FIELDS OF BOUNDED DEFORMATION FOR MESOSCOPIC DISLOCATIONS

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ABSTRACT. In this paper we discuss the consequences of the distributional approach to dislocations in terms of the mathematical properties of the auxiliary model fields such as displacement and displacement gradient which are obtained directly from the main model field here considered as the linear strain. We show that these fields cannot be introduced rigourously without the introduction of gauge fields, or equivalently, without cuts in the Riemann foliation associated to the dislocated crystal. In a second step we show that the space of bounded deformations follows from the distributional approach in a natural way and discuss the reasons why it is adequate to model dislocations. The case of dislocation clusters is also addressed, as it represents an important issue in industrial crystal growth while from a mathematical point of view, peculiar phenomena might appear at the set of accumulation points. The elastic-plastic decomposition of the strain within this approach is also given a precise meaning.

1. INTRODUCTION

In linear thermoelasticity, it is usually said that strain ($\mathcal{E}^\star$), displacement ($u^\star$) and rotation ($\omega^\star$) become "infinitesimal", and hence, that the reference and actual configurations coincide. In the absence of defect lines, the strain is everywhere compatible and hence single-valued rotation and displacement fields can be integrated from the strain field provided the domain be simply connected. However, when disclinations or dislocations are present, rotation and displacement become multiple-valued and hence, take their values on a domain called a Riemann foliation.

Let Ω be the actual configuration (the domain) and $\Omega_{\mathcal{L}} := \Omega \setminus \mathcal{L}$ with $\mathcal{L}$ the line defects, be the domain without dislocations and disclinations. In general, a multivalued function from $\Omega_{\mathcal{L}}$ to $\mathbb{R}^N$ consists of a pair of single-valued mappings with appropriate properties:

$$\mathcal{R} \to \Omega_{\mathcal{L}} \quad \text{and} \quad \mathcal{R} \to \mathbb{R}^3,$$

where F is the associated Riemann foliation [26, 27]. In the present case of meso-scale elasticity, we will limit ourselves to multivalued functions obtained by recursive line integration of single-valued mappings defined on $\Omega_{\mathcal{L}}$. Reducing these multiple line integrals to simple line integrals, the Riemann foliation shows to be the set of equivalence classes of paths inside $\Omega_{\mathcal{L}}$ from a given $x_0 \in \Omega_{\mathcal{L}}$ with homotopy as equivalence relationship. In particular, mappings of the following kind exist:

$$\Omega_{\mathcal{L}} \overset{\mathcal{P}}{\longleftarrow} \mathcal{R} \overset{\omega^\star, u^\star}{\longrightarrow} \mathbb{R}^3$$

where $\mathcal{R} := \{(x, \#\Gamma)$ for every $x \in \Omega_{\mathcal{L}}$ and every curve Γ joining x_0 to x, with $\#\Gamma$ the equivalence class of all curves homotopic to Γ in $\Omega_{\mathcal{L}}\}$ while $\mathcal{P}$ is the projection of $\mathcal{R}$ onto $\Omega_{\mathcal{L}}$, in such a way that $\mathcal{P}(x, \#\Gamma) = x$.

The Riemann foliation can be univoquely associated to the actual configuration if cuts are introduced in order to select one particular branch of the displacement and rotation. However, this approach causes major theoretical difficulties and will not be used in the sequel.

For this reason the distributional approach was introducted in [26, 27]. This approach does not consider rotation and displacement as model variables, and does not need the prescription of a reference configuration. Instead, it is based on the strain, itself defined from (single-valued) well-defined measurable quantities, namely the stress and the temperature distributions inside the body. The linear thermo-elasticity stress-strain-temperature relationship takes the following form (this assumption being generally valid in single-crystal growth):

$$\mathcal{E}^\star = (\mathbb{C}^\star)^{-1}\sigma^\star + \beta^\star(T^\star - T_0), \tag{1.1}$$

where $\sigma^\star$ denotes the stress field, $(\mathbb{C}^\star)^{-1}$ and $\beta^\star$ stand for the 4th- and 2nd-order compliance and thermal dilation tensors, and T_0 is the reference temperature.

Moreover, the main model field being the strain $\mathcal{E}^\star$, the distributional approach consists in assuming that $\mathcal{E}^\star$ has a locally integrable norm, which is consistent with the strain singularity as created by dislocations and disclinations. Then, derivatives of $\mathcal{E}^\star$ are taken in the distributional sense, thereby defining the Frank tensor $\bar{\partial}\omega^\star := -\mathcal{E}^\star \times \nabla$, and the Burgers tensor $\bar{\partial}b^\star := \mathcal{E}^\star + \big((x - x_0) \times \bar{\partial}\omega^\star\big)$, which both are order-one distributions (in the sense of L. Schwartz [18]). It should be emphasized that $\mathcal{E}^\star$ is not of square norm integrable, and hence the linear elastic energy might be unbounded. This well-known observation raises the open problem of searching an appropriate (nonlinear, nonlocal) constitutive law (an important step in this direction has been realized in [17]). We believe that an adequate constitutive law should incorporate strain derivatives, as for instance the Frank or Burgers tensors (see [21] for a discussion). It is remarkable that the strain curl appears instead of the strain gradient (cf. for instance [15] for gradient-based models).

Having said that, it is clear that with a view to a general model, (1.1) is an unproper constitutive law. It is nevertheless at the basis of our approach, but should here be considered as the definition of the linear strain $\mathcal{E}^\star$. For these reasons, the distributional approach is said to describe the geometry (or statics) of dislocations and disclinations in single crystals. Dynamical and energetical aspects at the mesoscale are for the moment beyond reach, though at the macroscale, dynamics is briefly addressed in two publications [22, 25].

Many other mathematical approaches to dislocations are based on the displacement (cf., e.g., [16, 17]). In general, an isothermal stress-free and defect-free reference configuration is considered on which the displacement is assumed of *bounded deformation* (in the sense of Temam and Strang [20]). This functional space is assumed because of its convenient decomposition property (the so-called BD decomposition theorem) of the symmetric part of the displacement gradient in a diffuse, norm-integrable part an a concentrated part on the set of displacement jump points. Moreover, the displacement jump is suitably identified with the *Burgers vector*, while the concentrated part of the strain is denoted as the *plastic* part.

Many questions arise from this formalism:

(1) how can one prove the identification of the displacement jump with the Burgers vector, being the latter classicaly defined as a uniform (i.e., constant for a given dislocation) line integral around the dislocation loop [10, 11, 26]?
(2) working with the displacement and a prescribed reference configuration implies that a cut in the Riemann foliation $\mathcal{R}$ has been implicitly assumed. Is this cut arbitrary or has it a physical meaning? In the latter case, it should be incorporated into the model, in the former, it is likely to generate gauge fields which in turn may have physical meaning.
(3) denoting the concentrated part as *plastic*, implicitely assumes that the diffuse part is elastic. Is this justified by any kind of constitutive law? Instead, shouldn't one assume that there might exist both elastic and plastic diffuse effects?
(4) by appropriately defining the plastic process together with a stress- and defect-free *intermediate*[1] configuration, the multiplicative (or Lee) decomposition of the deformation gradient F may nevertheless be such that the plastic strain be considered as purely concentrated. Then, assuming the elastic strain as a purely diffuse field allows us to identify the concentrated term of the BD decomposition with the plastic strain. The question raised by this procedure is that the reference configuration as defined by F must not be stress- and defect-free, while $\nabla u := F - I$ might not correspond to the gradient of the assumed BD displacement (because of an unspecified rotation). In addition ∇u cannot be decomposed in an elastic and plastic part, since obviously, no constitutive law for the rotation exists.
(5) assuming that the set of jump points Σ of the BD displacement field has a physical meaning would require to identify Σ with (a subset of) the glide planes of the dislocation $\mathcal{L}$. By definition, this would hold if both $\mathcal{L}$ and its Burgers vector would be contained in Σ. In particular, one should prove that the trace of the concentrated part of the strain vanishes, which is equivalent to a condition on the divergence of the BD displacement(and hence,again, on the chosen reference configuration).

The space of bounded deformation is probably the wright functional space to model dislocations. However, the aim of this paper is to justify the introduction of BD functions as a consequence of a

[1]Sometimes also called “plastic configuration“.

more general approach to model defect lines at the mesoscopic scale. Our objective is to rigourously introduce the physical and the mathematical concepts, and to emphasize their strong interrelation.

As a matter of fact, we start from the linear strain $\mathcal{E}^\star$, which is a well-defined, measurable quantity at the mesoscale, and which can be defined without appealing to any reference configuration. From well-known strain expressions for rectilinear dislocations and disclinations [26] we cannot assume that $\mathcal{E}^\star$ be more regular than $L^s_{loc}(\Omega)$ with $1 \leq s < 2$. This choice nonetheless allows us to define the strain derivatives as distribution tensors. In particular the Frank tensor and the strain incompatibility are defined and serve as the basis of our model. On the other hand, given the actual configuration Ω and a defect line $\mathcal{L}$ (or a set of lines Υ), the dislocation and disclination density *tensors* (remark that most of the available dislocation models are limited to scalar densities), are well-defined quantities explicitely given by the line location, orientation, and their Burgers or Frank vectors. A first issue was to relate the strain incompatibility to the defect densities. This has been completely answered in [26] for a finite family of rectilinear lines, in [27] for a countable family of such lines, in [23] for a finite family of skew lines, and in [24] for two kinds of planar dislocation loops[2].

In this paper we start from the main result of [24], (cf. Theorem 2 at the end of §2) relating strain incompatibility with the density of defects, namely with the so-called *contortion* tensor (this tensor is related to the crystal intrinsic torsion, cf. [12, 14, 21]), disclination density, and with the line curvature. From this result we show that appropriate completions of the Burgers and Frank tensors (cf. §3) can be introduced to generalize the relations valid for rectilinear lines. These so-called *completed* tensors are defined up to a gauge tensor field, which is nevertheless fixed (and its explicit expression given) for a particular case of $3D$ loops without disclinations, denoted as a simple dislocation loops in §2.1. In §4.14 we show that the distributional approach allows one to define a single-valued distortion field, which corresponds to the known distortion from which the dislocation theory is classically reported in the literature. In particular, its integral around $\mathcal{L}$ provides the Burgers vector (which in the distributional approach is merely defined from the single-valued strain and strain curl in [26]). In §4.2, it is shown that this distortion is indeed the gradient of a single-valued field, so far as general as a distribution vector. To this aim, one must introduce an arbitrary cut (related to aforementioned cut in Riemann foliation) on which the distortion shows concentrated effects. For this reason, another gauge vector field appears in the definition of the displacement. Eventually, in §5 we show that the symmetric part of the displacement gradient (note that at this stage, the latter does not coincide with the distortion introduced above) is a so-called *Radon measure*, and hence that the displacement is in fact of bounded deformation. Extension of these results to a finite and a countable family of loops, hence to dislocation clusters, including the peculiar phenomena at the accumulation set of lines, are discussed in §6. Finaly, a discussion on the consequences of these results with a view to the construction of general model is carried on in §6.3.

2. The distributional approach at the mesoscopic scale

The assumed open and connected domain is denoted by Ω, the defect line(s) are indicated by $\mathcal{L} \subset \bar{\Omega}$, and $\Omega_{\mathcal{L}}$ stands for $\Omega \setminus \mathcal{L}$. A family of lines will be denoted by Υ and is always assumed to be a closed subset of Ω, that is, the intersection of a closed subset of $\mathbb{R}^3$ with Ω.

Remark 1. *If $\Omega \subsetneq \mathbb{R}^3$, the given topological definition of Υ allows us to consider clusters of defects in $\partial\Omega$, which also corresponds to actual observation in single crystal growth technology. Indeed consider a sequence of $\{\mathcal{L}_k\}_k \in \Omega$ then its countable union is contained in $\Omega \cup \partial\Omega$.*

2.1. **Preliminary results.**

Notations 1. *For a second-order tensor E, we introduce the left (resp. right) curl operator $\nabla\times$ (resp. $\times\nabla$), i.e., $(\nabla \times E)_{ij} = \epsilon_{ikl}\partial_k E_{lj}$ and[3] $(E \times \nabla)_{ij} = \epsilon_{lkj}\partial_k E_{il}$ (otherwise written, $(E \times \nabla)^T = -\nabla \times E^T$), where E^T denotes the transpose of E. Note that $\nabla \times E$ might also be written as* curl E.

The incompatibility tensor associated to the symmetric second-order tensor E writes as

$$\text{inc } E := -\nabla \times E \times \nabla = \nabla \times (\nabla \times E)^T, \tag{2.1}$$

[2]In the latter, the loop curvature is shown to play a role.

[3]This notation is preferred to the other as found in [22, 23] with the opposite sign convention for the $\times\nabla$ operator.

i.e., written componentwise, $(\text{inc } E)_{ij} = \epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l E_{mn}$.

In the sequel, we say that a symmetric tensor E_{mn} is compatible on $U \subset \Omega$ if $\epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q E_{mn}$ vanishes on U. Moreover, as soon as $E \in L^1_{loc}(\Omega, \mathbb{R}^{3\times 3})$, the incompatibility of E, inc E is a distribution [18], that is, a linear and continous form on the space of test functions $\mathcal{C}^\infty_c(\Omega)$.

