mathematical properties of dislocations, we have already mentioned that in finite elasticity $F \in L^p(\Omega, \mathbb{M}^3)$ with $1 \le p < 2$ (see e.g. [33] for examples). In fact, this property 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 [23]. Here, classical examples show that deformation allowing for radial cavitation are such that $\operatorname{cof} F \in L^q(\Omega, \mathbb{M}^3)$ with $1 \le q < 3/2$

[1] This convention – of considering the inverse deformation gradient, defined in Ω –, can also be found in [1]. In fact, it is preferred to have a discontinuous reference configuration, while the current configuration is the continuous medium containing the –possibly time-evolving– dislocation network. Thus, the energy density of Ω will also depend on such a F.

[14]. Thus, one cannot restrict to the interval $3/2 \leq p < 2$ where some existence results in finite elasticity already exist [22], and must allow F, $\mathrm{cof}F \in L^p(\Omega, \mathbb{M}^3)$ in the whole range $1 \leq p < 2$. For this reason, as suggested in [22], *Cartesian maps* will be considered [13]. Moreover, nucleation of dislocation loops resulting from the collapse of a void will provoke locally high pressure gradient and hence the behavior of the Jacobian $J = \det F$ must be controlled. Therefore, classical pointwise conditions on J will be considered: these are the non-negativeness (to ensure orientation preserving deformation and non-interpenetration of matter) or the fact that $J \to 0^+$ is precluded by finite energy states. Finally, to avoid any spurious (i.e., *concentrated and dissipative*) effects away from the dislocation set, we will assume not only that $\det F$, $\mathrm{cof}F \in L^p(\Omega, \mathbb{M}^3)$ but also that their distributional counterparts have no s-dimensional ($0 \leq s \leq 3$) singular parts in $\Omega \setminus L$, that is, $\mathrm{Det}F$, $\mathrm{Cof}F \in L^p(\Omega, \mathbb{M}^3)$ locally away from L [21]. Indeed, the dislocations induce 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, $\mathrm{cof}F$ and $\det F$ and will be assumed polyconvex, i.e., convex in each variable separately, and satisfying the growth

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

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

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

allowing us to control pathological behaviors of dislocation clusters. Note that 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 5.3).

Scope and structure of the work. The variational framework is inspired by the pioneer paper [22], where a *single and fixed* dislocation loop is considered, and hence minimization is 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 with respect to the line location. With the aforementioned type of energy, our aim is twofold. In a first step, to define classes of admissible deformations F and admissible dislocations L satisfying (i) a boundary condition in terms of dislocation density and (ii) the geometric constraint (1.2). In a second step, to prove existence of solutions to

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

To achieve the proof of existence, a series of preliminary results must be proved and in particular we define and carefully analyze two classes of dislocations, at the *mesoscopic* and at the *continuum* scales. With this respect, an important result is Theorem 4.6 which states their equivalence under certain conditions. Let us stress that both these classes have a specific interest in terms of modeling, according to the choice of the dislocation variable: either the line per se (i.e., a current $\mathcal{L}$, which might

be followed with time – though in this work we restrict to statics), or its associated density (i.e., the measure $\Lambda_{\mathcal{L}}$). In the latter case, the associated line $\mathcal{L}$ must not be determined everywhere – it will be known on the geometric necessary parts. Then, the two existence results are Theorems 5.5 and 5.6, respectively for the class of mesoscopic and continuum dislocations.

Let us remark that by solving (1.5) we consider a statics problem, whereas dislocations are known to be moving defects inside the crystal by the action of mechanical and thermal forces [1, 16]. First, we should precise that by considering an equilibrium problem at fixed time t, we indeed define a thermodynamical ground-state on the base of which dynamical effects will be added in a second step, beyond the scope of this paper. Second, such minimization states are reached very fast in actual crystals such as pure copper, where resistance to dislocation motion is negligible [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 mean of *integer-multiplicity currents* with coefficients in a group. A similar approach to continuum dislocations by integral currents was already suggested in [16], [17], and [9], but without such a systematic description as we sought. 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 mutually be summed, possibly forming complex *transfinite* geometries (in the sense of Cantor [7]), with appropriate laws on their Burgers vectors at dislocation junctions.

Let us emphasize that the chosen approach to minimize jointly the deformation and the line location is more correct from a physics standpoint, since the deformation field is inherently bound up with the dislocation density. To our knowledge, the main results of this paper represent the first generalization in this 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 leave these considerations for future works. With this respect, thanks to our minimization results, the dynamics of the lines at optimality could be analyzed and discussed in a companion paper [25]. Nevertheless, in order to set apart the construction of the mathematical model and the discussion of the definitions and assumptions, we have chosen to defer a large portion of the model discussion to a specific section: about modeling considerations and model justifications, cf. Appendix A.

This paper is self-contained and can be read without previous notions neither on dislocations nor on currents. 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 4.6. In Section 4.4, we discuss the admissible deformations satisfying the constraint (1.2). In particular, we show that the class of admissible deformations satisfying the boundary conditions given in terms of the dislocation density is well defined and this allows us to solve the two minimum problems of Section 5. In section 5.3, we show how the concept of deformation in the presence of dislocations is related to the space of functions of *bounded higher variation* introduced in [18]. Conclusions and plans to further extend the range of applications of this approach

are drawn in Section 6. Lastly, in Appendix A, we propose a model discussion with emphasis on the physical justification of the chosen formalism.

2. Preliminary notions and results. The curl of a tensor A is defined componentwise as $(\operatorname{Curl} A)_{ij} = \epsilon_{jkl} D_k A_{il}$ where D denotes the distributional derivative. In particular one has

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

Note that with this convention one has $\operatorname{Div} \operatorname{Curl} A = 0$ in the sense of distributions, since componentwise the divergence is classically defined as $(\operatorname{Div} A)_i = D_j A_{ij}$.[2] For the remaining of this section, our main references are [11, 13].

2.1. Preliminaries on compact sets. Let C be a 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 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 and such that $\mathcal{H}^1(K_n) < \lambda < \infty$. Then K is connected, has Hausdorff dimension* 1*, and*

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

2.2. Currents and graphs of Sobolev functions. Let M, n be integers with $0 \le M \le n$. We denote by $\Lambda^M\mathbb{R}^n$ and $\Lambda_M\mathbb{R}^n$ the vector spaces of *M-covectors* and *M-vectors* respectively. A M-vector ξ is said *simple* if it can be written as a single wedge product of vectors, $\xi = v_1 \wedge v_2 \wedge \cdots \wedge v_M$. Details on exterior algebra can be found in [19]. Let α be a multi-index, i.e., an ordered (increasing) subset of

[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 [27]-[29] where it holds $\operatorname{Curl} A = -A \times \nabla$).

$\{1, 2, \dots, n\}$. We denote by $|\alpha|$ the length of α, and we denote by $\bar{\alpha}$ the complementary set of α, i.e., the multi-index given by the ordered set $\{1, 2, \dots, n\} \setminus \alpha$.

For a $n \times n$ matrix A with real entries and for α and β multi-indices such that $|\alpha| + |\beta| = n$, $M^{\beta}_{\bar{\alpha}}(A)$ denotes the determinant of the submatrix of A obtained by erasing the i-th columns and the j-th rows, for all $i \in \alpha$ and $j \in \bar{\beta}$. Moreover, symbol $M(A)$ denotes the n-vector in $\Lambda_n \mathbb{R}^{2n}$ given by

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

where $\{e_i, \varepsilon_i\}_{i \le n}$ 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,

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

For a matrix $A \in \mathbb{M}^3$, symbols adj A and $\det A$ stand for the adjunct, i.e. the transpose of the matrix of the cofactors of A, and the determinant of A, respectively. Explicitly,

$$M^i_j(A) = A_{ij}, \quad M^I_J(A) = M^{\bar{i}}_{\bar{j}}(A) = (\operatorname{cof} A)_{ij} \quad M^{\{1,2,3\}}_{\{1,2,3\}}(A) = \det A, \tag{2.3}$$

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

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

Let us also define

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

Currents. Let Ω be an open set in $\mathbb{R}^n$. For non-negative integers $M \le n$, the symbol $\mathcal{D}^M(\Omega) = \mathcal{D}(\Omega; \Lambda^M \mathbb{R}^n)$ stands for the topological vector space of C^∞-differential forms with degree M and compact support in Ω. The space of *M-dimensional currents on* Ω is defined as $\mathcal{D}_M(\Omega) := (\mathcal{D}(\Omega; \Lambda^M \mathbb{R}^n))'$, the class of continuous linear functionals on $\mathcal{D}^M(\Omega)$. Since $\mathcal{D}_M(\Omega)$ is 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 simple M-vector giving the orientation, the symbol $[\![S]\!] \in \mathcal{D}_M(\mathbb{R}^n)$ denotes the current obtained by integration on S, that is,

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

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

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

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

where $d\omega$ is the external derivative of ω. A current T is said *closed* if $\partial T = 0$. 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 defined the *push forward* of a current $T \in \mathcal{D}_M(U)$ by 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 which is equal to 1 on $\mathrm{spt}T \cap \mathrm{spt}F^\sharp\omega$ (here and below "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

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

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

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

Not to overburden some subsequent formulae, the notation will be employed:

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

whenever $T \in \mathcal{D}_M(\Omega)$ and $U \subset \Omega$ is an open set. Notice that this number, which measures both the mass of a current and of its boundary, is not a norm.

Rectifiable currents. A set $S \subset \mathbb{R}^n$ is said $\mathcal{H}^M$-*rectifiable* if it is contained in the union of a negligible set and a countable family of C^1-submanifolds. Moreover, a $\mathcal{H}^M$-rectifiable set S is said a M-*set* if it has $\mathcal{H}^M$-finite measure, whereas it is said locally finite if for each compact set $K \subset \mathbb{R}^n$ we have $\mathcal{H}^M(S \cap K) < \infty$. 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 $\lambda > 0$.

If $\tau : S \to \Lambda_M(\mathbb{R}^n)$ with $\tau(x) \in T_xS$ is a simple unit M-vector for $\mathcal{H}^M$-a.e. $x \in S$, and $\theta : S \to \mathbb{R}$ is $\mathcal{H}^M$-integrable, we can define the current

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

Every current for which there exists such S, τ, and θ is said a *rectifiable current*, and will be denoted by

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

Integral currents. A rectifiable current $T \in \mathcal{D}_M(\Omega)$ is said *rectifiable with integer multiplicity* if θ takes values in $\mathbb{Z}$. An integer-multiplicity current T such that $N(T) < \infty$ is called *integral current*. The following compactness theorem for integer multiplicity ("i.m.") currents holds:

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

$$N_U(T_i) < C < +\infty \qquad \text{for all } i \text{ and } U \subset\subset \Omega.$$

Then there exist an integer multiplicity current $T \in \mathcal{D}_k(\Omega)$ and a subsequence, still denoted by $\{T_i\}_i$, such that $T_i \rightharpoonup T$ weakly in Ω.