Assumption 1 (3D elastic strain)**.** *Let $\mathcal{L} \subset \Omega$ be a defect loop and let the elastic strain $\mathcal{E}^\star_{mn}$ be a given symmetric $L^s_{loc}(\Omega) \cap \mathcal{C}^\infty(\Omega_\mathcal{L})$-tensor compatible on $\Omega_\mathcal{L}$, with $1 \le s < 2$. In other words, the incompatibility tensor, as defined by the distribution $\eta^\star_{kl} := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathcal{E}^\star_{mn}$, vanishes everywhere on $\Omega_\mathcal{L}$.*

Definition 1 (Frank and Burgers tensors)**.** *The Frank tensor $\bar\partial\omega^\star$ is defined on the entire domain Ω as the following distribution:*

$$\bar\partial\omega^\star := -\mathcal{E}^\star \times \nabla, \tag{2.2}$$

that is, componentwise, $\bar\partial_m\omega^\star_k := \epsilon_{kpq}\partial_p\mathcal{E}^\star_{qm}$, in such a way that incompatibility writes as the following symmetric distribution tensor:

$$\eta^\star = \text{inc } \mathcal{E}^\star = -\nabla \times \mathcal{E}^\star \times \nabla, \tag{2.3}$$

that is, componentwise, $\eta^\star_{kl} = \eta^\star_{lk} := \epsilon_{lpm}\partial_p\bar\partial_m\omega^\star_k$. Moreover, for a selected $x_0 \in \Omega_\mathcal{L}$, the Burgers tensor is defined on the entire domain Ω as the distribution

$$\bar\partial b^\star := \mathcal{E}^\star + \left((x - x_0) \times \bar\partial\omega^\star\right), \tag{2.4}$$

that is, componentwise, as $\bar\partial_l b^\star_k(x) := \mathcal{E}^\star_{kl}(x) + \epsilon_{kpq}(x_p - x_{0p})\bar\partial_l\omega^\star_q(x)$.

Given $x_0 \in \Omega_\mathcal{L}$, the rotation $\omega^\star_{0k}$ and displacement $\omega^\star_{0k}$ at x_0, the multivalued rotation and displacement vectors at $x \in \Omega_\mathcal{L}$ are defined as

$$\omega^\star_k(x) = \omega^\star_{0k} + \int_\Gamma \bar\partial_m\omega^\star_k(\xi)d\xi_m, \tag{2.5}$$

$$u^\star_k(x) = u^\star_{0k} + \epsilon_{klm}\omega^\star_l(x_m - x_{0m}) + \int_\Gamma \bar\partial_l b^\star_k(\xi)d\xi_l, \tag{2.6}$$

where $\omega^\star_k$ and $u^\star_k$ obviously depends on the path $\Gamma \subset \Omega_\mathcal{L}$ from x_0 to x. It is well-known that $\omega^\star_k$ and $u^\star_k$ are single-valued fields if and only if the incompatibility $\eta^\star$ vanishes. To render these two fields single valued one can also introduce a cut in Ω in such a way that all path Γ are equivalent. This procedure introduces a jump set at the arbitrarily chosen cut, whose consequences must be carefully discussed.

Single defect line, denoted by $\mathcal{L}$, are in general either dislocations (translational defect) or disclinations (rotational defect) (cf. [11] and [26] for detail) or have a combined dislocation and disclination nature. Accordingly, we introduce the following concentrated distribution tensors.

Definition 2 (Defect densities and contortion)**.**

DISCLINATION DENSITY: $$\Theta^\star := \tau\delta_\mathcal{L} \otimes \Omega^\star \quad \left(\Theta^\star_{ij} := \tau_i\Omega^\star_j\delta_\mathcal{L}\right) \tag{2.7}$$

DISLOCATION DENSITY: $$\Lambda^\star := \tau\delta_\mathcal{L} \otimes B^\star \quad \left(\Lambda^\star_{ij} := \tau_i B^\star_j\delta_\mathcal{L}\right) \tag{2.8}$$

MESOSCOPIC CONTORTION: $$\kappa^\star := \alpha^\star - \frac{I}{2}\text{tr }\alpha^\star \quad \left(\kappa^\star_{ij} := \alpha^\star_{ij} - \frac{1}{2}\delta_{ij}\alpha^\star_{kk}\right), \tag{2.9}$$

where $\delta_\mathcal{L}$ denotes the 1-dimensional Hausdorff measure concentrated on $\mathcal{L}$, τ the unit tangent vector of $\mathcal{L}$, and with the auxiliary defect density measure:

$$\alpha^\star_{ij} := \Lambda^\star_{ij} - \epsilon_{jlm}(x_l - x_{0l})\Theta^\star_{im}, \tag{2.10}$$

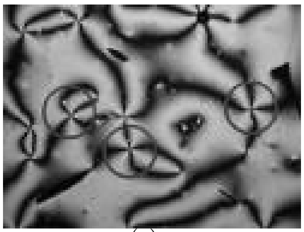
where x_{0m} is a point where rotation and Burgers fields are prescribed.

Typical disclination and dislocation loops are given in Figs. 1(a) and 1(b). We observe that the lines are either close or end at the crystal boundary. In fact, the following classical theorem is proved in, e.g. [11].

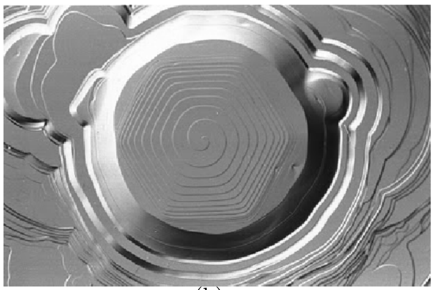
Theorem 1 (Conservation laws)**.** *Isolated defect lines are always closed or end at the boundary of Ω. Moreover, $\partial_i\Theta^\star_{ij} = \partial_i\Lambda^\star_{ij} = 0$ while $\partial_i\alpha^\star_{ij} = \epsilon_{jmn}\Theta^\star_{mn}$.*

Lemma 1. *The tensor $\tilde\eta^\star := -\kappa^\star \times \nabla$ is symmetric.*

Proof. The proof follows from Definition 2 and Theorem 1 by the simple computation of $\epsilon_{ijm}\epsilon_{jpq}\partial_p\kappa^\star_{iq}$ which shows to vanish identically. □



(a)



(b)

FIGURE 1. 1(a) Disclinations is a rotational defect, which is often present, although rare, in crystals growing from the melt, ©University of Cambridge; 1(b) Spiral screw dislocation in a crystal of silicon carbide ((IKZ, Berlin) Institute for Crystal Growth, Germany);

2.2. **General mesoscopic results for defect loops.** In general, a dislocation curve is of mixed screw-edge type. The type is determined by the scalar $\alpha(x) = \tau_i(x)B_i^\star$: if $\alpha = 0$ on $\mathcal{L}$ the curve is a pure edge dislocation, whereas pure screw curves (i.e., s.t. $\alpha = 1$) which are not rectilinear do not exist. The dislocation at x is of mixed screw-edge type as soon as $0 < \alpha(x) < 1$. The expression of the strain and Frank tensors for these two kinds of dislocations and this kind of discliantion are given for lines parallel to the z-axis for which the medium is assumed to be steady, body force free and isothermal (detail is given in [10, 26])[4].

Let us introduce the classes of torsion-free dislocations which will be considered in this paper.

Definition 3 (Smooth defect loop). *Let the dislocation and/or dislocation $\mathcal{L} \subset \Omega$ be a loop homeomorphic to the circle such that its tangent vector τ is almost everywhere Lipschitz continuous (and hence the loop curvature exists and is bounded almost everywhere).*

Precisely, the following assumption and lemma are required to prove Theorem 2 by extending the proof of the result holding for rectilinear defects (see [26]) to defect loops.

Assumption 2. *A smooth defect loop $\mathcal{L}$ is a simple*[5] *regular and closed Lipschitz curve contained in $\bar{\Omega}$, that is, a curve satisfying the following requirements:*

(1) *an admissible defect-line $\mathcal{L}$ is parametrically described by a continuous mapping*

$$\hat{x}_i : [0,1] \to \bar{\Omega}$$

where its restriction to the open interval $]0,1[$ takes its values in Ω.

(2) *the tangent vector τ exists everywhere and is Lipschitz continuous in $\in [0,1]$.*

(3) *if $\hat{x}_i(t) = \hat{x}_i(t')$ then $t = t'$ or $\{t,t'\} = \{0,1\}$. Moreover if $\{t,t'\} = \{0,1\}$ then $\hat{x}_i(0) = \hat{x}_i(1) \in \Omega$ and $\tau_p(0) = \tau_p(1)$.*

Assumption 2 allows one to define a tube surrounding the line $\mathcal{L} \in \Omega$ whose normal sections do not intersect.

Lemma 2. *For every smooth defect $\mathcal{L}$ and for every $\hat{x} \in \mathcal{L}$ there exists $\delta > 0$ with δ independent of $\hat{x}$ such that the closed disks $D_\delta(\hat{x})$ and $D_\delta(\hat{x}')$ for $\hat{x} \neq \hat{x}'$ have an empty intersection.*

Let ν be the inward normal to the loop $\mathcal{L}$ and introduce the normal vector $\sigma := \nu \times \tau$ in order to define the right-handed orthonormal basis $\{\sigma, \nu, \tau\}$ satisfying the usual Frenet's formulae on $\mathcal{L}$:

$$\tau' = \chi\nu, \qquad \nu' = -\chi\tau - \zeta\sigma, \qquad \sigma' = \zeta\nu, \tag{2.11}$$

where χ and ζ denote the loop curvature and torsion, respectively.

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[4]The explicit expressions given in [26] are not all identical to the classically reported ones [10]. However the difference in the strain expressions are explicitely known up to a compatible strain tensor, as discussed in [26].

[5]"Simple" means that there are no distinct values of the length parameter other than the start- and endpoints whose images may coincide on $\mathcal{L}$.

In the remaining of the paper the following abuse of notation will be tolerated: we will sometimes denote by σ, ν, τ their uniform extension in a neigbourhood of the line. In fact, the precise knowledge of the neigbourhood and in particular its width and the exact expression of the cut-off function (which must be smooth, with compact support, and take unit values in a neibourhood of $\mathcal{L}$) has no importance since σ, ν, τ are nevertheless multiplied by concentrated fields on the line. So, eventually, only the value of σ, ν, τ on the line matters, even if the extension must be considered to give a rigourous meaning to the products.

Assumption 3 (Mesoscopic nature of the Frank tensor). *The Frank tensor $-\mathcal{E}^\star \times \nabla$ is a first-order distribution assumed to be such that the projection $p^\star := (-\mathcal{E}^\star \times \nabla)\,\tau$ is a vector-valued Radon measure in the sense of Ambrosio et al. [1] on Ω, with a (vector) singular part $c^\star$ and (vector) regular part $r^\star := p^\star - c^\star \in L^1(\Omega)$ such that the following quantities are purely concentrated on $\mathcal{L}$:*

$$c^\star \quad , \quad \tau \cdot \nabla \times r^\star \quad \text{and} \quad \nabla(\tau \cdot r^\star), \tag{2.12}$$

with τ indicating the tangent vector of $\mathcal{L}$ (here understood as multiplied by a unit cut-off function around $\mathcal{L}$).

Theorem 2 (Incompatibility of a smooth loop). *Under Assumptions 1,2 & 3 and for a smooth loop $\mathcal{L}$ satisfying Assumption 2, incompatibility is the following first-order symmetric tensor distribution:*

$$\eta^\star_{mn} = \operatorname{inc}_{mn}(\mathcal{E}^\star) = \left[\tau_m\tau_k\hat{\eta}^\star_{kn} + \tau_m\tau_n\frac{1}{2}(B^\star_k\sigma_k)\,\chi\delta_{\mathcal{L}}\right]_{m\leftrightarrow n} \tag{2.13}$$

where the Einstein tensor reads

$$\hat{\eta}^\star_{kn} = \tilde{\tilde{\eta}}^\star_{kn} - \frac{\delta_{kn}}{2}\tilde{\tilde{\eta}}^\star_{pp}, \tag{2.14}$$

the Kröner's tensor is defined by

$$\tilde{\tilde{\eta}}^\star_{kn} = \Theta^\star_{kn} + \tilde{\eta}^\star_{kn}, \tag{2.15}$$

with the symmetric tensor,

$$\tilde{\eta}^\star_{kn} := \epsilon_{kij}\partial_i\kappa^\star_{nj}, \tag{2.16}$$

where the defect contortion $\kappa^\star$ are given by Definition 2, and symbol $A_{m\leftrightarrow n}$ means that sum of tensor A_{mn} and its transposed A_{nm} is taken.

Remark 2. *Theorem 2 has been proven in [23] for skew rectilinear dislocations and disclinations. For dislocation loops we refer to [24] where* (2.13) *has been verified explicitely for planar (of mixed edge-screw type) and pure edge dislocation loops. Recall also that the symmetry of $\tilde{\eta}^\star_{kn}$ has been proved in Lemma 1.*

In the following we will use the notation $B^\star_\sigma := B^\star_k\sigma_k$ and $B^\star_\nu := B^\star_k\nu_k$.