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-currents (see [11, Section 4.2.25]).

THEOREM 2.4 (Decomposition theorem). *For every integral current T there exists a sequence of indecomposable integral currents T_i such that*

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

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

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

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

Graphs of Sobolev functions. Given $u \in W^{1,p}(\Omega, \mathbb{R}^n)$, we define its *graph* $\mathcal{G}_u \subset \Omega \times \mathbb{R}^n$ as

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

The following theorem provides a sufficient condition to guarantee that the graph is a rectifiable set. We refer to [13, Section 3.1.5, Theorem 4] for the proof.

THEOREM 2.5. *Let $u \in W^{1,p}(\Omega, \mathbb{R}^n)$. 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 of ω 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 by the map $\mathrm{Id} \times u$, provided $u \in W^{1,p}(\Omega;\mathbb{R}^n)$. Let us consider $[\![\Omega]\!]$, the canonical current given by integration on Ω. We set $G_u := (\mathrm{Id} \times u)_\sharp [\![\Omega]\!]$, in such a way that for all ω satisfying (2.12), it holds

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

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 $i \neq j$. The *distributional cofactor* of Du, denoted as $\mathrm{Cof}Du$ is defined componentwise by

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

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 by 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 adj Du, $\det Du$ belong to $L^p(\Omega)$. The following result can be found in [13, Section 3].

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 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 $\mathcal{G}_u$.

For $p \geq 1$, we define the class of *Cartesian maps* as the function class

$$\mathrm{Cart}^p(\Omega,\mathbb{R}^n) := \{u \in \mathcal{A}^p(\Omega;\mathbb{R}^n) : \partial G_u \llcorner_{(\Omega\times\mathbb{R}^n)} = 0\}. \tag{2.13}$$

The following closure theorem for Cartesian maps holds (see [13, Section 3.3.3]):

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

$$u_k \rightharpoonup u \quad \textit{weakly in } L^p(\Omega, \mathbb{R}^n),$$
$$M^\beta_\alpha(Du_k) \rightharpoonup v^\beta_\alpha \quad \textit{weakly in } L^p(\Omega),$$

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

A 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 $\mathrm{Adj}Du \in L^p(\Omega, \mathbb{R}^{n\times n})$. This will be clear in Section 5.

3. Dislocation lines as currents. A dislocation in an elasto-plastic body arises as a closed arc, or a curve connecting two points of the boundary, to which a Burgers vector $b \in \mathbb{R}^3$ and a measure concentrated in the dislocation line (viz., the dislocation density) are associated. Since dislocation densities fulfill linear additivity when dislocation lines overlap, dislocations will be described by means of integer-multiplicity 1-currents with coefficients in a group. The group, in the crystallographic case, is assumed isomorphic to $\mathbb{Z}^3$. The coefficient θ represents the Burgers vector multiplicity. Moreover, 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). On the other hand, the tangent vector to the dislocation line represents the current orientation. Note that integer-multiplicity 1-currents are essentially Lipschitz curves, thanks to Theorem 2.4, and hence a description of dislocations without using the notion of currents is also possible. However the notion of currents, as we will see, simplifies some descriptions and provides more direct proofs of some of the following statements.

Let us introduce the class of Burgers vectors, that is, the group of the coefficients of the 1-integral currents representing dislocations. 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 defines the set of *admissible Burgers vectors* as

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

Accordingly, a dislocation whose Burgers vector belongs to the lattice $\mathcal{B}$ is called a *crystallographic dislocation*. Without loss of generality, we will assume that $\bar{b}^k = e_k$, the k-th base vector, that is, we set $\mathcal{B} := \mathbb{Z}^3$. With this definition we can identify each dislocation with a current with coefficients in the group $\mathbb{Z}^3$.

Figures 1, 2, 3 show how the Frank law applies at dislocation junctions, which indeed corresponds to how currents mutually operate, and the kind of geometries taking place when simple dislocation loops interact. It should be noticed that complex geometries with countable many loops should also be taken into account when developing a mathematical model, since such geometries are observed in actual crystals.

In this section, we introduce the dislocation as a precise mathematical object.

3.1. b-dislocations. The first notion is the class of b-dislocations, which are those dislocations associated to only one Burgers vector $b \in \mathbb{Z}^3$. Let Ω be a bounded simply-connected and smooth open set.

DEFINITION 3.1 (b-dislocation). *Let $b \in \mathbb{Z}^3$. A b-dislocation $\mathcal{L}^b$ is a family $\{\mathcal{L}^b_i\}_{i\in\mathcal{I}^b}$ of integral 1-currents such that*

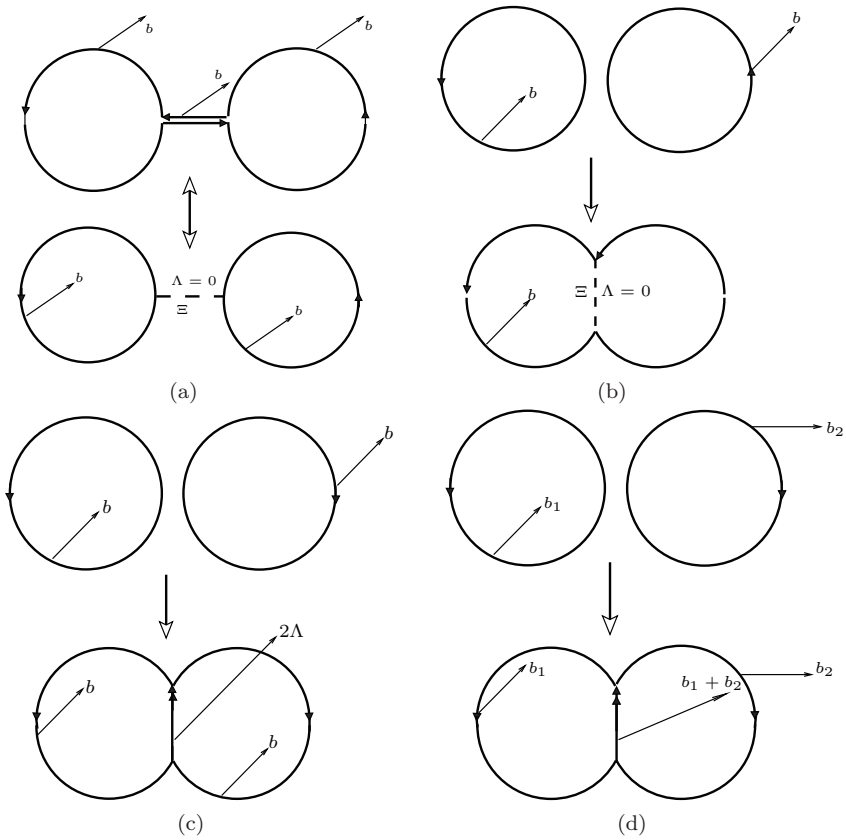


Fig. 1: *Typical indecomposable dislocation loops and the resulting dislocation currents: in (a), a single b-dislocation loop is equivalently viewed as two indecomposable b-loops with opposite orientations and connected by a geometrically unnecessary arc* Ξ*; the inverse property is observed in (b) where 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.*

(i) $\mathcal{I}^b$ *is finite with cardinality* $k_b \in \mathbb{N}$*,*

(ii) there exist k_b *Lipschitz functions* $\varphi_i^b : [0, T_i^b] \to \bar{\Omega}$ *with* $\mathrm{Lip}(\varphi_i^b) \leq 1$ *such that*

$$\mathcal{L}_i^b = \varphi_{i\sharp}^b([\![[0, T_i^b]]\!]). \tag{3.2}$$

Moreover, for all $1 \leq i \leq k_b$*, either* $\varphi_i^b(0) = \varphi_i^b(T_i^b)$ *or* $\varphi_i^b(0), \varphi_i^b(T_i^b) \in \partial\Omega$*.*

We set

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

The $\mathbb{Z}^3$-valued coefficient current associated *to a b-dislocation* $\mathcal{L}^b$*, denoted as* $\hat{\mathcal{L}}^b$*, is defined by*

$$\hat{\mathcal{L}}^b(\omega) := \mathcal{L}^b(\omega b), \tag{3.4}$$

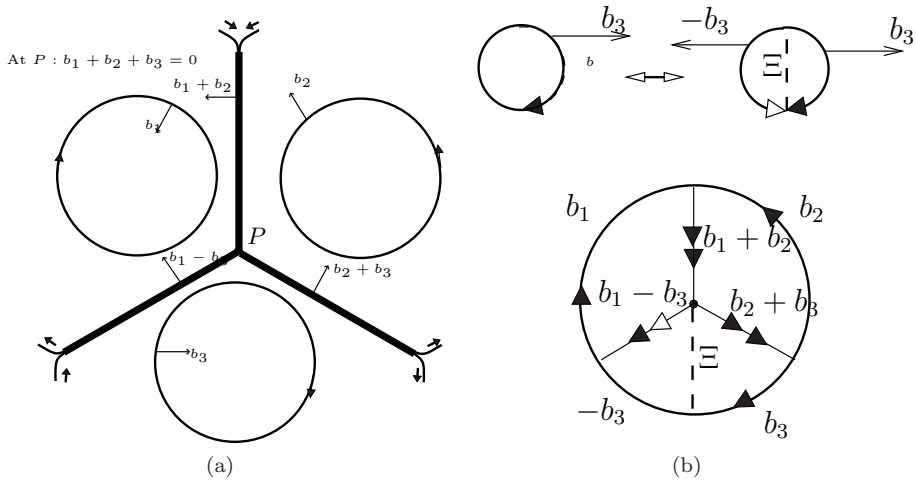


Fig. 2: *For certain combinations of Burgers vectors, the three separated loops of (a) might intersect and form the cluster element of (b) where the Frank law at the intersection points is satisfied.*

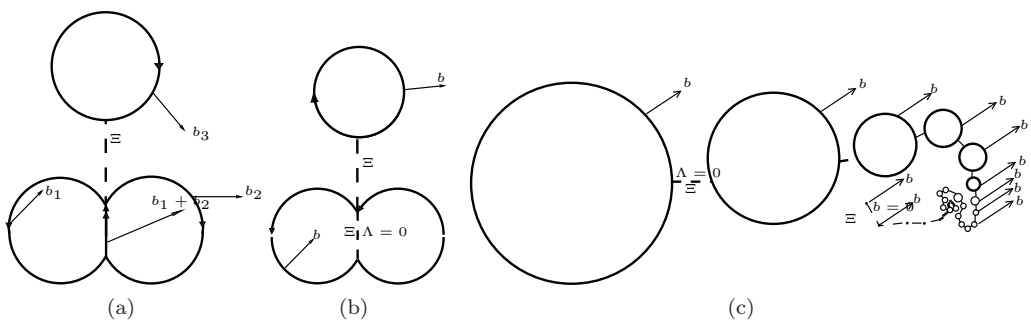


Fig. 3: *Different kinds of cluster components: in (a) the sum of b-current dislocations* $\mathcal{L}^{b_1}+\mathcal{L}^{b_2}+\mathcal{L}^{b_3}$ *is depicted, whereas (b) shows a single b-current constituted of three elementary b-loops. In (c) a b-dislocation cluster writing as* $\mathcal{L}^b = \varphi^b_\sharp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

for all 1*-form with vector-valued coefficients* $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$*. Here and below* $\mathcal{D}^1(\Omega, \mathbb{R}^3)$ *denotes the space of* 1*-forms with vector-valued smooth and compactly supported coefficients. Note that* ω *writes componentwise (with Einstein summation convention on* l*) as* $\omega_k := \omega_{lk} dx_l$*, with* ω *a* 2*nd-rank tensor. Moreover,* ωb *is defined componentwise as* $(\omega b)_j := \omega_{lj} b_j dx_l$ *(with no summation on* j*).*

Let us denote by l_i^b, the length of the current given by φ_i^b. Thanks to the Lipschitz continuity of the functions φ_i^b one has $\sum_{i=1}^{k_b} l_i^b := \sum_{i=1}^{k_b} \int_0^{T_i^b} \|\dot{\varphi}_i^b\| dt < \infty$, meaning that the total length of the supporting set of the current $\mathcal{L}^b$ (counted with possible overlapping) is finite.

By Theorem 2.4, one can always decompose $\mathcal{L}^b$ as follows: there is a countable index set $\mathcal{J}^b$ such that

$$\mathcal{L}^b = \sum_{j\in\mathcal{J}^b} \mathcal{L}^b_j, \tag{3.5}$$

with $\mathcal{L}^b_j$ indecomposable 1-currents such that $\sum_{j\in\mathcal{J}^b} N(\mathcal{L}^b_j) = N(\mathcal{L}^b)$. The components $\mathcal{L}^b_j$ are called *current loops*. Notice that even if the word loop usually refers to a closed curve, we use the same word when referring to a non-closed curve (with endpoints belonging to $\partial\Omega$).

By definition of rectifiable current, if $\mathcal{L}^b$ is a b-dislocation, there exists a rectifiable set (which, by the finiteness of its measure, is a 1-set) called *dislocation set* and denoted by L^b, such that

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

In general L^b is not unique, and we can choose

$$L^b := \bigcup_{i=1}^{k_b} \varphi^b_i([0, T^b_i]). \tag{3.7}$$

Therefore, we write $\mathcal{L}^b = \{L^b, \tau^b, \theta^b\}$.

To any b-dislocation we associate a *density* $\Lambda_{\mathcal{L}^b}$ which, since k_b is finite, turns out to be a Radon measure.

Definition 3.2. *The density of a b-dislocation $\mathcal{L}^b$ is the measure $\Lambda_{\mathcal{L}^b} \in \mathcal{M}_{\mathrm{b}}(\bar{\Omega}, \mathbb{M}^3)$ defined by*

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

for every $w := [w_{ij}] \in C^\infty_c(\Omega, \mathbb{M}^3)$, where we define componentwise $(wb)^*_j := w_{lj} b_j dx_l$ (j fixed).

Remark 3.3. *Note that, by* (3.4)*, 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* (3.4) *turn out to coincide.*

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

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

Definition 3.4 (Geometrically necessary dislocation set). *The geometric necessary dislocation set $L^\star$ is the support of $\Lambda_{\mathcal{L}}$.*

Note that in general the geometrically necessary dislocation set $L^\star$ does not coincide with the dislocation set L^b, since it may happen that $\theta^b = 0$ on some subset of L^b with $\mathcal{H}^1$ positive measure. Note that if $\mathcal{L}^b_j$ are the indecomposable components of $\mathcal{L}^b$ in (3.5), we write $\mathcal{L}^b_j = \{L^b_j, \tau^b, \theta^b\}$, in such a way that

$$L^\star = \bigcup_{j\in\mathcal{I}^b} L^b_j, \qquad L^b = L^\star \cup \Xi^b, \tag{3.10}$$

where Ξ^b is defined as the set $\{x \in L^b : \theta^b(x) = 0\}$.

3.2. Regular dislocation. The following definition extends the notion of b-dislocation to general dislocations. Since we are interested in the class of dislocations with finite mass, we will call them *regular*.

DEFINITION 3.5 (Regular dislocation). *Let $\mathcal{B}_{\mathcal{L}} \subset \mathbb{Z}^3$. A* regular dislocation *is a sequence of b-dislocations $\mathcal{L} := \{\mathcal{L}^b\}_{b\in\mathcal{B}_{\mathcal{L}}}$ whose total density (or associated current) has finite mass. According to the previous definition, the $\mathbb{Z}^3$-coefficient dislocation current, still denoted by $\hat{\mathcal{L}}$, and the* dislocation density $\Lambda_{\mathcal{L}}$, *are given by*

$$\hat{\mathcal{L}} := \sum_{b\in\mathcal{B}_{\mathcal{L}}} \hat{\mathcal{L}}^b, \qquad \Lambda_{\mathcal{L}} := \sum_{b\in\mathcal{B}_{\mathcal{L}}} \Lambda_{\mathcal{L}^b}. \tag{3.11}$$

The dislocation set L *is defined as*

$$L := \bigcup_{b\in\mathcal{B}_{\mathcal{L}}} L^b, \tag{3.12}$$

so that, according to the notation (2.11), *we can write $\hat{\mathcal{L}} = \{L, \tau, \theta\}$ with*

$$\tau \in \mathrm{Tan}L, \qquad \theta = \sum_{b\in\mathcal{B}_{\mathcal{L}}} \mathrm{sg}(\tau^b)\theta^b b, \tag{3.13}$$

where $\mathrm{sg}(\tau^b) = \{1, -1\}$ *is s.t.* $\tau = \mathrm{sg}(\tau^b)\tau^b$ *(note that $\theta \in \mathbb{Z}^3$, whereas $\theta^b \in \mathbb{Z}$).*

By (3.3), every dislocation current can also be written as

$$\hat{\mathcal{L}}(\omega) = \sum_{b\in\mathcal{B}_{\mathcal{L}}} \hat{\mathcal{L}}^b(\omega) = \sum_{b\in\mathcal{B}_{\mathcal{L}}} \sum_{1\le i\le k_b} \varphi^b_{i\sharp}[\![[0, T^b_i]]\!](\omega b), \tag{3.14}$$

for all $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$. Now, enumerating the family of generating functions $\{\varphi^b_i\}$, we construct a index set $\mathcal{J} = \mathcal{J}_{\mathcal{L}}$ such that

$$\sum_{b\in\mathcal{B}_{\mathcal{L}}} \sum_{1\le i\le k_b} \varphi^b_{i\sharp}[\![[0, T^b_i]]\!] = \sum_{j\in\mathcal{J}} \varphi_{j\sharp}[\![[0, T^b_j]]\!]. \tag{3.15}$$

Moreover, setting $S_j := \varphi_j([0, T_j])$, from (3.7) and (3.12), we have $L = \bigcup_{j\in\mathcal{J}} S_j$.

3.3. Canonical decomposition. Since every dislocation can be represented by different integral 1-currents, we introduce the following notion.

DEFINITION 3.6 (Equivalence between dislocations). *Two dislocations $\mathcal{L}$ and $\mathcal{L}'$ are said geometrically equivalent if*

$$\Lambda_{\mathcal{L}} = \Lambda_{\mathcal{L}'}. \tag{3.16}$$

Among all geometrically equivalent dislocations there exists one representation which is sharp in the sense that it is expressed in terms of the mutually independent elementary Burgers vectors. 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), for $k = 1, 2, 3$ we introduce

$$\mathcal{L}^{b,k} := \{L^b, \tau^b, \beta_k\theta^b\}, \tag{3.17}$$

with the corresponding density $\Lambda_{\mathcal{L}^{b,k}} := \mathcal{L}^{b,k} \otimes e_k = \mathcal{L}^b \otimes \beta_k e_k$. Observe that

$$\sum_{k=1}^{3} \Lambda_{\mathcal{L}^{b,k}} = \sum_{k=1}^{3} \mathcal{L}^{b,k} \otimes e_k = \sum_{k=1}^{3} \tau^b \otimes \beta_k e_k \; \theta^b \mathcal{H}^1 \llcorner_{L^b} = \Lambda_{\mathcal{L}^b}. \tag{3.18}$$

To any regular dislocation $\mathcal{L}$ we associate univoquely three currents

$$\mathcal{L}_k := \sum_{b \in \mathcal{B}(\mathcal{L})} \mathcal{L}^{b,k}, \quad \text{so that } \mathcal{L}_k = \{L, \tau, \theta_k\}, \tag{3.19}$$

for $k = 1, 2, 3$, where θ_k is defined by $\theta_k := \sum_{b \in \mathcal{B}} \mathrm{sg}(\tau^b)\beta_k \theta^b$, with $\tau = \mathrm{sg}(\tau^b)\tau^b$.

Definition 3.7. *The* canonical dislocation decomposition of *a regular dislocation current $\hat{\mathcal{L}}$ is*

$$\hat{\mathcal{L}} = \hat{\mathcal{L}}_1 + \hat{\mathcal{L}}_2 + \hat{\mathcal{L}}_3, \tag{3.20}$$

where $\hat{\mathcal{L}}_k$ is the kth component of $\hat{\mathcal{L}}$ defined as $\hat{\mathcal{L}}_k(\omega) := \mathcal{L}_k(\omega e_k)$ for all $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$, and $k = 1, 2, 3$. In other words

$$\hat{\mathcal{L}}_k = \{L, \tau, \theta_k e_k\}.$$

A useful property of the decomposition (3.20) 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 3.8. *Let $\mathcal{L}$ be a regular dislocation. The following assertions hold true:*

(a) The currents $\mathcal{L}_k$ ($k = 1, 2, 3$) are integer-multiplicity currents in Ω.