3. The completed Frank and Burgers tensors for dislocation loops

Definition 4 (Planar defects). *A planar defect $\mathcal{L}$ is a torsion-free (i.e., $\zeta = 0$) dislocation and/or a disclination loop such that either the Burgers vector lies in the plane of the loop (the so-called mixed-type loop) or the Burgers vector is purely out-of-plane (the so-called pure edge dislocation).*

We will also consider a particular class of $3D$ non-planar and torsion-free loops of mixed type

Definition 5 (Simple $3D$ defect). *A simple $3D$ defect $\mathcal{L}$ is a torsion-free dislocation and/or dislocation which is assumed to lie in the union of a finite number of parallel planes and skew segments. Moreover, the associated Burgers vector lies in one of those planes, which is referred to as the "plane of the loop". Thus, $\chi = 0$ on the skew segments, i.e., in the portions of $\mathcal{L}$ not lying in planes not parallel to the plane of the loop (where $B^\star_\sigma \neq 0$), while $B^\star_\sigma = 0$ on the planes parallel to the plane of the loop. Hence $B^\star\chi = 0$ on a simple $3D$ defect $\mathcal{L}$.*

Remark that a mixed-type planar defect is a particular kind of simple $3D$ defect where the finite number of planes reduces to the plane of the loop. Notice also that the Frank tensor can be arbitrary in Definitions 4 & 5.

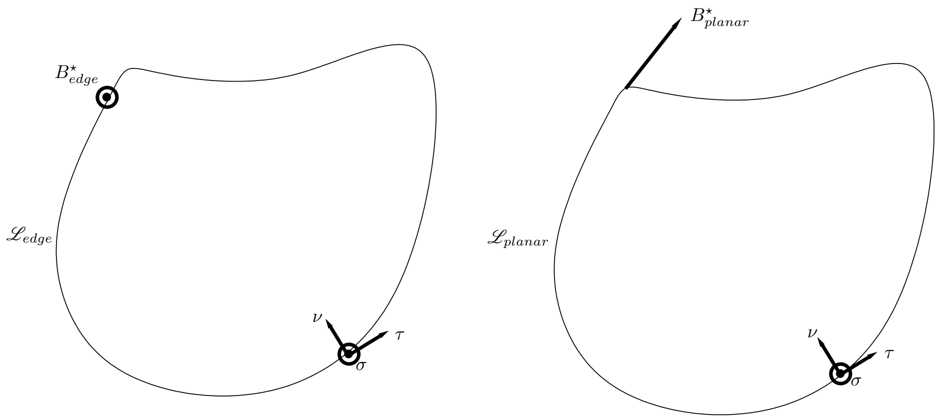

FIGURE 2. Left: pure edge dislocation loop. Right: the planar loop dislocation. The out-of-plane normal σ is pointing downwards.

The following decomposition theorem will be used in the sequel. It is well-known that any smooth vector field can be decomposed into a solenoidal and an irrotational part, and this property can be easily extended to distributional fields. Similar decomposition of any symmetric tensor field into a compatible and a solenoidal part will here be recalled (for a proof, we refer for instance to [8] or [27]).

Lemma 3 (Standard decomposition of a symmetric tensor). *Any symmetric 2^{nd}-order distribution tensor $\mathcal{E}$ can be decomposed into a compatible and a solenoidal symmetric part:*

$$\mathcal{E} = \mathcal{E}^c + \mathcal{E}^s, \tag{3.1}$$

with $\nabla \times \mathcal{E}^c \times \nabla = 0$ *(compatible part) and* $\nabla \cdot \mathcal{E}^s = 0$ *(solenoidal part).*

Notations 2. *For a second order tensor A, symbol A^{d*} will denote the tensor $A^{d*} := A - \frac{1}{2}\,\mathrm{tr}\; A$, where subscript $d*$ is chosen to remind that in $2D$ the operation consists in taking the deviatoric part of A.*

Lemma 4. *Eq.* (2.13) *can be rewritten as*

$$\left[\tau_i\tau_m\left(\epsilon_{mql}\partial_q\left(\bar\partial_l\omega^\star_j - \kappa^\star_{jl}\right)\right)^{d*}\right]_{i\leftrightarrow j} = \left[\tau_i\tau_m\left(\Theta^\star_{mj} - \chi B_\sigma\delta_{\mathcal{L}}\delta_{mj}\right)^{d*}\right]_{i\leftrightarrow j}. \tag{3.2}$$

Proof. First step. Let $\bar\eta_{mn} := \tau_m\tau_n\frac{1}{2}\left(B^\star_\sigma\right)\chi\delta_{\mathcal{L}}$. From (2.13)-(2.15) we have

$$\mathrm{tr}_\tau\eta^\star := \tau_k\eta^\star_{kl}\tau_l = \tau_k\left(\tau_k\tau_p\left(\hat\eta^\star_{pl} + \bar\eta^\star_{pl}\right) + \tau_l\tau_p\left(\hat\eta^\star_{pk} + \bar\eta^\star_{pk}\right)\right)\tau_l = 2\tau_p\left(\hat\eta^\star_{pl} + \bar\eta^\star_{pl}\right)\tau_l, \tag{3.3}$$

while obviously,

$$\mathrm{tr}_\nu\eta^\star := \nu_k\eta^\star_{kl}\nu_l = \mathrm{tr}_\sigma\eta^\star := \sigma_k\eta^\star_{kl}\sigma_l = 0. \tag{3.4}$$

On the other hand, it is easily computed by the definitions that

$$\begin{aligned}\tau_i\tau_m\eta^\star_{mj} &= \tau_i\tau_k\left(\hat\eta^\star_{kj} + \bar\eta^\star_{kj}\right) + \frac{1}{2}\tau_i\tau_j\,\mathrm{tr}_\tau\eta^\star \\ \tau_i\tau_m\eta^\star_{mj} + \tau_j\tau_m\eta^\star_{mi} &= \eta^\star_{ij} + \tau_i\tau_j\,\mathrm{tr}_\tau\eta^\star.\end{aligned} \tag{3.5}$$

Moreover we have the identity

$$\tau_i\tau_m\eta^\star_{mj} = \tau_i\tau_m\left(\eta^\star_{mj} - \frac{1}{2}\delta_{mj}\,\mathrm{tr}\;\eta^\star\right) + \frac{1}{2}\tau_i\tau_j\,\mathrm{tr}\;\eta^\star. \tag{3.6}$$

Therefore, by (3.3) & (3.4), $\mathrm{tr}\;\eta^\star = \mathrm{tr}_\tau\eta^\star$, and hence (3.5) & (3.6) and Notation 2 entail that

$$\eta^\star_{ij} = \left[\tau_i\tau_m\left(\eta^\star_{mj}\right)^{d^*}\right]_{i\leftrightarrow j}. \tag{3.7}$$

Second step. By the identity $\left(-\chi B_\sigma\delta_{\mathcal{L}}\delta_{mj}\right)^{d^*} = \frac{1}{2}\chi B_\sigma\delta_{\mathcal{L}}\delta_{mj}$ Eq. (2.13) rewrites by (3.7) as

$$\eta^\star_{ij} = \left[\tau_i\tau_m\left(\eta^\star_{mj}\right)^{d^*}\right]_{i\leftrightarrow j} = \left[\tau_i\tau_m\left(\tilde\eta^\star_{mj}\right)^{d^*}\right]_{i\leftrightarrow j} + \left[\tau_i\tau_m\left(\Theta^\star_{mj} - \chi B_\sigma\delta_{\mathcal{L}}\delta_{mj}\right)^{d^*}\right]_{i\leftrightarrow j} \tag{3.8}$$

and hence by (2.14) & (2.15), (2.16), (2.1) & (2.2) (i.e., $\eta^\star_{mj} = \epsilon_{mql}\partial_q\bar\partial_l\omega^\star_j$) rewrites as (3.2). □

Eq. (3.2) indicates that $\bar{\partial}_q\omega_j^\star - \kappa_{jq}^\star$ is a meaningfull quantity. Therefore, we recall the $2D$ expression of the so-called completed Frank and Burgers tensors (as introduced in [26, 27]).

Definition 6 ($2D$ completed Frank and Burgers tensors). *By Lemma 4, the completed Frank and Burgers tensors of a planar defect loop $\mathcal{L}$ are defined as follows:*

$$\text{2D COMPLETED FRANK TENSOR:} \quad \eth_q\omega_j^\star \;:=\; \bar{\partial}_q\omega_j^\star - \kappa_{jq}^\star, \tag{3.9}$$

$$\text{2D COMPLETED BURGERS TENSOR:} \quad \eth_q b_j^\star \;:=\; \mathcal{E}_{qj}^\star + \epsilon_{jkp}(x_k - x_{0k})\eth_q\omega_p^\star. \tag{3.10}$$

Corollary 1. *By (3.2), (3.9) & (3.10) the following relations hold:*

$$\epsilon_{ipq}\partial_p\eth_q\omega_j^\star = \Theta_{ij}^\star + \theta_{ij}^\star - \chi B_\sigma^\star\delta_{\mathcal{L}}\delta_{ij}, \tag{3.11}$$

$$\epsilon_{ipq}\partial_p\eth_q b_j^\star = \Lambda_{ij}^\star + \epsilon_{jpk}(x_p - x_{0p})\left(\theta_{ik}^\star - \chi B_\sigma^\star\delta_{\mathcal{L}}\delta_{ik}\right), \tag{3.12}$$

where $\theta^\star$ is a trace-free distribution tensor of order 2 obtained by spanning the base tensors $\sigma\otimes\sigma, \nu\otimes\nu, \sigma\otimes\nu, \nu\otimes\sigma, \sigma\otimes\tau$ and $\nu\otimes\tau$.

Proof. Posing $\theta_{ij}^\star = \epsilon_{ipq}\partial_p\eth_q\omega_j^\star - \Theta_{ij}^\star + \chi B_\sigma\delta_{\mathcal{L}}\delta_{ij}$, Eq. (3.2) rewrites as

$$0 = \left[\tau_i\tau_m\left(\theta_{mj}^\star\right)^{d*}\right]_{i\leftrightarrow j} = \tau_i\tau_m\theta_{mj}^\star + \tau_j\tau_m\theta_{mi}^\star - \tau_i\tau_j\theta_{pp}^\star,$$

which implies that $\theta^\star$ is a trace-free tensor spanned by $\sigma\otimes\sigma, \nu\otimes\nu, \sigma\otimes\nu, \nu\otimes\sigma, \sigma\otimes\tau$ and $\nu\otimes\tau$.
Then (3.12) follows from (3.11) as a consequence of Definiton 2. □

At this stage, we consider a simple $3D$ dislocation loop, by which we mean a defect satisfying Definition 5 with in addition $\Omega^\star = 0$, that is, we consider a simple dislocation $\mathcal{L}$ in the absence of disclinations and such that $B_\sigma^\star\chi = 0$ almost everywhere on $\mathcal{L}$.

For a simple dislocation, Corollary 1 and Eq. (3.9) entail that

$$\theta^\star = \nabla\times\eth\omega^\star = \text{curl }\eth\omega^\star = \eta^\star + \kappa^\star\times\nabla, \tag{3.13}$$

where as a consequence of $\text{tr }\theta^\star = 0$ one has $0 = (\nu\otimes\nu + \sigma\otimes\sigma)\cdot(\kappa^\star\times\nabla)$ (to check the detail, cf. step 1 of the proof of Lemma 6)[6].

The completed Frank and Burgers tensors must be redefined to generalize their $2D$ counterparts of Definition 6. First observe that by Theorem 1 and Eqs. (3.11) & (3.12) one has

$$\partial_i\Theta_{ij}^\star = 0 \quad\Rightarrow\quad \partial_i\theta_{ij}^\star = \partial_j\left(\chi B_\sigma^\star\delta_{\mathcal{L}}\right), \tag{3.14}$$

$$\partial_i\Lambda_{ij}^\star = \epsilon_{jmn}\Theta_{mn}^\star \quad\Rightarrow\quad \epsilon_{jik}\theta_{ik}^\star = -\epsilon_{jmn}\Theta_{mn}^\star. \tag{3.15}$$

Therefore $\Theta^\star = 0$ implies that $\theta^\star$ is symmetric and hence Lemma 3 entails that $\theta^\star = (\nabla\psi)^S - \nabla\times\varphi^\star\times\nabla$ for some distribution tensors ψ and $\varphi^\star$, with $\varphi^\star$ solenoidal. As a consequence $\text{inc }\theta^\star = \text{inc}\,(\text{inc }\varphi^\star) = \Delta\Delta\varphi^\star$, while in the absence of disclinations, Eq. (3.11) rewrites as

$$\epsilon_{ipq}\partial_p\left(\eth_q\omega_j^\star - \epsilon_{jmn}\partial_m\varphi_{qn}^\star\right) = -\chi B_\sigma^\star\delta_{\mathcal{L}}\delta_{ij} + (\nabla\psi)_{ij}^S. \tag{3.16}$$

This conduct us to the following definition.