(b) The mass of the currents and the total variation of the associate measures are related by

$$|\mathcal{L}_k|_\Omega = |\hat{\mathcal{L}}_k|_\Omega = \|\Lambda_{\mathcal{L}_k}\|_{\mathcal{M}_\mathrm{b}(\Omega)} \le \|\Lambda_{\mathcal{L}}\|_{\mathcal{M}_\mathrm{b}(\Omega)} = |\hat{\mathcal{L}}|_\Omega, \tag{3.21}$$

for $k = 1, 2, 3$.

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

Proof. Assertion (a) follows by Theorem 2.3 since $\sum_{b \in \mathcal{B}} N(\mathcal{L}^{b,k}) < \infty$ by definition of a regular dislocation. The equalities in (3.21) follow by definitions and identifying forms with smooth functions. Moreover, by (3.18) and (3.19), it holds

$$\Lambda_{\mathcal{L}} = \sum_{b \in \mathcal{B}_{\mathcal{L}}} \Lambda_{\mathcal{L}^b} = \sum_{k=1}^{3} \Lambda_{\mathcal{L}_k} = \sum_{k=1}^{3} \mathcal{L}_k \otimes e_k, \tag{3.22}$$

in such a way that inequality

$$\|\Lambda_{\mathcal{L}}\|_{\mathcal{M}} \ge \|\Lambda_{\mathcal{L}_k}\|_{\mathcal{M}} \qquad \text{for } k = 1, 2, 3, \tag{3.23}$$

follows by the matrix inequality $|\sum_{k=1}^{3} a_k \otimes e_k| \ge |a_k \otimes e_k| = |a_k|$ for every $a_k \in \mathbb{Z}^3$. To prove (c), observe first that $\mathcal{L}_k = \{L, \tau, \theta_k\}$ and by definition of $\mathcal{L}_k$ and $\Lambda_{\mathcal{L}_k}$ it easily

follows that $\mathrm{spt}\mathcal{L}_k = \mathrm{spt}\Lambda_{\mathcal{L}_k}$. So we only need to prove that $\mathrm{spt}\Lambda_{\mathcal{L}} = \bigcup_{k=1}^{3} \mathrm{spt}\Lambda_{\mathcal{L}_k}$. But this is a direct consequence of the fact that $\Lambda_{\mathcal{L}_k}$ acts on orthogonal subspaces of $C_c^\infty(\mathbb{R}^3, \mathbb{M}^3)$. □

Definition 3.9 (Unnecessary dislocations). *The* set of unnecessary dislocations *is defined as* $\Xi = \bar{L} \setminus L^\star$.

4. Classes of admissible dislocations and deformations for the minimum problem. With a view to studying the dislocation motion, two classes of dislocations will now be introduced, the first being useful if one wishes to follow (for instance, with time) each line as it deforms, intersect with others etc., whereas the second will be more appropriate if the model relevant quantity is the dislocation density, instead of the single lines themselves. In the latter case, dislocations are determined up to the equivalence relation (3.16) and the clusters might exhibit locally dense subsets of unnecessary dislocation segments.

4.1. Admissible dislocations.

4.1.1. 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). *Let $\mathcal{L}$ be a regular dislocation. We assume that the number of generating loops is finite, i.e.,*

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

with k_b as introduced in Definition 3.1.

The class of dislocations at the mesoscale is defined as:

Definition 4.2 (Mesoscopic dislocation).

$$\mathcal{MD} := \{\mathcal{L} = \{\mathcal{L}^b\}_{b \in \mathcal{B}_{\mathcal{L}}} : \mathcal{L}^b \text{ takes the form (3.3) and satisfies Assumption 4.1.}\}.$$

Remark 4.3. *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 countably intersections of arcs may take place (in other words, with this approach, it is accounted for possibly large Burgers vectors, provided they are attached to small enough arcs). Moreover, the cluster of Fig. 3(c) made of countably many loops whose lengths are summable, and which are interconnected by unnecessary segments, turns out to be a mesoscopic dislocation, since it can be generated by a single b-loop.*

From Definition 4.2 and Assumption 4.1 the next lemma is readily proved.

Lemma 4.4. *The following properties hold for a dislocation at the mesoscopic scale $\mathcal{L}$:*

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

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

(b) The dislocation current $\hat{\mathcal{L}}$ is an integral current with coefficients in $\mathbb{Z}^3$ satisfying $|\hat{\mathcal{L}}|_\Omega = \|\Lambda_{\mathcal{L}}\|$. In particular θ and θ_k, for $k = 1, 2, 3$, are all summable functions with respect to $\mathcal{H}^1 \llcorner L$.

(c) The dislocation set L of the current $\hat{\mathcal{L}}$ (defined in (3.12)) 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 $\|\Lambda_{\mathcal{L}}\| \leq \sum_{b\in\mathcal{B}_{\mathcal{L}}} \|\mathcal{L}^b \otimes b\| \leq \sum_{\substack{b\in\mathcal{B}_{\mathcal{L}}\\ i=1,\dots,k_b}} \|\mathcal{L}^b_i \otimes b\| \leq \sum_{\substack{b\in\mathcal{B}_{\mathcal{L}}\\ i=1,\dots,k_b}} |b| l^b_i < \infty$ by Assumption 4.1 (i.e., the sum is made on a finite number of Lipschitz loops). Statement (b) follows from (a) and property (b) of Lemma 3.8. Property (c) is a straightforward consequence of the fact that $\mathcal{H}^1(L) \leq \sum_{\substack{b\in\mathcal{B}\\ i=1,\dots,k_b}} l^b_i < \infty$. ∎

4.1.2. 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 4.5 (Continuum dislocation).

$$\mathcal{CD} := \{\mathcal{L}_{\mathcal{I}}, \mathcal{I} \subset \mathbb{N} : \textit{there exists a continuum } \mathcal{K} \textit{ such that } L^\star \subset \mathcal{K}\}. \tag{4.3}$$

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.

4.2. An equivalence result. In the applications, the notion of continuum dislocations is useful to study the cases in which Assumption 4.1 is not satisfied. Moreover, if one is not interested in the particular dislocation current associated to a given dislocation density, mesoscopic dislocations become a superfluous notion. In fact, crystallographic mesoscopic dislocations turn out to be equivalent to continuum dislocations, in the sense that, for any continuum dislocation $\mathcal{L}$, there is a mesoscopic dislocation $\mathcal{L}'$ such that $\mathcal{L} \equiv \mathcal{L}'$ in the sense of Definition 3.6. The proof of this fact is based on the following theorem

Theorem 4.6. *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 $\mathcal{L} = \alpha_\sharp[\![S^1]\!]$.*

The proof of Theorem 4.6 requires some preliminary lemmas.

Lemma 4.7. *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

$$\mathcal{S} := \{\phi : S^1 \to K \text{ satisfying the following three properties:}\} \tag{4.4}$$

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

It is easily seen that $\mathcal{S}$ is not empty, since K is a rectifiable set. 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 $j_k \to \sup J$, for each $k \in J$, it holds $C_k \subseteq C$, and hence it remains 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 $\mathrm{Lip}(\phi_j) \le \frac{L}{\pi}$ imply that $\mathrm{Lip}(\phi) \le \frac{L}{\pi}$. Thus, (i) and (iii) are readily fulfilled. Relation (ii) is easy to check, too. Let Φ_j be the homotopy map between $\Phi_j(\cdot, 1) = \phi_j$ and the constant $\Phi_j(\cdot, 0) \equiv P$. Then, up to a rescaling, we may suppose that for all $x \in S^1$, the map $\Phi_j(x, \cdot)$ is Lipschitz with $\mathrm{Lip}(\Phi_j(x, \cdot)) \le L$. 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 these two intervals, ψ_1 and ψ_2. Then it is readily seen that the arc $\psi_1 \star \alpha \star \alpha_{-1} \star \psi_2$, if suitably rescaled as a function on S^1, is a map in $\mathcal{S}$ that is strictly greater than ψ, contradicting the maximality of ψ. Hence the thesis follows. □

Lemma 4.8. *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 that $K \subset \mathbb{R}^2$. 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 and which does not intersect K, so that any connected component of B has positive Lebesgue measure. Therefore, 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 and set $\hat{T} = \psi_\sharp[\![S^1]\!] - T$. 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) twice, one time by α and another time by $\hat{\alpha}$ with opposite direction. But this contradicts 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 (4.6).

Proof of Theorem 4.6. 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 4.7, so that there are points $x_j \in S^1$ such that $\psi(x_j) = \beta_j(1)$. Suppose for simplicity that $x_1 = 1$ and x_j are clockwise ordered on S^1. Setting $\psi_j := \psi \llcorner [x_j, x_{j+1}]$, the chain

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

as suitably rescaled, will match the required conditions, since ψ, being homotopic to the constant map by Lemma 4.8, satisfies $\psi_\sharp[\![S^1]\!] = 0$. □

The precise equivalence theorem is stated as follows.

THEOREM 4.9. *Let $\mathcal{L} = \mathcal{L}_{\mathcal{B}_\mathcal{L}}$ be a continuum dislocation such that $\mathcal{B}_\mathcal{L} \subset \mathbb{Z}^3$ and $\Lambda_\mathcal{L}$ is finite. Then $\mathcal{L}$ is a mesoscopic dislocation.*

Proof. Considering the canonical dislocation current $\hat{\mathcal{L}}$ equivalent to $\mathcal{L}$ (cf. Eq. (3.20)), the thesis follows from Eq. (3.21) and Theorem 4.6. Indeed the latter provides three Lipschitz functions α_k $(k = 1, 2, 3)$ such that $\alpha_{k\sharp}[\![S^1]\!] = \mathcal{L}_k$, hence it follows $\Lambda_\mathcal{L} = \sum_k \alpha_{k\sharp}[\![S^1]\!] \otimes e_k$. □

In particular Theorem 4.9 tells us that continuum and mesoscopic dislocations 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 $\mathbb{Z}^3$).

4.3. Boundary conditions for dislocations. Let us introduce the mechanical setting for our minimization problem.

ASSUMPTION 4.10. *We consider a bounded smooth and simply-connected open set Ω. Let U be a bounded and smooth open set such that $\Omega \cap U \neq \emptyset$, and let $\partial_D\Omega := \partial\Omega \cap U$. We also denote $\hat{\Omega} := \Omega \cup U$.*

DEFINITION 4.11 (Boundary conditions). *A boundary condition is a triple $(N, \mathcal{P}, \alpha_D)$ satisfying:*

(i) $N \geq 0$ is a natural number.

(ii) $\mathcal{P}$ is a triple $(P_i, Q_i, \mathcal{B}_D)_{1\leq i\leq N}$ with $\{P_i\}$ and $\{Q_i\}$ sequences of points in $\partial_D\Omega$, and $\mathcal{B}_D = \{b^i_D\}_{1\leq i\leq N}$ a sequence of vectors belonging to $\mathbb{Z}^3$. We associate to $\mathcal{P}$ the 0-current with coefficients in $\mathbb{Z}^3$

$$\hat{T}_D := \sum_{1\leq i\leq N} \delta_{P_i} b^i_D - \delta_{Q_i} b^i_D,$$

with δ_P being the Dirac delta 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 $\Lambda_{\alpha_D} = \sum_{1\le i\le M} \alpha_{b^i_\alpha} \otimes b^i_\alpha + \sum_{1\le i\le N} \alpha_{b_{\hat\alpha^i}} \otimes b^i_D$ as 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 4.12. *We say that the boundary condition $(N, \mathcal{P}, \alpha_D)$ is* admissible *if the following condition is satisfied: there exists a regular dislocation $\mathcal{L}$ with support in $\bar\Omega$ 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 $\bar U \cup \bar\Omega$.

4.4. The class of admissible deformations. In the setting of Assumption 4.10, 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 $\mathcal{L}' := \mathcal{L} + \hat\alpha$ 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 $-\operatorname{Curl} \bar F = (\Lambda_\alpha)^{\mathrm{T}}$ in U.

Definition 4.13.

$$\mathcal{F} := \{(F, \mathcal{L}) \in L^p(\Omega, \mathbb{M}^3) \times \mathcal{MD} : F \text{ satisfies (i)-(iii) below:}\} \tag{4.5}$$

(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 $\hat\Omega$ (with χ_A denoting the characteristic function of A).

(ii) 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 $\phi \in \mathrm{Cart}^p(B; \mathbb{R}^3)$ 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 in B, then it is readily satisfied that the distributional determinant $\mathrm{Det}(F)$ and adjoint $\mathrm{Adj}(F)$ of F are elements of $L^1(B, \mathbb{M}^3)$ and coincide with $\det(Du)$ and $\mathrm{adj}(Du)$ respectively. It is also straightforward that smooth functions $u \in C^1(B, \mathbb{R}^3)$ 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 finite mutual intersections coinciding with α in $\partial\Omega_D$. In the following theorem, we will use the identity:

$$-\operatorname{Curl} F = b \otimes \tau\, \mathcal{H}^1 \llcorner L \quad \text{if and only if} \quad \int_{C_L} F\, \underline{e}_\theta d\mathcal{H}^1 = b. \tag{4.6}$$

for all Lipschitz-continuous closed path C_L in Ω enclosing once L and with unit tangent vector $\underline{e}_\theta$. To check identity (4.6), observe that, if S_L is a Lipschitz and compact surface in Ω with boundary L and unit normal ν, then $\Omega \setminus S_L$ is simply-connected and there exists a function $\phi \in W^{1,p}(\Omega \setminus S_L)$ such that $F = \nabla\phi$ in $\Omega \setminus S_L$. By (4.6), ϕ has a constant jump on S_L equal to 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, by (2.1), one has $\langle \operatorname{Curl}(b \otimes \nu\mathcal{H}^2 \llcorner S_L), \psi\rangle = \langle b \otimes \nu\mathcal{H}^2 \llcorner S_L, \operatorname{Curl} \psi\rangle$. By Stokes theorem, this writes componentwise as

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

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

Proof. We first construct an admissible function for a simple geometry. Consider the circle $L := \{(x,y,z) \in \mathbb{R}^3 : |x|^2 + |y|^2 = R^2,\ z = 0\}$ as a dislocation loop with Burgers vector $b = \beta_1 \underline{e}_1 + \beta_2 \underline{e}_2 + \beta_3 \underline{e}_3 = \beta_R \underline{h}_R + \beta_l \underline{h}_l + \beta_z \underline{h}_z$, where we have used the local basis on L, $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\} = Q(l)\{\underline{e}_1, \underline{e}_2, \underline{e}_3\}$. Here, $Q(l)$ is the matrix of rotation around $\underline{e}_3 = \underline{h}_z$ by the 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 as follows: 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 $a > 0$ (to be fixed later); the coordinate r is the distance from the set L; l, as before, is R times the angle around the z axis. Corresponding to these coordinates, the local cylindrical basis defined on the normal sections of V_δ are denoted by $\underline{g} := (\underline{g}_r, \underline{g}_\theta, \underline{g}_l)$, with $\underline{g}_l = \underline{h}_l$.

We then consider the function $\hat{F}$ inside V_δ whose components in the basis $\{\underline{h}_R, \underline{h}_l, \underline{h}_z\}$ read

$$\hat{F}(r,\theta,l) = \zeta(\theta) \begin{pmatrix} -\frac{\sin\theta}{r}\beta_R & +\frac{\cos\theta}{r}\beta_R & 0 \\ -\frac{\sin\theta}{r}\beta_l & +\frac{\cos\theta}{r}\beta_l & 0 \\ -\frac{\sin\theta}{r}\beta_z & +\frac{\cos\theta}{r}\beta_z & 0 \end{pmatrix}. \tag{4.7}$$

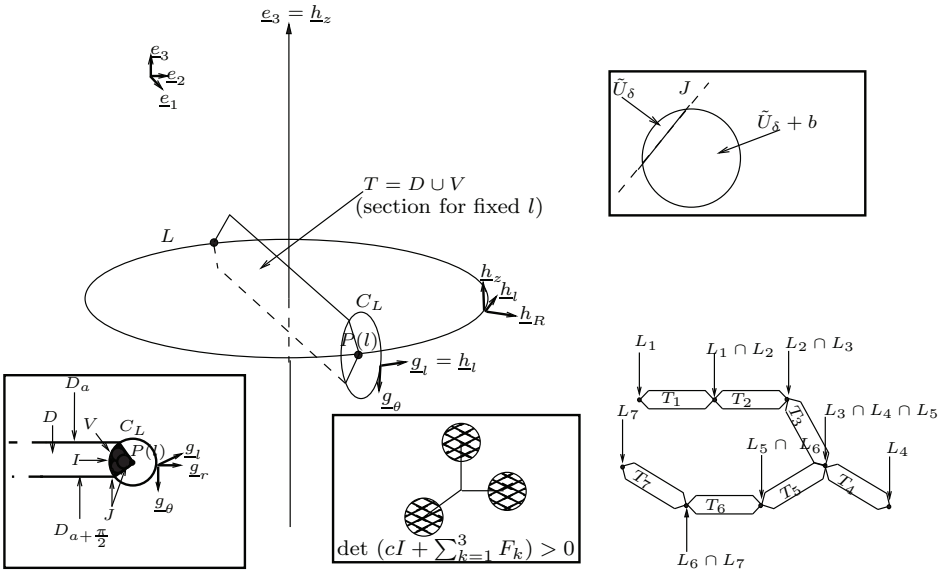
Here (r, θ, l) are the coordinates associated to the basis system $\underline{g}$, and ζ is a smooth function on $[0, 2\pi)$ which is non-negative in $(a, a+\pi/2)$, zero outside, and has integral equal to 1. It is readily checked that curl F $= 0$ in $V_\delta \setminus L$. It is known that there exists a solution to equation $\hat{F} = \nabla\phi_\delta$ in the simply-connected domain $S = S_l := \{(r,\theta,l) : a < \theta < a + \pi/2, 0 < r < \delta\}$ with $0 \le l \le 2\pi$, and satisfying $\phi_\delta = 0$ on $\bar{S} \cap \{\theta = a\}$ 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 ϕ_δ is constant on the sets $C_{\bar\theta} := \{(\delta, \bar\theta, l) : 0 \le l \le 2\pi R\}$ for every $a < \bar\theta < a + \pi/2$. Let $D_{\bar\theta}$ be the disk with boundary $C_{\bar\theta}$. 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 finally set $\phi_\delta = 0$ in $\Omega \setminus (V \cup D)$. Notice that ϕ_δ 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 $\|\nabla\tilde\phi_\delta\|_{L^\infty(D\cap\mathcal{V})} \le 2\|\nabla\phi_\delta\|_{L^\infty(D\cap\mathcal{V})}$ 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 $\tilde\phi_\delta$). As for the jump set J, the jump part of $D\tilde\phi_\delta$ reads $b \otimes \nu\ \mathcal{H}^2 \llcorner J$. Moreover, (4.6) and (4.7) entail that $-\operatorname{Curl} F = b \otimes \tau\ \mathcal{H}^1$ on L. As a consequence, the function F turns out to be smooth outside L, vanishes outside $T := V \cup D$, while, from expression (4.7), $F \in L^p(\Omega)$ for $p \in [1, 2)$, since

$$\|\hat{F}\|^p_{L^p(\Omega)} \le C|b|(R\delta^{2-p} + \delta^{1-p}R^2), \tag{4.8}$$

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, has null curl, and hence there exists $\phi \in C^\infty(B)$ 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 cancelling the discontinuity due to the jump. Thus ϕ is smooth, and hence is a Cartesian map.



(a) (b)

Fig. 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 $c > 0$ multiplying the identity 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 $1 \le k \le K$ with the associated $T_k := V_k \cup D_k$ constructed as described above, and observe that (by possibly adapting the amplitude of the solid angle S_k, i.e., replacing $\pi/2$ by π/N) the T_k's only intersect at points in L_k for some k's, while keeping the V_k's with empty mutual intersection (cf. Fig 4(b) below left). Let F_k be defined as (4.7) with β_k in place of β and a_k in place of a, chosen in order that $f_k(\theta, l) := \beta_l^k(l)\cos\theta - \beta_R^k(l)\sin\theta = \beta_2^k \cos(\theta + \frac{l}{R}) - \beta_1^k \sin(\theta + \frac{l}{R}) \ge 0$ (for instance, if $\beta_1, \beta_2 > 0$, then $a_k := \frac{3\pi}{2} - \frac{l}{R}$). Defining $F := \sum_{k=1}^{K} F_k + cI$, (4.8) entails that F, $\det F$, $\mathrm{adj} F$ belong to L^p, that

$$\det F = \frac{c^2}{r} f_k(\theta, l)\zeta(\theta) + c^3 \ge 0 \quad \text{in } V_k, \tag{4.9}$$

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).