Definition 7 ($3D$ completed Frank and Burgers tensors). *By Lemma 4, the completed Frank and Burgers tensors of a simple dislocation loop $\mathcal{L}$ are defined as follows:*

$$\text{COMPLETED FRANK TENSOR:} \quad \bar{\eth}_q\omega_j^\star \;:=\; \bar{\partial}_q\omega_j^\star - \kappa_{jq}^\star - (\text{curl }\varphi^\star)_{jq} \tag{3.17}$$

$$\text{COMPLETED BURGERS TENSOR:} \quad \bar{\eth}_q b_j^\star \;:=\; (\mathcal{E}^\star - \varphi^\star)_{jq} + ((x - x_0)\times(\eth\omega^\star - \text{curl }\varphi^\star))_{jq}, \tag{3.18}$$

where $\varphi^\star$ is a symmetric solenoidal distributional solution of

$$\Delta\Delta\varphi^\star = \text{inc }\theta^\star = \text{inc curl }\eth\omega^\star. \tag{3.19}$$

Remark 3. *It is immediately observed from the identity* $\text{tr inc }E = \Delta\Delta\,\text{tr }E - \nabla\cdot E\cdot\nabla$ *that*

$$\text{tr }\varphi^\star = 0, \tag{3.20}$$

since $\theta^\star$ is trace-free and divergence-free for simple dislocation loops by (3.14).

[6]The latter can easily be verified by simple calculations since $\epsilon_{jpq}\partial_p(\tau_i B_q^\star\delta_{\mathcal{L}}) = -\sigma_j\nu_i B_\nu^\star\chi\delta_{\mathcal{L}} + \nu_i\nu_j B_\sigma^\star\chi\delta_{\mathcal{L}} + \tau_i B_q^\star\epsilon_{jpq}\partial_p\delta_{\mathcal{L}}$, while $\epsilon_{jpq}\partial_p(\delta_{iq}\tau_l B_l^\star\delta_{\mathcal{L}}) = \epsilon_{ijp}\partial_p(\tau_l B_l^\star\delta_{\mathcal{L}})$, where all terms vanish as multiplied by $\nu_i\nu_j + \sigma_i\sigma_j$ (recalling also that $\chi B_\sigma^\star = 0$).

Definition 8 (Completed strain)**.** *Let us define the completed strain as*

$$\text{COMPLETED STRAIN:} \qquad \bar{\mathcal{E}}^\star := \mathcal{E}^\star - \varphi^\star, \tag{3.21}$$

where by Remark 3 tr $\bar{\mathcal{E}}^\star =$ tr $\mathcal{E}^\star$. *Let us also define*

$$\bar{\bar{\partial}}_q \omega_j := \epsilon_{jlm} \partial_l \bar{\mathcal{E}}^\star_{mq}. \tag{3.22}$$

Remark 4 (A-priori regularity of the completed strain)**.** *Observe by* (2.2) *&* (3.10) *that* curl $\eth\omega^\star = \eta^\star - \kappa^\star \times \nabla$ *has by Theorem 2 the same regularity as* $\kappa^\star \times \nabla$. *On the other hand, since* $\kappa^\star$ *is a Radon measure it belongs to* $H^{-2}_{loc}(\Omega)$, *whereby the RHS of* (3.19) *belongs to* $H^{-5}_{loc}(\Omega)$. *Then, by elliptic regularity results [28] one has* $\varphi^\star \in H^{-1}_{loc}(\Omega)$, *whereby Lemma 3 entails that* $\varphi^\star = \nabla \times \Psi \times \nabla$ *with* $\Psi \in H^1_{loc}(\Omega)$ *(cf. also, e.g., [19]).*

By elliptic regularity results, it is however observed from (4.1) that $\varphi^\star \in L^2_{loc}(\Omega)$. This will be proved in Lemma 6.

Recalling (2.2), (3.17) & (3.18) rewrite as

$$\text{COMPLETED FRANK TENSOR:} \qquad \bar{\bar{\eth}}_q \omega^\star_j := \bar{\bar{\partial}}_q \omega_j - \kappa^\star_{jq} \tag{3.23}$$

$$\text{COMPLETED BURGERS TENSOR:} \qquad \bar{\bar{\eth}}_q b^\star_j := \bar{\mathcal{E}}^\star_{jq} + \left((x - x_0) \times \bar{\bar{\eth}}_q \omega^\star \right)_{jq}, \tag{3.24}$$

recovering the exact counterpart of (3.9) & (3.10) with the complete strain instead of the strain.

4. Further results for a simple 3D dislocation loop

In this and the following sections we consider a simple 3D dislocation loop (i.e., with $\Omega^\star = 0$ and $B^\star_\sigma \chi = 0$ a.e. on $\mathcal{L}$, cf. Definition 5).

Remark 5. *For a simple dislocation loop one has an explicit expression of the trace-free* $\theta^\star$, *viz. (cf. step 5 of the proof of Lemma 6)*

$$\theta^\star_{ij} = -(\nu_i \sigma_j + \sigma_i \nu_j) \chi \nu_l B^\star_l \delta_{\mathcal{L}}, \tag{4.1}$$

which shows the following: $\varphi^\star$, *solution of* (3.19), *which is also identified with a diffuse residual strain in Definition 8 (see also §5), is a contribution to the total strain which is due to the curvature of the line (recall that* $B^\star_\nu$ *never identically vanishes for any planar loop).*

From the definitions of the 3D completed Frank and Burgers tensors, the aim of this section is to show existence of single-valued distortion and displacement fields, and to prove that the displacement is of bounded deformation.

4.1. Existence of a single-valued distortion for a simple dislocation.

Lemma 5 (Canonical relations for simple dislocations)**.** *For a simple dislocation, Eq.* (3.11) *&* (3.12) *rewrites as*

$$\epsilon_{ipq} \partial_p \bar{\bar{\eth}}_q \omega^\star_j = 0, \tag{4.2}$$

$$\epsilon_{ipq} \partial_p \bar{\bar{\eth}}_q b^\star_j = \Lambda^\star_{ij}. \tag{4.3}$$

Proof. By (3.15), the skew-symmetric parts of $\Theta^\star$ and $\theta^\star$ mutually cancel and (3.11) rewrites as

$$\epsilon_{ipq} \partial_p \eth_q \omega^\star_j = \frac{1}{2} \left(\Theta^\star_{ij} \right)_{i \leftrightarrow j} + \frac{1}{2} \left(\theta^\star_{ij} \right)_{i \leftrightarrow j} - \chi B^\star_\sigma \delta_{\mathcal{L}} \delta_{ij}. \tag{4.4}$$

Moreover, by Theorem 3, $\frac{1}{2} \left(\theta^\star_{ij} \right)_{i \leftrightarrow j}$ can be rewritten as $\epsilon_{ipq} \epsilon_{jkl} \partial_p \partial_k \varphi^\star_{ql} + \frac{1}{2} \left(\partial_i \psi_j + \partial_j \psi_i \right)$ for some distributions tensor $\varphi^\star$ and vector ψ. Then (3.11) & (3.12) rewrite as

$$\epsilon_{ipq} \partial_p \left(\eth_q \omega^\star_j - \epsilon_{jkl} \partial_k \varphi^\star_{ql} \right) = \frac{1}{2} \left(\Theta^\star_{ij} \right)_{i \leftrightarrow j} + \frac{1}{2} \left(\partial_i \psi_j + \partial_j \psi_i \right) - \chi B^\star_\sigma \delta_{\mathcal{L}} \delta_{ij}. \tag{4.5}$$

Taking the divergence on both sides of (4.5) entails that

$$0 = \mathcal{L}_{0,1}(\psi_j) - \partial_j \left(\chi B^\star_\sigma \delta_{\mathcal{L}} \right) + \frac{1}{2} \partial_i \Theta^\star_{ji}, \tag{4.6}$$

with the Lamé operator $\mathcal{L}_{\lambda,\mu}(\psi_j) := \mu \Delta \psi_j + (\lambda + \mu) \partial_j \partial_k \psi_k$.

Moreover, since $\mathcal{L}$ is a simple dislocation, $\Omega^\star = 0$ and $B^\star_\sigma \chi = 0$ almost everywhere on $\mathcal{L}$, and hence from (4.6) one has $\psi = 0$ (recall that ψ is given by convolution with the Kelvin matrix [2]). Thus, (4.5) rewrites as

$$\epsilon_{ipq}\partial_p\left(\bar{\eth}_q\omega^\star_j - \epsilon_{jkl}\partial_k\varphi^\star_{ql}\right) = 0, \tag{4.7}$$

with the solenoidal $\varphi^\star$ solution of $-\Delta\Delta\varphi^\star = \text{inc } \theta^\star$ (in the sense of distributions, see [27] for detail), thereby proving (4.2). In particular, by (3.15) & (4.4),

$$\epsilon_{ipq}\partial_p\bar{\eth}_q\omega^\star_j = \frac{1}{2}\left(\theta^\star_{ij}\right)_{i\leftrightarrow j} = \theta^\star_{ij} = \epsilon_{ipq}\epsilon_{jmn}\partial_p\partial_m\varphi^\star_{qn}. \tag{4.8}$$

By (3.12) and (4.4), and recalling that $\varphi^\star_{lk} = \varphi^\star_{kl}$, it is easily verified by part integration that

$$\epsilon_{jlk}(x_l - x_{0l})\epsilon_{ipq}\epsilon_{kmn}\partial_p\partial_m\varphi^\star_{qn} = \epsilon_{ipq}\partial_p\left(\epsilon_{jlk}(x_l - x_{0l})\epsilon_{kmn}\partial_m\varphi^\star_{qn}\right) + \epsilon_{ipq}\partial_p\varphi^\star_{jq},$$

achieving the proof by (3.18). □

Thus, for a simple dislocation, according to Eq. (4.2) of Lemma 5, there exists a distribution vector $\omega^{\star(S)}_j$ satisfying

$$\bar{\bar{\eth}}_m\omega^\star_j \quad = \quad \partial_m\omega^{\star(S)}_j. \tag{4.9}$$

Specifically, $\omega^{\star(S)}$ is the solution to

$$-\Delta\omega^{\star(S)} = -\nabla\cdot\bar{\bar{\eth}}\omega^\star, \tag{4.10}$$

with $\bar{\bar{\eth}}\omega^\star$ given by (3.17). Remark that $\omega^\star$ will be uniquely defined as soon as appropriate boundary conditions are provided. Here the subscript (S) serves to emphasize that the field is single-valued.

Let us now introduce the 2^{nd} order "Bravais distortion" $\beta^\star$, which we identify with the completed Burgers tensor of Eq. (3.18) or (3.24)

BRAVAIS DISTORTION
$$\beta^\star = \bar{\bar{\eth}}b^\star \qquad (\beta^\star_{qj} = \bar{\bar{\eth}}_q b^\star_j), \tag{4.11}$$

with $\bar{\bar{\eth}}b^\star$ given by (3.24) and which satisfies by (4.3),

$$\nabla\times\nabla\times\beta^\star = -\left(\Delta - \nabla\nabla\cdot\right)\beta^\star = \nabla\times\Lambda^\star. \tag{4.12}$$

The field $\beta^\star$ is called "distortion" since by (2.8), (4.3) and (4.11), one formaly recovers the classical formula (provided $\beta^\star \in \mathcal{C}(\Omega_\mathcal{L})$)

$$B^\star_j = \int_{S_C}\Lambda^\star_{ij}dS_i = \int_C \beta^\star_{qj}dx_q, \tag{4.13}$$

where C is a sectional loop with index 1 with respect to $\mathcal{L}$ (that is, C encloses $\mathcal{L}$ ones and lies in a plane perpendicular to $\mathcal{L}$), and where S_C is the planar surface enclosed by C with normal vector τ.

Remark 6. *From* (4.13) *one deduces that*

$$\beta^\star(x) = O\left((1/d(x,\mathcal{L})\right) \tag{4.14}$$

where d denotes the Euclidean distance. It is remarquable that this aymptotic behaviour is solely due to the constraint (4.11) *and not the any chosen constitutive behaviour (see also [17]).*

4.2. **Existence of a displacement of bounded deformation for planar dislocation loops.** The existence of a single-valued *distortion* field in the absence of disclinations has been justified above, but so far there is no proof of existence of a single-valued *displacement*[7]. In this section we show that, for a simple dislocation $\mathcal{L}$, the Bravais distortion is indeed the gradient of a single-valued displacement field here denoted by $u^{\star(S)}$. This will show possible if a cut surface, that is, a smooth surface $S \in \overline{\Omega}$ supported by $\mathcal{L}$ on one side and passing across Ω, is introduced in order to avoid field multivaluedness.

The formalism of "Functions of Bounded Deformations", BD [20], and of "Special functions of Bounded Deformations", SBD [5], is by now classical in Mechanics and is not new in field of dislocation modeling (see for instance [16]). However, to the knowledge of the author this formalism has

[7]For a discussion on field multivaluedness, we refer to [26].

yet not been systematically considered for dislocations, and when it is, the SBD space is generally postulated as appropriate for the displacement. Moreover, it is usualy considered that elastic/plastic strain decomposition coincides with the mathematical diffuse/concentrated decomposition of the distributional derivative Du. Rather, there might be diffuse plastic and concentrated elastic strain contributions. In the present paper, the SBD formalism appears as a natural consequence of another "distributional" formalism where multivalued fields, such as the rotation $\omega^{\star(S)}$, displacement $u^{\star(S)}$ or even distortion $\beta^\star$ are avoided in a first step [23, 26]. Moreover the field regularity (and in particular their concentration properties) appear in a subseqyent step, as the solution of PDEs.

We have just showed that in the absence of disclinations a distortion field could be rigourously introduced, but this "Bravais distortion" however is not, so far, the gradient of displacement field. We show in this section that provided the introduction of a cut surface S, the displacement field naturally appears as a special function of bounded deformation. Although the case of one single line is natural, the case of clusters is more envolved and appeals to compactness results in the class of BD functions.