Notice that the arguments presented above for a finite family of circular loops remain valid for a Lipschitz deformation of such loops, with appropriate Lipschitz deformations of the T_k's. In particular, it is valid for the boundary current α, and for any finite family of curves in Ω joining P_i's to the Q_i's without self-intersections (an

admissible F can be constructed as above in $\hat{\Omega} \supset \Omega$ and then restricted to Ω with its curl restricted to $\bar{\Omega}$). The proof is achieved. ∎

5. Existence of minimizers. Our mechanical setting for the minimum problem is the one of Assumption 4.10. Here 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 (but this is 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.

5.1. Existence result in $\mathcal{F} \times \mathcal{MD}$. We are given a potential $\mathcal{W} : \mathcal{F} \times \mathcal{MD} \to [0, +\infty]$ such that there are positive constants C and β for which

$$\mathcal{W}(F, \mathcal{L}) := \int_\Omega \mathrm{W_e}(F)dx + \mathcal{W}_{\mathrm{defect}}(\Lambda_\mathcal{L}) \geq C\big(\|\mathcal{M}(F)\|_p^p + \sum_{j \leq k_\mathcal{L}} b^j \|\dot{\varphi}_j\|_{L^1} + k_\mathcal{L}\big) - \beta, \tag{5.1}$$

with the notation

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

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 3.3, 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 $g : \mathbb{M}^3 \times \mathbb{M}^3 \times \mathbb{R}^+ \to \mathbb{R}^+$ 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 $\mathcal{W}^2_{\mathrm{defect}}(\Lambda_\mathcal{L}) = \kappa_2 \sum_{1 \leq j \leq k_\mathcal{L}} b^j \|\dot{\varphi}_j\|_{L^1}$, for some constitutive material positive parameters κ_1 and κ_2.

(W4) $\mathcal{W}^1_{\mathrm{defect}}$ 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 $\mathcal{M}_\mathrm{b}(\bar{\Omega}, \mathbb{M}^3)$.

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 5.1. *The term involving $\|\dot{\varphi}_j\|_{L^1}$ in the energy bound is mandatory for mesoscopic dislocations, since it controls the length of the lines. In fact, minimizing sequences of Lipschitz maps (describing minimizing sequences of lines) might become locally dense, a phenomenon which should be prohibited to get existence. For a physical viewpoint this term is questionable since dense arcs of the dislocation cluster might be nonnecessary, and hence admissible from an energetical standpoint. This drawback is addressed in the second existence result for continuum dislocations in Section 5.1. Moreover, recalling* (4.2)*, this term implies a bound on the densities.*

Before stating the existence of minimizers of the problem

$$\inf_{\substack{(F,\Lambda_\mathcal{L}) \in \mathcal{F} \times \mathcal{MD} \\ -\operatorname{Curl} F = \Lambda_\mathcal{L}^\mathrm{T}}} \mathcal{W}(F, \Lambda_\mathcal{L}), \tag{5.2}$$

some technical results should be stated and proven.

LEMMA 5.2. *Let* $(F_k, \mathcal{L}_k)$ *be a minimizing sequence for the problem* (5.2)*, 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 $0 = \liminf \int_A \det F_k > 0$ since $\chi_A \in L^q(A)$, a contradiction. Hence from condition $(W1)$, we must have $\mathcal{W}(F_k, \Lambda_{\mathcal{L}_k}) \geq \int_A W_{\mathrm{e}}(F_k)dx \geq \int_A h(\det F_k)dx$. By Fatou's Lemma and the fact that $(F_k, \mathcal{L}_k)$ is a minimizing sequence, the contradiction follows, and hence A must be negligible, achieving the proof. □

LEMMA 5.3. *Let* γ_n *be a sequence of* 1*-currents in* $\bar{\Omega}$ *such that* $\gamma_n = \varphi_{n\sharp}[\![[0, M]]\!]$ *for Lipschitz functions* φ_n *with* $\mathrm{Lip}(\varphi_n) \leq 1$ *for all* $n > 0$*. 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 uniformly bounded and uniformly continuous 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 5.4. *Let* $\hat{\mathcal{L}}_n = \{S_n, \tau_n, \theta_n\}$ *be a sequence of uniformly bounded dislocation currents of the form* (3.20) *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* $\Lambda_n := \Lambda_{\mathcal{L}_n}$*, the sequence of densities of* $\mathcal{L}_n$*, weakly converges to* $\Lambda \in \mathcal{M}_{\mathrm{b}}(\bar{\Omega}, \mathbb{M}^3)$*, as* $n \to \infty$*. Moreover,* $\hat{\mathcal{L}}$ *satisfies the boundary condition, it has density* $\Lambda = \Lambda_{\mathcal{L}}$*, and for all* $k = 1, 2, 3$*,* $(\mathcal{L}_n)_k \rightharpoonup \mathcal{L}_k$*, and* $(\Lambda_n)_k \rightharpoonup \Lambda_k = \mathcal{L}_k \otimes e_k$ *(with the notation* (3.9)*).*

Proof. As in (3.20), 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 $(\Lambda_n)_k = \mathcal{L}_n \otimes e_k$. By assumption $(\mathcal{L}_n)_k$ are closed in Ω and, thanks to (3.21), $(\mathcal{L}_n)_k$ are uniformly bounded. Thus, Theorem 2.3 implies existence of 3 integral currents $\{\mathcal{L}_k\}_{k=1}^3$ s.t. $(\mathcal{L}_n)_k \rightharpoonup \mathcal{L}_k$, as $n \to \infty$. Since

$$\hat{\mathcal{L}}_n(\omega) = \sum_{k=1}^{3} (\mathcal{L}_n)_k(\omega_k) \to \sum_{k=1}^{3} \mathcal{L}_k(\omega_k), \tag{5.3}$$

for all $\omega \in \mathcal{D}^1(\Omega, \mathbb{R}^3)$, we get $\hat{\mathcal{L}}_n \rightharpoonup \hat{\mathcal{L}} := \sum_{k=1}^3 \hat{\mathcal{L}}_k$. The fact that $\hat{\mathcal{L}}$ satisfies the boundary condition follows from the convergence $\partial\hat{\mathcal{L}}_n \rightharpoonup \partial\hat{\mathcal{L}}$. 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 $\mathcal{M}_{\mathrm{b}}(\bar{\Omega}, \mathbb{M}^3)$, with $(\Lambda_n)_k \rightharpoonup \Lambda_k$ weakly in $\mathcal{M}_{\mathrm{b}}(\bar{\Omega}, \mathbb{M}^3)$, and $\Lambda_k = \mathcal{L}_i \otimes e_k$ for all $k = 1, 2, 3$. □

Now we are ready to solve Problem (5.2).

THEOREM 5.5 (Existence in $\mathcal{F} \times \mathcal{MD}$). *Assume* $(W1) - (W4)$ *and assume existence of an admissible* $(F, \mathcal{L}) \in \mathcal{F} \times \mathcal{MD}$ *such that* $\mathcal{W}(F, \Lambda_{\mathcal{L}}) < \infty$*. Then, there is at least a solution of the minimum problem* (5.2)*.*

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

$$F_n \rightharpoonup F \quad \text{weakly in } L^p(\Omega, \mathbb{M}^3), \tag{5.4a}$$

$$\text{adj } F_n \rightharpoonup A \quad \text{weakly in } L^p(\Omega, \mathbb{M}^3), \tag{5.4b}$$

$$\det F_n \rightharpoonup D \quad \text{weakly in } L^p(\Omega). \tag{5.4c}$$

By condition (i) of Definition 4.5 and since F_n satisfy the same boundary condition, we can consider $\hat{F}_n$ the extensions of F_n on $\hat{\Omega}$ in such a way that $\hat{F}_n = \bar{F}$ on $\hat{\Omega} \setminus \Omega$ for a fixed $\bar{F}$. In particular, also $\hat{F}_n$ satisfies the convergences (5.4a)-(5.4c) for some $\hat{F}$, $\hat{A}$, and $\hat{D}$ extensions of F, A, and D, respectively. It also follows that at the limit $\hat{F} = \bar{F}$ on $\hat{\Omega} \setminus \Omega$ and thus F satisfies the same boundary condition. Moreover, By the uniform bound on $\sum_{j \le k_{\mathcal{L}}} b^j \|\dot{\varphi}_j\|_{L^1}$ in (5.1) and by (4.2), $\Lambda_n^T := -\operatorname{Curl} \hat{F}_n$ are uniformly bounded. Hence, there is a measure $\Lambda \in \mathcal{M}_{\mathrm{b}}(\bar{\Omega}, \mathbb{M}^3)$ such that, as $n \to \infty$,

$$\Lambda_n \rightharpoonup \Lambda \ \text{ weakly in } \mathcal{M}_{\mathrm{b}}(\bar{\Omega}, \mathbb{M}^3). \tag{5.4d}$$

Now 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.

It remains to check this fact. Since the energy values at $(F_n, \mathcal{L}_n)$ are uniformly bounded by $k_{\mathcal{L}}$ in (5.1), 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.,

$$\hat{\mathcal{L}}_n(\omega) = \sum_{j=1}^K \varphi_{n\sharp}^j [\![0, M]\!](\omega b^j) \qquad \text{and} \qquad \Lambda_n = \sum_{j=1}^K \varphi_{n\sharp}^j [\![0, M]\!] \otimes b^j u \tag{5.5}$$

for all $\omega \in \mathcal{D}^1(\hat{\Omega}, \mathbb{R}^3)$. By Lemma 5.3, we can suppose that for every j we have

$$\varphi_{n\sharp}^j [\![0, M]\!] \rightharpoonup \varphi_\sharp^j [\![0, M]\!],$$

for some 1-Lipschitz functions $\{\varphi^j\}_{j=1}^K$. By Lemma 5.4 we have $\hat{\mathcal{L}}_n \rightharpoonup \hat{\mathcal{L}}$, with $\hat{\mathcal{L}}(\omega) := \sum_j \varphi_\sharp^j [\![0, M]\!](\omega b^j)$ for all $\omega \in \mathcal{D}^1(\hat{\Omega}, \mathbb{R}^3)$, and $\Lambda_n \rightharpoonup \sum_j \varphi_\sharp^j [\![0, M]\!] \otimes b^j$ weakly in $\mathcal{M}_{\mathrm{b}}(\hat{\Omega}, \mathbb{M}^3)$. Therefore, from (5.4d) we get

$$\Lambda = \sum_j \varphi_\sharp^j [\![0, M]\!] \otimes b^j. \tag{5.6}$$

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

$$\langle \operatorname{Curl} \hat{F}_n, w \rangle = \langle \hat{F}_n, \operatorname{Curl} w \rangle \to \langle \hat{F}, \operatorname{Curl} w \rangle = \langle \operatorname{Curl} \hat{F}, w \rangle, \tag{5.7}$$

as $n \to \infty$. Since the first term in the left-hand side of (5.7) also tends to $\langle -\Lambda^T, w \rangle$, we finally get

$$-\operatorname{Curl} \hat{F} = \sum_j b^j \otimes \varphi_\sharp^j [\![0, M]\!]. \tag{5.8}$$

Let us set $L_n := \bigcup_{j=1}^K \varphi_n^j([0, M])$ and $L := \bigcup_{j=1}^K \varphi^j([0, M])$. 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 $u \in \mathrm{Cart}^p(B, \mathbb{R}^n)$ such that $Du = F$ in B. Let x be such a point. By the uniform convergence $\varphi_n^j \to \varphi^j$, it follows that L_n tends to L in the Gromov-Hausdorff topology, so we have $B \cap L_n = \varnothing$ for n sufficiently large. In such a ball, by hypotheses, there are maps $u_n \in \mathrm{Cart}^p(B, \mathbb{R}^n)$ satisfying $Du_n = F_n$, and, up to summing suitable constants to u_n, we can also suppose u_n have all zero average in B. The Poincaré inequality provides u such that $u_n \rightharpoonup u$ weakly in $W^{1,p}(B, \mathbb{R}^3)$. Hence Theorem 2.6 implies that $A = \mathrm{adj}F$ and $D = \det F$. Thesis follows from (5.4a)-(5.4c) and Lemma 5.2. ∎

We remark that with the formulation (5.1) the potential $W(F, \Lambda_{\mathcal{L}})$ depends explicitly on the dislocation current.

5.2. 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 line itself might 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:

$$\mathcal{F}' := \{F \in L^p(\Omega, \mathbb{M}^3) : F \text{ satisfies (i)-(iii) below:}\} \tag{5.9}$$

(i) There exists a continuum dislocation $\mathcal{L} := \mathcal{L}_{\mathcal{I}} \in \mathcal{CD}$ satisfying the boundary condition and 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 for every $x \in \Omega \setminus \mathcal{C}$, there is a ball $B \subset \Omega \setminus \mathcal{C}$ centered at x and a function $\phi \in \mathrm{Cart}^p(B; \mathbb{R}^3)$ 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 are positive constants C and β such that

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

with

$$G(\mathcal{L}) := \inf_{\mathcal{K} \in \mathcal{C}_{\mathcal{L}}} \left(\mathcal{H}^1(\mathcal{K}) + \kappa \#\mathcal{K}\right), \tag{5.10}$$

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

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

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

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 $\mathcal{W}_{\mathrm{defect}} = \mathcal{W}^1_{\mathrm{defect}} + \mathcal{W}^2_{\mathrm{defect}}$, with, for instance, $\mathcal{W}^2_{\mathrm{defect}} = \kappa G$ for some $\kappa > 0$, whereas a typical example for $\mathcal{W}^1_{\mathrm{defect}}$ reads

$$\mathcal{W}^1_{\mathrm{defect}}(\Lambda) = \int_L \psi(\theta b, \tau) d\mathcal{H}^1, \tag{5.11}$$

where b, θ, and τ represent the Burgers vector, its multiplicity, and the tangent vector to the dislocation L, respectively. Under suitable hypotheses on the function ψ, $\mathcal{W}^1_{\text{defect}}$ is proved to be lower semicontinuous in the sense of $(W6)$ (see [9]).

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

THEOREM 5.6 (Existence in $\mathcal{F}'$). *Assume* $(W5)$ *and* $(W6)$ *and assume existence of an admissible* $F \in \mathcal{F}'$ *with* $\mathcal{W} := \int_\Omega W(F) < \infty$. *Then, there exists a minimizer to 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, arguing as in the proof of Theorem 5.5, 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 as $n \to \infty$. Thanks to (3.21), $\{\hat{\mathcal{L}}_n\}$ are uniformly bounded, so that one has by Theorem 2.3 the existence of an integer multiplicity current $\hat{\mathcal{L}}$ such that $\hat{\mathcal{L}}_n \to \hat{\mathcal{L}}$, while by Lemma 5.4, $\Lambda = \Lambda_{\hat{\mathcal{L}}} = (-\operatorname{Curl} \hat{F})^T$ 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 $G(\mathcal{L}_n) = \big(\mathcal{H}^1(\mathcal{K}_n) + \kappa \# \mathcal{K}_n\big)$ are uniformly bounded. By $(W5)$, Blaschke and Golab theorems, $\mathcal{K}_n$ converges 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 supports are 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. Now $\hat{\mathcal{L}} = (\hat{L}, \tau, \theta)$ is admissible since $L^\star := \operatorname{spt}\Lambda \subset \mathcal{K}$. Taking any ball in $\Omega \setminus \mathcal{K}$, we conclude as in the proof of Theorem 5.5. $\square$

The physical interpretation of $G(\mathcal{L})$ is the following. To create a new loop at some finite distance d from the current dislocation $\mathcal{L}$, it is worth to nucleate (i.e., add a connected component) rather than deforming the existent dislocation, as soon as $d > \kappa$. It basically means that the continuum dislocation lies in a compact 1-set which keeps as minimal the balance between the number of its connected subsets (of the continuum, not of the dislocation cluster) and its length. However, it should be admitted that (5.10) is so far a mere mathematical assumption whose physical meaning remains to be elucidated.

5.3. A weak notion of Jacobian for displacements in the presence of dislocations. Let us firstly introduce some conventions.

DEFINITION 5.7 (Hodge identification). *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* $w_i := (-1)^{i+1}\omega_{\bar{i}}$.

As a consequence, the curl operator on $C_c^\infty(\mathbb{R}^3, \mathbb{R}^3)$ satisfies

$$\operatorname{curl} w := d\omega, \tag{5.12}$$

for all $\omega \in \mathcal{D}^1(\mathbb{R}^3)$, where in the right-hand side we first identify w with the 1-form ω, then we compute the external derivative, and identify the resulting 2-form with the corresponding vector field in $\mathbb{R}^3$.

DEFINITION 5.8. *We also identify elements* $v \in \mathbb{R}^3$ *with* 2*-vectors by* $\Lambda_2(\mathbb{R}^3) \ni v = v_i e_{\bar{i}}$. *Similarly, elements* $v \in \mathbb{R}^3$ *are seen as* 1*-vectors, as* $v = v_i e_i \in \Lambda_1(\mathbb{R}^3)$. *From these correspondences it is possible to identify either*

- *a distribution* $T \in \mathcal{D}'(\mathbb{R}^3, \mathbb{R}^3)$ *with a* 2*-current in* $\mathcal{D}_2(\mathbb{R}^3)$*,*
  or
- *a distribution* $T \in \mathcal{D}'(\mathbb{R}^3, \mathbb{R}^3)$ *with a* 1*-current in* $\mathcal{D}_1(\mathbb{R}^3)$*.*

In particular, thanks to this identification, we can define the Curl of a current as follows

$$\langle \operatorname{Curl} \mathcal{T}, \omega \rangle := \langle T, \operatorname{curl} w \rangle,$$

where in the right-hand side we have identified the current with a distribution, and the form with a smooth fields, as in the previous definition.

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

$$\partial \mathcal{S}(\omega) = \mathcal{S}(d\omega) = \langle S, \operatorname{curl} w \rangle = \langle \operatorname{Curl} \mathcal{S}, w \rangle. \tag{5.13}$$

We now collect two classical results.

THEOREM 5.9. *Let* Ω *be a bounded and simply-connected open set. Let* $\lambda \in \mathcal{M}_{\mathrm{b}}(\Omega, \mathbb{R}^3)$ *be a Radon measure such that* $\operatorname{Curl} \lambda = 0$ *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 [20]. The following results provides a chain rule to compute the derivative of the composition of a smooth function with a function with bounded variation (see [3] or [30]).

THEOREM 5.10. *Let* $u \in BV(\Omega)$ *with* $\Omega \subset \mathbb{R}^3$ *a bounded open set, and let* $f \in C^1(\mathbb{R}^3)$*. Then the distributional derivative of* $f \circ u$ *is given by*

$$D(f \circ u) = Df(u) D^a u \mathcal{L}^n + Df(\tilde{u}) D^c u + (f(u^+) - f(u^-)) \nu_{J_u} \mathcal{H}^2 \llcorner_{J_u}, \tag{5.14}$$

where $\tilde{u}$ *is the Lebesgue representative of* u *(i.e.,* $\tilde{u}(x)$ *is the Lebesgue value of* u *at* x*),* $D^a u$ *and* $D^c u$ *are the absolutely continuous part and the Cantor part of the derivative of* u*. Moreover* J_u *is the jump set of* u *with unit normal* ν*, while* u^+ *and* u^- *are the traces of* u *on* J_u*, from the two sides of* J_u*, respectively.*

Now, let us prove the following result, stating that each strain F in the presence of dislocations can be written by means of the gradient of a Sobolev map with value in $(S^1)^3$.