Consider a simple dislocation loop $\mathcal{L}$ and a tensor test-function $\varphi^\star$ (with compact support in Ω). By (4.3) & (4.11), and by Stokes theorem, one has

$$\begin{aligned}\langle \epsilon_{ipq}\partial_p\beta^\star_{qj}, \varphi^\star_{ij}\rangle =< \Lambda^\star_{ij}, \varphi^\star_{ij} > &= < B^\star_j \tau_i \delta_{\mathcal{L}}, \varphi^\star_{ij} >= B^\star_j \int_{\mathcal{L}} \varphi_{ij}\tau_i d\mathcal{H}^1 = B^\star_j \int_{S_{\mathcal{L}}} \epsilon_{ipq}\partial_p\varphi_{ij} n_q d\mathcal{H}^2 \\ &= < B^\star_j n_q \delta_{S_{\mathcal{L}}}, \epsilon_{ipq}\partial_p\varphi_{ij} >=< -\epsilon_{ipq}\partial_p\left(B^\star_j n_q \delta_{S_{\mathcal{L}}}\right), \varphi_{ij} >, \quad (4.15)\end{aligned}$$

where $S_{\mathcal{L}}$ is a smooth closed surface enclosed by $\mathcal{L}$ and n the inward unit normal vector to $S_{\mathcal{L}}$[8].

By (4.15) one has

$$\beta^\star_{qj} = -B^\star_j n_q \delta_{S_{\mathcal{L}}} + \partial_q \Psi_j^{(S_{\mathcal{L}})} \quad (4.16)$$

where $\Psi^{(S_{\mathcal{L}})}$ is an arbitrary vector distribution at this stage. Moreover by (3.21), (3.24), (4.9) and (4.11), the Bravais distortion rewrites as

$$\begin{aligned}\beta^\star_{qj} &= \mathcal{E}^\star_{qj} + \epsilon_{jpl}(x_p - x_{0p})\partial_q \omega_l^{\star(S)} - \varphi^\star_{qj} \\ &= \partial_q\left(\epsilon_{jpl}(x_p - x_{0p})\omega_l^{\star(S)}\right) + \mathcal{E}^\star_{qj} + \omega_{jq}^{\star(S)} - \varphi^\star_{qj} \quad (4.17)\end{aligned}$$

with the skew-symmetric $\omega_{jq}^{\star(S)} := -\epsilon_{jql}\omega_l^{\star(S)}$. By (4.9), (4.15), (4.16) and (4.17), there exists a distribution vector field $u_j^{\star(S)}$,

DISPLACEMENT FIELD:
$$u_j^{\star(S)} := \Psi_j^{(S_{\mathcal{L}})} - \epsilon_{jpl}(x_p - x_{0p})\omega_l^{\star(S)}, \quad (4.18)$$

with $\omega^{\star(S)}$ solution of (4.10), and such that

DISPLACEMENT GRADIENT:
$$\partial_q u_j^{\star(S)} = B^\star_j n_q \delta_{S_{\mathcal{L}}} + \left(\mathcal{E}^\star_{qj} + \omega_{jq}^{\star(S)} - \varphi^\star_{qj}\right), \quad (4.19)$$

where subscript (S) again means "single-valued" but also recalls that the field depends on the arbitrary choice of the cut surface $S = S_{\mathcal{L}}$. In the sequel, $u^{\star(S)}$ will be considered as un unknown (instead of the gauge $\Psi^{(S_{\mathcal{L}})}$), which will be determined in an appropriate function space as soon as constitutive and conservative laws are provided and with chosen boundary conditions.

Let us rewrite Eq. (4.19) as

DISPLACEMENT GRADIENT DECOMPOSITION:
$$\partial_q u_j^{\star(S)} = e^\star_{qj} + p^\star_{qj}, \quad (4.20)$$

DIFFUSE DISTORTION:
$$e^\star_{qj} := \mathcal{E}^\star_{qj} - \varphi^\star_{qj} + \omega_{jq}^{\star(S)}, \quad (4.21)$$

CONCENTRATED DISTORTION:
$$p^\star_{qj} := B^\star_j n_q \delta_{S_{\mathcal{L}}}. \quad (4.22)$$

Remark 7. *Let us emphasize that $p^\star$ is not an physical observable field, since it is not invariant by change of admissible $S_{\mathcal{L}}$.*

Remark 8. *If and only if there are no dislocations, one recovers the classical formula*

$$\nabla u^{\star(S)} = \mathcal{E}^\star + \omega^{\star(S)}.$$

[8]Here and in the sequel symbol δ_S denotes the concentrated two-dimensional Hausdorff measure on S ($\delta_S \equiv \mathcal{H}^2_S$).

Moreover, one has tr $p^\star = 0$ *if and only if* $B^\star \cdot n = 0$*, that is, if the dislocation is a conservative planar defect (i.e., lying in* $S_{\mathcal{L}}$ *and with Burgers vector in* $S_{\mathcal{L}}$*). Moreover, one also has* tr $(p^\star)^S = 0$*. Remark that the skew-symmetric part of* $p^\star$*, viz.* $w^{\star P}_{jq} := \frac{1}{2}\left(B^\star_j n_q - B^\star_q n_j\right)\delta_{S_{\mathcal{L}}}$ *is called the "plastic spin" [6].*

Now, taking the symmetric part of (4.19), one defines

SYMMETRIC PART: $$\frac{1}{2}\left(\partial_q u^{\star(S)}_j + \partial_j u^{\star(S)}_q\right) = e_{qj}\left(u^{\star(S)}\right) := \mathcal{E}^\star_{jq} - \varphi^\star_{jq} + \frac{1}{2}\left(B^\star_j n_q + B^\star_q n_j\right)\delta_{S_{\mathcal{L}}}, \tag{4.23}$$

SKEW-SYMMETRIC PART: $$\frac{1}{2}\left(\partial_q u^{\star(S)}_j - \partial_j u^{\star(S)}_q\right) = w^{\star T}_{jq} := \omega^{\star(S)}_{jq} + \frac{1}{2}\left(B^\star_j n_q - B^\star_q n_j\right)\delta_{S_{\mathcal{L}}}. \tag{4.24}$$

Remark 9. *Observe that the displacement gradient symmetric part* (4.23) *is made of (i) a diffuse elastic part* $\mathcal{E}^\star$ *(the linear elastic strain tensor), (ii) a diffuse "residual" part* $-\varphi^\star$*, (iii) a "plastic" concentrated part. Moreover, the displacement gradient skew-symmetric part* (4.24) *is made of (i) a diffuse part* $\omega^{\star(S)}$ *(the infinitesimal rotation tensor), (ii) a concentrated part* $w^{\star P}$ *(the skew-symmetric plastic spin).*

The following definitions are made[9]:

Definition 9.

TOTAL COMPATIBLE STRAIN: $$\mathcal{E}^{\star T} := \frac{1}{2}\left(\nabla u^{\star(S)} + u^{\star(S)}\nabla\right) \tag{4.25}$$

RESIDUAL STRAIN: $$\mathcal{E}^{\star R} := -\varphi^\star \tag{4.26}$$

PLASTIC CONCENTRATED STRAIN: $$\mathcal{E}^{\star p} := \frac{1}{2}\left(B^\star \otimes n + n \otimes B^\star\right)\delta_{S_{\mathcal{L}}}, \tag{4.27}$$

PLASTIC STRAIN: $$\mathcal{E}^{\star P} := \mathcal{E}^{\star R} + \mathcal{E}^{\star p} \tag{4.28}$$

where by "plastic strain" it is meant non linear-elastic strain.

Remark 10. *It should be noted that by the trace and divergence- free properties of* $\mathcal{E}^{\star R}$ *(cf. Eqs.* (3.19) *and* (3.20)*), the residual strain is impactless on the equilibrium, i.e.,* $-\nabla\cdot\left(\mathbb{C}^\star\bar{\mathcal{E}}\right) = -\nabla\cdot\left(\mathbb{C}^\star\mathcal{E}^\star\right) = f$ *where* f *is the external body force, and* $\mathbb{C}^\star$ *the isotropic elasticity tensor. This justifies the term "residual".*

In Definition 9, $\varphi^\star$ is a solution of (3.19) which a priori belongs to $H^{-1}_{loc}(\Omega)$ (cf. Remark 4). Moreover, $u^{\star(S)} = \Psi^{(S_{\mathcal{L}})} - (x - x_0)\times\omega^{\star(S)}$ is a distribution depending on the arbitrary distribution $\Psi^{(S_{\mathcal{L}})}$.

Eq. (4.23) can be rewritten as

TOTAL STRAIN DECOMPOSITION: $$\mathcal{E}^{\star T} = \mathcal{E}^\star + \mathcal{E}^{\star P} = \bar{\mathcal{E}}^\star + \mathcal{E}^{\star p}. \tag{4.29}$$

Remark from (4.29), (4.23) & (4.24) that

$$\nabla u^{\star(S)} = \mathcal{E}^{\star T} + \omega^{\star T}, \tag{4.30}$$

where $\mathcal{E}^{\star T}$ and $\omega^{\star T}$ have each elastic and plastic parts.

Moreover, it is observed from Remark 3 that tr $\mathcal{E}^{\star R} = 0$, and hence tr $\mathcal{E}^{\star P} = 0$ if and only if tr $\mathcal{E}^{\star p} = B^\star \cdot n = 0$, that is, if $S_{\mathcal{L}}$ is contained in the glide planes.

The linear elastic strain is defined from the stress $\sigma^\star$ by

$$\mathcal{E}^\star = (\mathbb{C}^\star)^{-1}\sigma^\star + \beta^\star(T^\star - T_0), \tag{4.31}$$

where $\sigma^\star$ denotes the mesoscopic stress field, $(\mathbb{C}^\star)^{-1}$ and $\beta^\star$ stand for the 4th- and 2nd-order mesoscopic compliance and thermal dilation tensors, and T_0 is the reference temperature. Thus $\mathcal{E}^{\star P}$ is the part of the strain wich represents mechanical properties which depart from the linear elasticity assumption, also including diffuse and concentrated plastic effects. Moreover, $\mathcal{E}^{\star P}$ " accomodates" the linear strain in the sense that its incompatibility verifies by (4.23)

$$\text{inc } \mathcal{E}^{\star P} = -\text{inc } \mathcal{E}^\star = -\eta^\star.$$

[9]The notation ∇u means $\nabla \otimes u$ while $u\nabla$ means $u \otimes \nabla$.

Let us emphasize that the aforementioned decomposition (4.29) has been made possible provided we had shown first that there exists a displacement gradient (4.20), itself guaranteed as soon as a cut surface S was introduced, in order to render any reference configuration unambiguously defined.

Definition 10 (Glide surface)**.** *The glide surface associated to a defect line $\mathcal{L}$ is a particular smooth surface $\mathcal{G}_{\mathcal{L}} \subset \bar{\Omega}$ containing $\mathcal{L}$ and such that its tangent plane at $\mathcal{L}$ is spanned by $\tau^{\mathcal{L}}$ and $B^{\star\mathcal{L}}$.*

For a planar dislocation, $\mathcal{G}_{\mathcal{L}}$ coincides with the plane of the loop. For a pure edge dislocation, $\mathcal{G}_{\mathcal{L}}$ is the cylinder whose section is the loop. For rectilinear defects, the glide plane can be taken arbitrary as any plane containg the line.

Definition 11 (Particular glide surface $S^\circ_{\mathcal{L}}$)**.** *A particular choice of $S_{\mathcal{L}}$ in* (4.15) *(and hence in* (4.27)*) consists in taking the particular $S_{\mathcal{L}} = S^\circ_{\mathcal{L}}$ contained in $\mathcal{G}_{\mathcal{L}}$. For a planar dislocation, $S^\circ_{\mathcal{L}}$ coincides with the planof the loop, whereas for a pure edge dislocation, $S^\circ_{\mathcal{L}}$ is the closed surface made of the half cylinder whose section is the loop and whose uper base is a subset of $\partial\Omega$ (the half cylinder is chosen on the side of $\mathcal{L}$ corresponding to its out-of-plane Burgers vector).*

5. The displacement field is of bounded deformation

It remains to observe that the functional space which naturally appears in the distributional approach and with simple dislocation loops is the set of *functions of Bounded Deformation $BD(\Omega)$*. Let us start with a definition.

Definition 12 (Radon measures)**.** *A (tensor-valued) Radon measure $\mu \in \mathcal{M}(U)$ is a linear and continuous functional on $\mathcal{C}_c(U)$, the set of continuous functions with compact support in U. Moreover for any Borel set $A \subset U$, $\mu(A)$ is a set function such that (i) $\mu(\emptyset) = 0$, (ii) $\mu(\bigsqcup_i A^i) = \sum_i \mu(A_i)$ for any collection of pairwise disjoint sets $\{A^i\}$, and (iii) $\mu(K)$ is scalar- or tensor-valued (i.e., finite) as soon as $K \subset U$ is compact.*

Let us emphasize that in mechanical terms, a field is an *extensive* model variable if it is a Radon measure. In particular condition (ii) of Definition 12 does not hold for a general distribution (and in particular for the general $\mathcal{E}^{\star R}$ of §4.2 which is not a-priori more regular than the curl of a L^2 function.)

However, let us now prove that the residual strain $\mathcal{E}^{\star R}$, or equivalently $\varphi^\star$, is not a general order-one distribution but a locally square integrable field. We would like to define our fields on an extension domain $\hat{\Omega}$ defined as follows. If $\Omega = \mathbb{R}^3$ then $\hat{\Omega} = \Omega$, whereas if $\Omega \subsetneq \mathbb{R}^3$ then $\hat{\Omega}$ is an open connected subset of $\mathbb{R}^3$ such that $\Omega \subsetneq \hat{\Omega}$. The elastic strain and defect densities, and hence the $2D$ completed Frank and Burgers tensors, and $\theta^\star$, are suitably extended in $\hat{\Omega} \setminus \bar{\Omega}$.

Lemma 6. *For a simple dislocation loop, let φ be a distributional solution of $\Delta\Delta\varphi =$ inc $\theta^\star$ on $\hat{\Omega}$. Then $\varphi^\star \in L^2_{loc}(\hat{\Omega})$.*

Proof. First step. From Lemma 1, we know that $\tilde{\eta}^\star$ is symmetric. Moreover, recall that as a consequence of tr $\theta^\star = 0$, one has tr $\tilde{\eta}^\star = \tau \otimes \tau \cdot \tilde{\eta}^\star$. In particular $\sigma \otimes \sigma \cdot \tilde{\eta}^\star = -\nu \otimes \nu \cdot \tilde{\eta}^\star$. To check this, consider Theorem 2 and the proof of Lemmas 4, and compute in the local basis (τ, σ, ν),

$$\begin{aligned}
0 = \epsilon_{jpq}\partial_p \bar{\partial}_q \omega^\star_j &= \epsilon_{jpq}\partial_p \left(\bar{\partial}_q \omega^\star_j - \kappa^\star_{jq}\right) = \eta^\star_{jj} - \epsilon_{jpq}\partial_p \kappa^\star_{jq} \\
&= 2\tau_p\tau_l \hat{\eta}^\star_{pl} - \epsilon_{jpq}\partial_p\kappa^\star_{jq} = 2\tau_p\tau_l \left(\epsilon_{pij}\partial_i\kappa^\star_{lj} - \delta_{pl}\frac{1}{2}\epsilon_{mnq}\partial_n\kappa^\star_{mq}\right) - \epsilon_{pij}\partial_i\kappa^\star_{pj} \\
&= 2\tau_p\tau_l\epsilon_{pij}\partial_i\kappa^\star_{lj} - 2\left(\tau_p\tau_l + \nu_p\nu_l + \sigma_p\sigma_l\right)\epsilon_{pij}\partial_i\kappa^\star_{lj} = -2\left(\nu_p\nu_l + \sigma_p\sigma_l\right)\epsilon_{pij}\partial_i\kappa^\star_{lj}.
\end{aligned}$$

Second step. Let us explicitely compute $\theta =$ curl $\bar{\partial}\omega^\star = \eta^\star + \kappa^\star \times \nabla$. By Theorem 2 one has componentwise, and by the properties of $\tilde{\eta}^\star$ as established in the first step,

$$\begin{aligned}
\theta^\star_{ij} &= \tau_i\tau_k\left(\tilde{\eta}^\star_{kj} - \frac{1}{2}\delta_{kj}\tilde{\eta}^\star_{pp}\right) + \tau_j\tau_k\left(\tilde{\eta}^\star_{ki} - \frac{1}{2}\delta_{ki}\tilde{\eta}^\star_{pp}\right) - (\tau_i\tau_k + \nu_i\nu_k + \sigma_i\sigma_k)\tilde{\eta}^\star_{kj}. \\
&= -\tau_i\tau_j\tilde{\eta}^\star_{pp} - \left(\nu_i\nu_l + \sigma_i\sigma_l\right)\tilde{\eta}^\star_{lj} + \left(\tau_i\tau_l + \nu_i\nu_l + \sigma_i\sigma_l\right)\tilde{\eta}^\star_{lk}\tau_k\tau_j \\
&= -\tau_i\tau_j\tilde{\eta}^\star_{pp} + \tau_i\tau_k\tilde{\eta}^\star_{kl}\tau_l\tau_j - \left(\nu_i\nu_l + \sigma_i\sigma_l\right)\tilde{\eta}^\star_{lk}\left(\nu_k\nu_j + \sigma_k\sigma_j\right) \\
&= -\left(\nu_i\nu_l + \sigma_i\sigma_l\right)\tilde{\eta}^\star_{lk}\left(\nu_k\nu_j + \sigma_k\sigma_j\right) = \left(\nu_i\nu_j - \sigma_i\sigma_j\right)\sigma_k\tilde{\eta}^\star_{kl}\sigma_l - (\nu_i\sigma_j + \sigma_i\nu_j)\sigma_k\tilde{\eta}^\star_{kl}\nu_l. \quad (5.1)
\end{aligned}$$

Third step. Let us now show that $\sigma_i\tilde{\eta}^\star_{ij}\sigma_j$ and hence the first term on the RHS of (5.1) vanishes. Recall that $\tilde{\eta}^\star_{ij} = \epsilon_{jpq}\partial_p(\tau_i B^\star_q\delta_{\mathcal{L}}) - \frac{1}{2}\epsilon_{jpq}\partial_p(\delta_{iq}\tau_l B^\star_l\delta_{\mathcal{L}})$. Then, by considering the Frenet's formulae (i.e., $\partial_s\tau_i = \chi\nu_i, \partial_s\nu_i = -\chi\tau_i, \partial_s\sigma_i = 0$, with τ_i, σ_i, ν_i uniformly extended in a neigbourhood of $\mathcal{L}$), it can easily be verified that $\epsilon_{jpq}\partial_p(\tau_i B^\star_q\delta_{\mathcal{L}}) = -\sigma_j\nu_i B^\star_\nu\chi\delta_{\mathcal{L}} + \nu_j\nu_i B^\star_\sigma\chi\delta_{\mathcal{L}} + \tau_i B^\star_q\epsilon_{jpq}\partial_p\delta_{\mathcal{L}}$, while $\epsilon_{jpq}\partial_p(\delta_{iq}\tau_l B^\star_l\delta_{\mathcal{L}}) = \epsilon_{ijp}\partial_p(\tau_l B^\star_l\delta_{\mathcal{L}})$, whereby all terms vanish as multiplied by $\sigma_i\sigma_j$.

We now consider the last term on the RHS of (5.1). Recalling that $\chi B^\star_\sigma = 0$, we multiply the terms $-\sigma_j\nu_i B^\star_\nu\chi\delta_{\mathcal{L}}$, $\tau_i B^\star_q\epsilon_{jpq}\partial_p\delta_{\mathcal{L}}$ and $\epsilon_{ijp}\partial_p(\tau_l B^\star_l\delta_{\mathcal{L}})$ by $\sigma_i\nu_j$, and observe that they all vanish except the last one which rewrites as $\tau_p\partial_p(\tau_l B^\star_l\delta_{\mathcal{L}}) = \partial_s(\tau_l B^\star_l\delta_{\mathcal{L}})$. Moreover, multiplying the terms $-\sigma_j\nu_i B^\star_\nu\chi\delta_{\mathcal{L}}$, $\tau_i B^\star_q\epsilon_{jpq}\partial_p\delta_{\mathcal{L}}$ and $\epsilon_{ijp}\partial_p(\tau_l B^\star_l\delta_{\mathcal{L}})$ by $\sigma_i\nu_j$ yields the single term $\partial_s(\tau_l B^\star_l\delta_{\mathcal{L}})$, whereby the RHS of (5.1) can be rewritten as

$$\theta^\star_{ij} = -(\nu_i\sigma_j + \sigma_i\nu_j)\partial_s(\tau_l B^\star_l\delta_{\mathcal{L}}) = \frac{1}{2}(\nu_i\sigma_j + \sigma_i\nu_j)\chi\nu_l B^\star_l\delta_{\mathcal{L}} + \frac{1}{2}(\nu_i\sigma_j + \sigma_i\nu_j)\tau_l B^\star_l\partial_s\delta_{\mathcal{L}}. \tag{5.2}$$

Fourth step. The last term of (5.2) vanishes. In fact, considering a test function ψ_{ij} one has

$$\langle\frac{1}{2}(\nu_i\sigma_j + \sigma_i\nu_j)\tau_l B^\star_l\partial_s\delta_{\mathcal{L}}, \psi\rangle = -\langle\delta_{\mathcal{L}}, \partial_s(\frac{1}{2}(\nu_i\sigma_j + \sigma_i\nu_j)\tau_l B^\star_l\psi_{ij})\rangle = 0,$$

since $\mathcal{L}$ is a loop (i.e., the variation at the endpoints vanishes). Thus

$$\theta^\star_{ij} = -(\nu_i\sigma_j + \sigma_i\nu_j)\chi\nu_l B^\star_l\delta_{\mathcal{L}} \tag{5.3}$$

shows to be a concentrated Radon measure. Therefore $\theta^\star$ belongs to $H^{-2}_{loc}(\hat{\Omega})$ (cf. Remark 4), whereby inc $\theta^\star$ belongs to $H^{-4}_{loc}(\hat{\Omega})$. Then, by elliptic regularity results [28] one has $\varphi^\star \in L^2_{loc}(\hat{\Omega})$. This achieves the proof. □

Remark 11. *If U is a bounded subset of $\hat{\Omega}$ with Lipschitz boundary, then $\varphi^\star \in L^2(U)$. In particular if Ω is bounded and Lipschitz then $\varphi^\star \in L^2(\Omega)$.*

Theorem 3. *The displacement field $u^{\star(S)}$ of Eq.* (4.18) *is of bounded deformation in $\hat{\Omega}$.*

Proof. Let us first recall that according to a famous theorem by Temam and Strang [20], a distribution field is in BD (and hence in L^1_{loc}) if the symmetric part of its gradient is a Radon measure. Consider Eq. (4.23). By Assumption 1, $\mathcal{E}^\star \in L^1(\hat{\Omega})$, while by Lemma 6 $\mathcal{E}^{\star R} \in L^1_{loc}(U)$ on every bounded subset U of $\hat{\Omega}$. Thus $\mathcal{E}^\star + \mathcal{E}^{\star R}$ is a Radon measure on $\hat{\Omega}$. Moreover, $\mathcal{E}^{\star p}$ is obviously a concentrated Radon measure on $\hat{\Omega}$ by its explicit expression (4.27), thereby achieving the proof. □

It is observed from (4.23) that the singular measure is here purely concentrated, whereby the $L^1(\hat{\Omega})$-displacement field $u^{\star(S)}$ belongs to a subset of $BD(\hat{\Omega})$ known as the space of *Special functions of Bounded Deformation* $SBD(\hat{\Omega})$ [1,5].

Remark 12. *As a field of bounded deformation $u^{\star(S)}$ is allowed to exhibit jumps*[10] *in $\hat{\Omega}$. Recall that $u^{\star(S)} = \Psi^{S_{\mathcal{L}}} - (x - x_0) \times \omega^{\star(S)}$ with $\omega^{\star(S)}$ solution of* (4.10). *As soon as the displacement $u^{\star(S)}$ is found (as a function of bounded deformation) the gauge field $\Psi^{S_{\mathcal{L}}}$ is fixed. Recall that the smooth surface $S_{\mathcal{L}}$ could also be chosen "arbitrarily".*

A crucial consequence of the dispacement field belonging to $SBD(\hat{\Omega})$ space, is that the surface $S_{\mathcal{L}}$ cannot anymore be selected completely freely, since it was proved in, e.g., [5], that it must coincide with the set of jump points $\Sigma_{\mathcal{L}}$ of $u^{\star(S)}$. Therefore, the concentrated plastic strain $\mathcal{E}^{\star p}$ is a physical observable field. Moreover, by (4.27), the jump of $u^{\star(S)}$ on $S_{\mathcal{L}}$, $[\![u^{\star(S)}]\!]$, is constant and equal to the Burgers vector $B^{\star\mathcal{L}}$ of $\mathcal{L}$, while $[\![u^{\star(S)}]\!] = 0$ in $\Omega \setminus S_{\mathcal{L}}$.

Remark 13. *The canonical choice $S_{\mathcal{L}} = S^\circ_{\mathcal{L}}$ is not a consequence of the dispacement being in $SBD(\hat{\Omega})$. Rather, it results from the postulate that the Burgers vector is restricted to lie in $\Sigma_{\mathcal{L}}$.*

[10] A function is alllowed to have jumps, though that function is considered as single-valued, the latter term having an instrinsic meaning at every $x \in \hat{\Omega}$ which is distinct from having jumps [26,27].