THEOREM 5.11. *Let* Ω *be a bounded and simply-connected open set. Let* $\mathcal{L} \in \mathcal{D}_1(\Omega)$ *be a closed* 1*-integral current and suppose* $F \in L^1(\Omega, \mathbb{R}^3)$ *is such that* $\operatorname{Curl} F = \mathcal{L}$ *(with the identification* (5.13)*). Then there exists* $u \in W^{1,1}(\Omega, S^1)$ *such that* $F = u_1 Du_2 - u_2 Du_1$ *in* Ω*.*

Proof. Since $\mathcal{L}$ is a closed 1-integer multiplicity current, there exists a 2-integral current $\mathcal{S}$ such that $-\partial \mathcal{S} = \mathcal{L}$. Let us now define the distribution $\lambda \in \mathcal{D}'(\Omega, \mathbb{R}^3)$ 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 5.7. The distribution λ is easily seen to be a Radon measure with finite mass. Computing the Curl of λ, we get

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

for all $\varphi \in C_c^\infty(\Omega, \mathbb{R}^3)$, by definition of $\mathcal{S}$. Then, Theorem 5.9 implies that there exists $v \in SBV(\Omega)$ such that $Dv = \lambda = \mathcal{S} + F$. 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 (5.14) 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 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. ∎

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 $-u_2^i D_j u_1^i + u_1^i D_j u_2^i = F_{ij}$ in Ω, for $i = 1, 2, 3$. The above statement and the proof is found in the simpler 1-dimensional case, but it can be generalized, as applied to every row of F.

In some sense, also the opposite of Theorem 5.11 holds true.

THEOREM 5.12. *Let $u \in W^{1,1}(\Omega, S^1)$ and assume that u satisfies*

$$\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) \in \mathcal{M}_{\mathrm{b}}(\Omega, \mathbb{R}^3). \tag{5.15}$$

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 hypothesis (5.15), $\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) = 2\pi\mathcal{L}$ is a closed 1-current $\mathcal{L}$, possibly with nonfinite mass. A constructive proof of Theorem 5.12 can be found in [24, Theorem 2.3.9].

In the theory of functions of bounded higher variation, introduced by Jerrard and Soner [18], 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

$$[J(u)] := dj(u), \tag{5.16}$$

which is a 2-form on Ω. Using identification (5.7) and (5.8), it turns out that $[Ju]$ is exactly $\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2)$. Hence, standing to the notations of [18], condition (5.15) is equivalent to requiring 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

$$\begin{aligned}\mathcal{U} := \{u \in W^{1,1}(\Omega, (S^1)^3) :\ &\operatorname{Curl}\,(-u_2 Du_1 + u_1 Du_2) \text{ is an integral}\\ &\text{1-current with coefficients in } \mathbb{Z}^3\},\end{aligned} \tag{5.17}$$

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

$$\begin{aligned}\mathcal{U}_c := \{u \in B2V(\Omega, (S^1))^3 :\ &[Ju] \text{ belongs to } \mathcal{CD},\\ &\text{and } u \in \operatorname{Cart}^p(B, (S^1)^3) \text{ whenever } B \cap L = \emptyset\},\end{aligned} \tag{5.18}$$

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

THEOREM 5.13. *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*

$$\mathcal{W}^1_{\mathrm{defect}}([Ju]) = \kappa_2 |[Ju]|(\Omega), \tag{5.19}$$

for some $\kappa_1, \kappa_2 > 0$. Then, there exists a minimizer $u \in \mathcal{U}_c$ of $\mathcal{W}(F)$, where $F_{ij} = u^i_1 D_j u^i_2 - u^i_2 D_j u^i_1$.

In the previous result, it is tacitly assumed that also a boundary condition is fixed.

5.4. 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 the following example we show that under suitable boundary condition, the dislocation of a minimizer will not be in U but will stay inside Ω. We consider the map $\bar{F} : \hat{\Omega} \to \mathbb{M}^3$ defined as

$$\bar{F}(\rho, \theta, z) = \zeta(\theta) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{\sin\theta}{\rho}\beta & \frac{\cos\theta}{\rho}\beta & 1 \end{pmatrix}, \tag{5.20}$$

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

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

This means that $\bar{F}$ shows a screw dislocation on the z-axis $\hat{z}$ with Burgers vector $b = (0, 0, \beta)$. We want to minimize the energy (5.1) 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 (4.5) with $\bar{F}$ as boundary condition. Let us suppose that the defect part of the energy takes the form

$$\mathcal{W}_{\mathrm{defect}}(\Lambda_{\mathcal{L}}) = \gamma \int_0^1 \|\dot{\varphi}(s)\| ds + \sum_{1 \le i < k_{\mathcal{L}}} \gamma \int_{S^1} \|\dot{\varphi}_i(s)\| ds + \mu |\Lambda_{\mathcal{L}}(\Omega)|, \tag{5.21}$$

for $\gamma > 0$ and $\mu > 0$, two material parameters, where the mesoscopic dislocation $\mathcal{L}$ is the image of $k_{\mathcal{L}}$ closed loops φ_i with Burgers vector b^i, with $\varphi_1 = \varphi$ being a dislocation with endpoints $P := (0, 0, h)$ and $Q := (0, 0, -h)$ and Burgers vector $b_1 = b$. 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

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

Let us now take another admissible deformation F^1 with the dislocation path φ_1 connecting P and Q 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

$$\mathcal{W}_{\text{defect}}(\mathcal{L}^1) \geq \gamma \int_0^1 \|\dot{\varphi}_1(s)\| ds + \mu |\Lambda_{\mathcal{L}}|(\Omega) \geq 2\gamma (R_t^2 + h^2)^{1/2} + 2h\mu\beta.$$

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

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

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

6. 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. To justify this generality, 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 related by $-\operatorname{Curl} F = \Lambda^T$.

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 networks, 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 the *deformation* internal variable F and the *defect* internal variable Λ. From this point of view, the individuality of the lines is replaced by a tensor density measure and hence all geometrically unnecessary dislocation segments are effectless in the model. These two approaches are connected, since the mass of a current is finite as soon as its density is bounded, at least as long as the Burgers vectors are crystallographic, that is, when dislocation currents are written by means of canonical dislocations.

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 in 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 behavior is precluded by the presence of the embedding continuum.

Furthermore, 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 range of p between 1 and 2. Let us mention a partial answer in a companion paper [26].

The described mathematical framework will be considered for future work in order to describe evolution problems involving the dissipation due to dislocation motion. Here a preliminary step before the complete dynamics will be the quasi-statics problem, that is, dynamics under the assumption that optimality (i.e., global minimization) is reached within each time step.

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 whether it is a measure, and homogenization of a countable family to the continuum to the macroscale (see, eg., [10, 12]). 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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Appendix A. Modeling discussion. So far, dislocations are mathematically represented by currents but it is crucial to keep in mind their physical origin and formation. A dislocation loop in the bulk results from nucleation, that is, the collapse of a void (i.e., a cavitation formed by aggregation of vacancies) which has become unstable. Another source of dislocations is the flux of vacancies or interstitials at the crystal boundary. In each case, the basic dislocation is a loop which is associated to a single Burgers vector that depends on the crystal structure. Submitted to thermal and mechanical forces, to diffusion, annihilation, recombination and any kind of mutual interactions, these loops might in turn deform and move inside the crystal and through its boundary, but also form clusters which themselves will either evolve or behave as fixed obstacle to the motion of other loops, provoking material hardening.

These considerations are at the basis of the notion of *regular dislocation* introduced above. According to the dislocation physics, the basic object are the loops associated to a given Burgers vector b, i.e., the functions φ_j^b introduced in Definition 3.1. These simple *generator* loops will then be smoothly deformed and summed (in the sense of currents) in order to form dislocation clusters. Moreover, it should be emphasized that the limited number of Burgers vectors of the generating loops might increase significantly as clusters are considered since Frank law applies at dislocation junctions [15]. For this reason, our restriction to finite families of regular loops associated to a finite number of distinct Burgers vectors (Assumption 4.1) does not preclude the formation of complex structures. As a consequence, a dislocation of this kind might be formed by countably regular loops connected by arcs which are effectless in terms of the intrinsic geometry of the crystal, and therefore referred to as *geometrically unnecessary* Ξ (Definition 3.9). Moreover, though being 1-sets, the clusters might exhibit complex geometries at the countable intersections or at the sets of accumulation points of their generating loops. It should nevertheless be specified that since overlapping of dislocations is not acceptable from a physical viewpoint, it

should be equivalently understood as a single curve associated to a scalar multiple of the Burgers vector.

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

Let us now describe a dislocation cluster which is not a mesoscopic dislocation. Consider the cluster of Fig. 3(c) but instead of assuming that each loop possesses the same Burgers vector b, suppose that the family $\mathcal{B}_\mathcal{I} \nsubseteq \mathcal{B}$ of Burgers vectors is non-crystallographic, that means that if $\mathcal{B}_\mathcal{I} = \{b_i\}_{i\in\mathbb{N}}$ then the ratios b_i/b_j is never rational for every $i \neq j$. Thus, it clearly appears that this cluster cannot be made of regular dislocations without violating Assumption 4.1. Instead, it turns out that the broader notion of continuum dislocation holds for this kind of pathological cluster, as long as the sum of the length of the loops is finite. We emphasize that from a strictly mesoscopic standpoint allowing the Burgers vectors to take countably many values ($\mathcal{B}_\mathcal{I} \nsubseteq \mathcal{B}$ non-crystallographic) is not physical, all the more for bounded crystals. However it can become important to permit this limit case, for instance if one considers homogenization, or from a statistical viewpoint, ensemble averaging of dislocations.

If $\mathcal{L}$ is a regular mesoscopic dislocation, the fact that $\mathcal{L} \in \mathcal{CD}$ does not imply that $\mathcal{H}^1(L) < \infty$, even if $\Lambda_\mathcal{L}$ is finite. Indeed *continuum dislocations* in $\mathcal{CD}$ might be quite wild, since they can consist of countable fully disconnected loops and may admit geometrically unnecessary arcs which are locally dense, i.e., $\mathcal{H}^1(\bar{\Xi}) = \infty$. Moreover, since disconnected pieces of a dislocation can be connected by adding geometrically unnecessary arcs Ξ (cf. Fig 3), it might also happen that $\mathcal{H}^1(\Xi) = \infty$.

The introduction of continuum dislocations might be convenient for some other reasons. First, considering time-evolution of dislocations, this latter class, as opposed to the former, allows us to consider an evolution of the unnecessary part $\Xi(t)$ such that $\mathcal{H}^1\left(\Xi(t)\right) \to \infty$ (or $\mathcal{H}^1\left(\bar{\Xi}(t)\right) \to \infty$) as t converges to some limit time. Time-evolution of some subset of $\mathcal{K}$ to a pathological Ξ is also possible within this setting, and it might be taken into account since unnecessary dislocations play an effective role in dynamics (as obstacle to motion, i.e. *hardening*), whereas they do not contribute to the dislocation density. Second, continuum dislocations conceptually suits better engineer models of dislocations in which necessary and unnecessary dislocations are treated by distinct, though coupled, equations.

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