6. Results for a family of defect lines

We would like to extend the results obtained and discussed above to a family $\Upsilon := \{\mathcal{L}^k\}_k$ of defect lines $\mathcal{L}^k$. Let us introduce

Definition 13 (Defect densities of a family of defect lines)**.**

DISCLINATION DENSITY: $$\Theta^\star_{ij} := \sum_{\mathcal{L}\in\Upsilon} \Theta^{\star\mathcal{L}}_{ij} \quad \textit{with} \quad \Theta^{\star\mathcal{L}}_{ij} := \Omega^{\star\mathcal{L}}_j \delta_{i\mathcal{L}} \tag{6.1}$$

PURE DISLOCATION DENSITY: $$\Lambda^\star_{ij} := \sum_{\mathcal{L}\in\Upsilon} \Lambda^{\star\mathcal{L}}_{ij} \quad \textit{with} \quad \Lambda^{\star\mathcal{L}}_{ij} := B^{\star\mathcal{L}}_j \delta_{i\mathcal{L}} \tag{6.2}$$

CONTORTION: $$\kappa^\star_{ij} := \sum_{\mathcal{L}\in\Upsilon} \kappa^{\star\mathcal{L}}_{ij} \quad \textit{with} \quad \kappa^{\star\mathcal{L}}_{ij} := \alpha^{\star\mathcal{L}}_{ij} - \frac{1}{2}\alpha^{\star\mathcal{L}}_{mm}\delta_{ij}, \tag{6.3}$$

with the auxiliary defect density measure:

$$\alpha^{\star\mathcal{L}}_{ij} := \Lambda^{\star\mathcal{L}}_{ij} - \epsilon_{jlm}(x_l - x_{0l})\Theta^{\star\mathcal{L}}_{im}, \tag{6.4}$$

and where x_{0m} is a point where rotation and Burgers fields are prescribed independently of $\mathcal{L}$.

Moreover, let us introduce

Definition 14.

ELASTIC STRAIN: $$\mathcal{E}^\star := \sum_{\mathcal{L}\in\Upsilon} \mathcal{E}^{\star\mathcal{L}} \tag{6.5}$$

PLASTIC CONCENTRATED STRAIN: $$\mathcal{E}^{\star p} := \sum_{\mathcal{L}\in\Upsilon} \mathcal{E}^{\star p\mathcal{L}} \quad \textit{with} \quad \mathcal{E}^{\star p\mathcal{L}} := \left(B^{\star\mathcal{L}} \otimes n\right)^S \delta_{S_\mathcal{L}}, \tag{6.6}$$

RESIDUAL STRAIN: $$\mathcal{E}^{\star R} := \sum_{\mathcal{L}\in\Upsilon} \mathcal{E}^{\star R\mathcal{L}} \quad \textit{with} \quad \mathcal{E}^{\star R\mathcal{L}} := -\varphi^{\star\mathcal{L}}, \tag{6.7}$$

where $\varphi^{\star\mathcal{L}}$ is a solution of $\Delta\Delta\varphi^{\star\mathcal{L}} = \operatorname{inc}\theta^{\star\mathcal{L}} = \nabla \times \left((\nu^\mathcal{L} \otimes \sigma^\mathcal{L} + \sigma^\mathcal{L} \otimes \nu^\mathcal{L})\chi^\mathcal{L}\nu^\mathcal{L} \cdot B^{\star\mathcal{L}}\delta_\mathcal{L}\right) \times \nabla$.

Here subscript $\mathcal{L}$ means that the quantity (tangent, Burgers or Frank vector, etc.) on which it is appended is relative to the isolated line $\mathcal{L} = \mathcal{L}^k \in \Upsilon$, for some index k (limited or not).

6.1. Case of finite family of defect lines.

The results of previous sections can immediately be extended to a finite number Υ of isolated lines $\mathcal{L}^k$. By isolated it is meant that $\mathcal{L}^i \cap \mathcal{L}^j = \emptyset$ whenever $i \neq j$. In fact, finite sums of L^1 functions, of Radon measures, and of order-1 distributions are still of the same functional type. Hence, Theorems 2 and 3 are straightforwardly extended to the finite family $\Upsilon := \{\mathcal{L}^k\}_{1\le k\le K}, (K \in \mathbb{N}^*)$.

Let us first give the following result which holds for a finite number of planar defects or simple $3D$ defect loops.

Theorem 4 (Incompatibility of a finite family of line defects)**.** *For a finite family of defect lines Υ, incompatibility writes in compact form as*

$$\eta^\star = \sum_{\mathcal{L}\in\Upsilon} \eta^{\star\mathcal{L}} = \operatorname{inc}(\mathcal{E}^\star) = -\nabla \times \mathcal{E}^\star \times \nabla = \left[\left(\tilde\eta^{\star\mathcal{L}}\right)^{d*} + \frac{I}{2}B^{\star\mathcal{L}}_\sigma \chi^\mathcal{L}\delta_\mathcal{L}\right]_\Upsilon, \tag{6.8}$$

where, given the second-order tensor A, A_Υ is the notation $A_\Upsilon := \sum_{\mathcal{L}\in\Upsilon} 2\left(\left(\tau^\mathcal{L} \otimes \tau^\mathcal{L}\right) A\right)^S$.

As the generalization of Theorem 3 and from Definition 14, the following result holds true for finite number of simple $3D$ dislocation loops.

Theorem 5. *For a finite family of simple dislocations Υ, one has*

TOTAL COMPATIBLE STRAIN: $$\mathcal{E}^{\star T} = \nabla^S u^\star = \mathcal{E}^\star + \mathcal{E}^{\star p} + \mathcal{E}^{\star R}, \tag{6.9}$$

where $\mathcal{E}^{\star T} := (\nabla u^\star)^S$ with the displacement field $u^\star := \sum_{\mathcal{L}\in\Upsilon} u^{\star\mathcal{L}(S)}$ of bounded deformation.

6.2. **Case of countable family of defect lines.** Let us introduce the finite family $\mathcal{L}^K := \bigcup_{1\le k\le K} \mathcal{L}^k$, $(K \in \mathbb{N}^*)$ and consider the case of a countable family $\Upsilon := \lim_{K\to\infty} \mathcal{L}^K$ (also denoted by $\bigcup_{\mathcal{L}\in\Upsilon} \mathcal{L}$).

Assumption 4 (Regularity of the cluster)**.** *It is assumed that Υ is a closed subset of Ω with finite $\mathcal{H}^1$ measure, that is, that Υ is a rectifiable one-dimensional set (or a curve-like one set in the temrinology of Falconer [7]) belonging to $\bar{\Omega}$. Moreover it is assumed that $\mathcal{H}^1$-almost everywhere, Υ has a Lipschitz continous tangent vector, that is, that its curvature χ exists $\mathcal{H}^1$-almost everywhere and is bounded.*

The following Lemma proved in [25,27] illustrates the kind of result required if a countable, instead of a finite family, is considered.

Lemma 7. *Let $\delta^{(i)}$, $i \in \mathcal{I} \subset \mathbb{N}$, stand for the Dirac measure at $\hat{x}^{(i)} \in l_0$ and $\sum_{i\in\mathcal{I}} C^{(i)}\delta^{(i)}$ be a Radon measure on $\Omega_{z_0} = \Omega \cap \{z = z_0\}$. Then the sum of the weights $C^{(i)}$ is locally absolutely convergent, this meaning its absolute convergence on any bounded subset $\{\hat{x}^{(i)}, i \in \mathcal{I}' \subset \mathcal{I}\}$ of l_0.*

Remark 14 (The difficulty dealing with a countable family of defects)**.** *As opposed to the finite case, it is false to claim that a concentrated first-order distribution on a countable set is a sum of Dirac masses and Dirac mass derivatives, as $1D$ counter-examples can show: the series $F = \sum_{i\in\mathbb{N}^*} C^{(i)}(H^0 - H^{(i)})$, with $H^{(i)} = H(x - \hat{x}^{(i)})$, $\hat{x}^{(i)} = 1/i$, $H^0 = H(x)$ and H the step function, may be L^1_{loc} converging even if the sum of the weights $C^{(i)}$ diverges. To show this, it suffices to select suitable $C^{(i)}$ such that the partial sums defining F are enclosed between the L^1_{loc} functions $G(x)$ and $-G(x)$, with $G(x) = \log((1 + x)/x)$ for $x > 0$ and $G(x) = 0$ for $x \le 0$. Then $F \in L^1_{loc}$, in such a way that the distributional derivative of F, which cannot be the diverging series $-\sum_{i\in\mathbb{N}^*} C^{(i)}\delta^{(i)}$, exhibits a special behaviour near the origin to recover convergence. Moreover, another difficulty arises from the different kinds of convergence that could be required. For instance, Lemma 7 is false if a (coarser) distributional convergence is considered.*

The mathematical problem raised by the example of Remark 14 will appear if an arbitrary countable family of simple $3D$ dislocation loops is considered. Peculiar concentration phenomena will appear at accumulation sets, in the form of distributional terms which are not measures (and hence, are not extensive quantities of the model). Moreover, since the loops are not restricted to by planar, the geometry of the accumulation set might also cause mathematical difficulties. In particular, the formalism of functions of bounded deformation would fail to be valid. To bypass this difficulty the following postulate is made.

Postulate 1. *It is assumed that there exists a finite family of glide planes $\mathcal{G} := \{\mathcal{G}_m\}_{m\le l\le M}$ in Ω such that $\Upsilon \subset \bigcup_{1\le 1\le M} \mathcal{G}_m$. Moreover, the canonical choice of Remark 11 will be adopted, that is, given $\mathcal{L} \subset \Upsilon$, we take $S_{\mathcal{L}} = S^\circ_{\mathcal{L}} \subset \mathcal{G}_m$ for some $1 \le m \le M$.*

The following assumption will also be made.

Assumption 5 (Total Burgers vector)**.** *The total Burgers vector, as defined by $B^\star := \sum_{\mathcal{L}\subset\Upsilon} B^{\star\mathcal{L}}$ has locally a finite norm, i.e., $\|B^\star\| \le \sum_{\mathcal{L}\subset\Upsilon\cap U} \|B^{\star\mathcal{L}}\| < \infty$ where U is an open and bounded subset of Ω.*

Remark 15. *It is shown in [27] that Assumption 5 is in fact a consequence of the set of assumptions on the strain curl, which are required to prove Theorem 4 for a countable family of lines (cf. [23, 25]).*

Let us now assume that Ω has a Lipschitz boundary and hence that $\mathcal{E}^\star$ can be continuously extended in a neigbourhood of $\partial\Omega$ while assumed of compact support in $\hat{\Omega}$. Moreover, the completed Frank and Burgers tensors, and $\theta^\star$, are extendend by 0 on $\hat{\Omega} \setminus \bar{\Omega}$.

Referring to Kleinert [11], the explicit complete strain expression[11] for a curve $\mathcal{L} \in \Upsilon$ (in a isotropic elastic crystal in equilibrium with no external body forces, nor inertial effects) reads componentwise

$$\bar{\mathcal{E}}_{ij}^{\star\mathcal{L}}(x) = \frac{B_r^{\star\mathcal{L}}}{8\pi}\epsilon_{uvr}[\epsilon_{j\kappa l}\epsilon_{vil}]_{i\leftrightarrow j}\oint_{\mathcal{L}}\tau_\kappa^{\mathcal{L}}(x')\partial_u 1/R dL(x') + \frac{B_r^{\star\mathcal{L}}}{8\pi(1-\nu)}\epsilon_{klr}\oint_{\mathcal{L}}\tau_\kappa^{\mathcal{L}}(x')\partial_i\partial_j\partial_l R dL(x'), \quad (6.10)$$

for every $x, x' \in \hat{\Omega}$ and with the notation $R := \|x - x'\|$. Integrating in a system of polar (spherical-type) coordinates, it is observed that $\mathcal{E}^{\star\mathcal{L}} \in L^s(\hat{\Omega})$ for $1 \le s < 3/2$.[12]

Therefore $\int_{\hat{\Omega}} \sum_{\mathcal{L}\in\mathcal{L}^K} \mathcal{E}^{\star\mathcal{L}} dV \le C\mathcal{H}^1(\Upsilon)\sum_{\mathcal{L}\in\Upsilon}\|B^{\star\mathcal{L}}\| < \infty$ by Assumption 5, by the hypothese $\mathcal{H}^1(\Upsilon) < \infty$, and with C is a positive constant independent of K. Thus $\{\mathcal{E}^{\star\mathcal{L}}\}_{\mathcal{L}\in\Upsilon}$ is equibounded in $L^s(\hat{\Omega})$ with $1 \le s < 3/2$. The explicit expression (6.10) shows that is also equicontinuous in $L^s(\hat{\Omega})$, and hence by Riesz-Kolmogorov's compactness theorem [4], for every bounded $U \subset \hat{\Omega}$ and up to a subsequence,

$$\bar{\mathcal{E}}^\star(\Upsilon) := \lim_{K\to\infty}\sum_{\mathcal{L}\in\mathcal{L}^K}\bar{\mathcal{E}}^{\star\mathcal{L}} \in L^s(U), \quad (6.11)$$

strongly in $L^s(U)$ ($1 \le s < 3/2$). Likewise, one also has (up to a non-relabeled subsequence),

$$\mathcal{E}^{\star R}(\Upsilon) := \lim_{K\to\infty}\sum_{\mathcal{L}\in\mathcal{L}^K}\mathcal{E}^{\star R\mathcal{L}} \in L^2_{loc}(\hat{\Omega}), \quad (6.12)$$

whereby we define

$$\mathcal{E}^\star(\Upsilon) := \bar{\mathcal{E}}^\star(\Upsilon) - \mathcal{E}^{\star R}(\Upsilon). \quad (6.13)$$

From Postulate 1 and Assumption 5, compacity of the Radon measures again entails that

$$\mathcal{E}^{\star p}(\Upsilon) := \lim_{K\to\infty}\sum_{\mathcal{L}\in\mathcal{L}^K}\left(B^{\star\mathcal{L}}\otimes n\right)^S\delta_{S^\circ_{\mathcal{L}}} \in \mathcal{M}(U), \quad (6.14)$$

(again up to a non-relabeled subsequence), where the uniform bound on $\mathcal{H}^2(S^\circ_{\mathcal{L}})$ is provided by the assumed finite number of glide planes and the boundedness of $U \subset \hat{\Omega}$.

Thus from (6.11)-(6.12), one deduce from the identity

$$\nabla\times\left(\bar{\mathcal{E}}^{\star\mathcal{L}} + \mathcal{E}^{\star p}(\Upsilon)\right)\times\nabla = 0, \quad (6.15)$$

that there exist a distribution field $u^\star := \lim_{K\to\infty}\sum_{\mathcal{L}\in\mathcal{L}^K} u^{\star(S)\mathcal{L}} =: \sum_{\mathcal{L}\in\Upsilon} u^{\star(S)\mathcal{L}}$ which belongs to $SBD(U)$ for every bounded $U \subset \hat{\Omega}$, and satisfies

$$\nabla^S u^\star = \bar{\mathcal{E}}^{\star\mathcal{L}} + \mathcal{E}^{\star p}(\Upsilon). \quad (6.16)$$

Let now U be a bounded subset of $\hat{\Omega}$ with a Lipschitz boundary, and $1 < s < 3/2$. From the above definitions and results we have the following uniform bound,

$$\begin{aligned}&\sum_{\mathcal{L}\in\mathcal{L}^K}\left(\|u^{\star(S)\mathcal{L}}\|_{L^1(U)} + \|\bar{\mathcal{E}}^{\star\mathcal{L}}\|^s_{L^s(U)} + |\mathcal{E}^{\star p\mathcal{L}}|(U) + \mathcal{H}^2(S^\circ_{\mathcal{L}})\right)\\ \le\ & \|u^\star\|_{L^1(\Omega)} + \|\bar{\mathcal{E}}^{\star\mathcal{L}}\|^s_{L^s(U)} + |\mathcal{E}^{\star p}(\Upsilon)|(U) + \mathcal{H}^2(\Upsilon) \le C < \infty,\end{aligned} \quad (6.17)$$

for some C independent of K.

Therefore, it results from a compactness result in $SBD(U)$ [3, 5] that there exists a displacement field (identified with $u^\star$) such that $u^\star \in SBD(U)$ and a rectifiable set $\Sigma \subset U$ defined as the jump set

[11]Expression (3.16) of [11] corresponds to our Eq. (4.20) since by Remark 10, $\nabla\cdot(\mathbb{C}\bar{\mathcal{E}}) = \nabla\cdot(\mathbb{C}\mathcal{E}^\star) = 0$. Note also that for a nonvanishing body force an extra impactless term should be added.

[12]Indeed $\mathcal{E}^{\star\mathcal{L}}$ can be integrated over $\hat{\Omega}$ by means of a system of polar (spherical-type) coordinates (R, s, Ψ) with s the abcissa of $\mathcal{L}$ and with volume element $dV := R^2 dR ds d\Psi$. Then, since $\partial_i R^{-1}, \partial_{ijl}R = O(R^{-2})$, one has $\int_{\hat{\Omega}}\|\mathcal{E}^{\star\mathcal{L}}\|^s(x)dV(x) = \oint_{\mathcal{L}} ds\int_{-\pi}^{\pi} d\Psi\int_0^\infty\|\mathcal{E}^{\star\mathcal{L}}\|^s(R, s, \Psi)R^2 dR$ which is bounded if $1 \le s < 3/2$.

of $u^\star$ such that

$$\sum_{\mathcal{L}\in\mathcal{L}^N} u^{\star(S)\mathcal{L}} \rightarrow u^\star \quad \text{strongly in} \quad L^1_{loc}(U;\mathbb{R}^3) \tag{6.18}$$

$$\sum_{\mathcal{L}\in\mathcal{L}^N} (\bar{\mathcal{E}}^{\star\mathcal{L}}) \rightharpoonup \mathcal{E}^{\star\mathtt{diff}}(\Upsilon) := \mathcal{E}^\star(\Upsilon) + \mathcal{E}^{\star R}(\Upsilon) \quad \text{weakly in} \quad L^1(U;\mathbb{R}^{3\times 3}) \tag{6.19}$$

$$\sum_{\mathcal{L}\in\mathcal{L}^N} \mathcal{E}^{\star p\mathcal{L}} \rightharpoonup \mathcal{E}^{\star p}(\Upsilon) \quad \text{weakly-}\star \text{ in} \quad \mathcal{M}(U;\mathbb{R}^{3\times 3}) \tag{6.20}$$

$$\mathcal{H}^2(\Sigma) \leq \liminf_{K\to\infty} \mathcal{H}^2(\bigcup_{\mathcal{L}\in\mathcal{L}^K} S^\circ_{\mathcal{L}}). \tag{6.21}$$

Remark 16. *In particular if Ω is a bounded, Lipschitz and connected set, take U s.t. $\Omega \subsetneq U \subset \hat{\Omega}$. Then $\Sigma \cap \partial\Omega$ must not be empty. Recall that $\Upsilon \cap \partial\Omega$ must not be empty, since Υ was assumed a closed subset of Ω. Thus the dislocations clustering at the crystal boundary (i.e., the accumulation points belonging to $\partial\Omega$) are identified with the jump points of $u^\star$ in $\partial\Omega$. Moreover, $\mathcal{E}^\star(\Upsilon) \in L^1(\Omega)$ and $\mathcal{E}^{\star R}(\Upsilon) \in L^2(\Omega)$.*

As the generalization of Theorem 3, the following result holds true for countable number of simple $3D$ dislocation loops.

Theorem 6. *Let U be a bounded subset of $\hat{\Omega}$ with a Lipschitz boundary. For a countable family of simple dislocations Υ, one has*

TOTAL COMPATIBLE STRAIN:
$$\mathcal{E}^{\star T} = \nabla^S u^\star = \mathcal{E}^{\star p}(\Upsilon) + \mathcal{E}^{\star diff}(\Upsilon), \tag{6.22}$$

where $\mathcal{E}^{\star T} := (\nabla u^\star)^S$ with the displacement field $u^\star := \sum_{\mathcal{L}\in\Upsilon} u^{\star\mathcal{L}(S)}$ of bounded deformation in U, with $\mathcal{E}^{\star diff}(\Upsilon)$ defined by (6.19) *and $\mathcal{E}^{\star p}(\Upsilon)$ given by*

$$\mathcal{E}^{\star p}(\Upsilon) = ([\![u^\star]\!] \otimes n)^S \delta_\Sigma. \tag{6.23}$$

In particular, the BD formalism has permitted to fix all gauge fields (and surfaces) unambiguously, therefore rendering the model fields physically as well as mathematically well defined.

6.3. **Discussion.** It appears from this compactness result that the *diffuse* part of the strain, $\mathcal{E}^{\star\mathtt{diff}}(\Upsilon)$, cannot be qualified of *elastic* anymore. In particular it must not verify any constitutive relation with the stress. Let us emphasize that the qualification *plastic* to denote $\mathcal{E}^{\star p}$ is also a nomenclature postulate, since so far this term only appears as the concentrated part of the total strain. This observation is also justified by the fact that $\mathcal{E}^{\star\mathtt{diff}}(\Upsilon)$ is neither elastic nor plastic, while of course, there is no way to set appart (with physical meaning) the displacement (or its gradient) in elastic and plastic parts.

However, by observing that

$$\mathcal{E}^{\star p}(\Upsilon) = \lim_{K\to\infty} \sum_{\mathcal{L}\in\mathcal{L}^K} \left(B^{\star\mathcal{L}} \otimes n\right)^S \delta_{S^\circ_{\mathcal{L}}} = ([\![u^\star]\!] \otimes n)^S \delta_\Sigma, \tag{6.24}$$

with $\Upsilon = \lim_{K\to\infty} \mathcal{L}^K \subset \Sigma \subset \bigcup_{\mathcal{L}\in\Upsilon} S^\circ_{\mathcal{L}}$ assumed as a subset of the glide plane family $\mathcal{G}$, the term plastic to denote the concentrated part $\mathcal{E}^{\star p}(\Upsilon)$ could be justified by the fact that the plastic effects are known to be due to the *motion* of the dislocations on their glide planes (which are always finitely many in actual materials). However, we believe that as far as statics is concerned and since the diffuse strain is not elastic, it is not physically justified to denote the concentrated part as *plastic*.

Moreover, from (6.24), we can define the Burgers vector at the accumulation set of the dislocation lines[13] as the jump of $u^\star$.

[13]which is a "curve-like" set and which is of course is not isolated, whereby any classical definition of the Burgers vector would fail to hold.

Nevertheless, it is observed from (4.1) that $\operatorname{tr}\mathcal{E}^{\star R}=0$, and since the jump set has been assumed as a subset of the glide planes in Postulate 1 one also has $\operatorname{tr}\mathcal{E}^{\star p}=B^\star\cdot n=0$. Then,

$$\mathcal{E}^{\star P}:=\mathcal{E}^{\star p}+\mathcal{E}^{\star R}$$

is trace-free and hence could be qualified as the plastic, or *nonelastic*, strain of the model, with a concentrated part $\mathcal{E}^{\star p}$ and a diffuse part $\mathcal{E}^{\star R}$. In fact, in many model of plasticity (see, e.g., [6]) the plastic strain is assumed trace free, in the sense that plastic strains do not affect the density (no changes in volume), but only appear as shear effects (as the creation of shear bands for instance). In our model, the concentrated nonelastic strain is related to the presence of the glide planes on which the dislocations lie and move, whereas the diffuse part is due to dislocation line curvature. It can also be observed that the non-elastic diffuse part is not affected by the out-of-plane "skew" edge segments.

As already mentioned, the search for the appropriate function space has allowed us to rigourously define the model fields, both from a physical (through the notion of "observability" of a physical field) and a mathematical point of view, since the gauge fields and surfaces have been fixed, while a precise meaning has been given to dislocation clusters.

In particular, we have shown that the displacement gradient can be decomposed in several physically meaningfull ways, among which (i) an elastic/plastic decomposition (4.20), a symmetric/skew-symmetric decomposition (4.30). Let us emphasize that (4.20) coincides to a diffuse/concentrated decomposition, but this must not be a necessarily condition, since $p^\star$ as well as $p^\star+\mathcal{E}^{\star R}$ are both trace-free and hence could both be considered as plastic parts. It should also be stressed that the importance of having at hand a well-defined displacement gradient, instead of its sole symmetric part, is justified by the necessity of taking into account the plastic spin in dislocation models. Quoting Gurtin in [9]: "Unless the plastic spin is constrained to be zero, constitutive dependencies on the Burgers tensor necessarily involve the infinitesimal plastic rotation".

From the present work one can now address the issue of (i) the choice of the relevant model internal variables, (ii) the appropriate constitutive laws (let us refer to [23] for a discussion). Some remarks can already be made.

In [6] a time-dependent plasticity model is considered with a free energy of the type

$$\Psi(\nabla u,p,\operatorname{curl}p,\gamma):=\Psi_{\rm e}(\varepsilon_e)+\Psi_{\rm curl}(\operatorname{curl}p)+\Psi_{\rm iso}(\gamma),\tag{6.25}$$

with $\nabla u=e+p$, $\varepsilon_e:=e^S$, and where $\Psi_{\rm iso}$ represents isotropic hardening. Within our model, this free energy would be written with $\varepsilon_e=\bar{\mathcal{E}}^\star$ and $p=p^\star$ or with $\varepsilon_e=\mathcal{E}^\star$ and $p=p^\star-\varphi^\star$, since by Remark 3, $\operatorname{tr}p=0$. Other choices could also be made (for instance $p=-\beta^\star$) since decompostion (4.20) is not unique whereby the exact meaning of the plastic spin remains unclear (about this issue, read also [13]). Moreover this second-order model is considered with the implicit assumption that ε_e and $\operatorname{curl}p$ are square-integrable, which is certainly not verified in our distributional model.

In fact we should first consider a time-independent model with a free energy of the type

$$\hat\Psi(e^\star,\Lambda^\star):=W_{\rm deform.}(e^\star)+W_{\rm defect}(\Lambda^\star),\tag{6.26}$$

where the energy is decomposed in a two terms involving the first-order deformation internal variable, $e^\star$ (with $(e^\star)^S=\bar{\mathcal{E}}^\star$), and the first-order defect internal variable[14] $\Lambda^\star$ (or equivalently $\kappa^\star$), respectively. Moreover, by (4.3), (4.16) and & (4.17), it is observed that $\operatorname{curl}e^\star=\operatorname{curl}\beta^\star=\Lambda^\star=-\operatorname{curl}p^\star$. Thus there is a link with (6.25) but problem of minimizing (6.26) is hard to address because (i) it explicitely takes into account the constraint $\operatorname{curl}e^\star=\Lambda^\star$, (ii) $e^\star$ is a multivalued field and $\Lambda^\star$ a Radon measure, (iii) $e^\star$ is not square integrable. To address this problem, a convincing approach using Cartesian currents has been proposed in [17]. Note that the stress is subsequently obtained by computing $\sigma^\star=\frac{\partial\hat\Psi}{\partial e^\star}(e^\star_{\rm min},\Lambda^\star)$, while $\mathcal{E}^\star$ is provided by Eq. (1.1).

Work towards an answer to these open questions and further generalizations will be proposed in future publications.

[14] For the terminology, see [13,23]

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