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Strain incompatibility in single crystals: Kröner's formula revisited

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Abstract In this paper we prove under precise working assumptions a famous relation originally due to Ekkehart Kröner [10] relating linear elastic strain incompatibility and dislocation and disclination densities. The $3D$ case with a set of isolated skew[1] defect lines in a single crystal is considered according to a mathematical approach taking into account the combined effects of field multivaluedness and concentration properties.

Keywords Dislocations, disclinations, single crystals, defect density tensors, multiple-valued fields, strain incompatibility, contortion tensor

Mathematics Subject Classification (2000) 74A05,74A60,74B05,74-01

1 Introduction

The study of dislocations in crystals began about one century ago with the pioneer works by Volterra [18]. About 30 years later, the work of Burgers [2], and then of Eshelby, Frank and Nabarro [5], Kondo [9] and Nye [13], among others, paved the way for major progress in understanding the dislocation physics. In the second half of the 20th century one of the most prolific and authoritative authors is certainly Ekkehart Kröner (1919-2000) who can be considered as a key contributor to the field. He showed how the dislocated crystal was embedded in a geometry whose intrinsic torsion [4] was directly related to the dislocation density [10, 12]. Moreover, he included disclinations– which are a more resistant and hence rarer (in fact, as compared to dislocations, they require higher energy to be created), in his analysis and showed how their presence was responsible for the intrinsic curvature of the body.

In this paper, we focus on one of the key formulae of the kinematic theory of line defects in linear elastic bodies relating the elastic strain incompatibility $inc\ \mathcal{E}$ [16] to

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[1] Skew lines are lines which do not intersect but are not parallel either.

the contortion tensor κ and the disclination density tensor Θ. This formula is

$$(inc\ \mathcal{E})^{KR} = \Theta + \nabla^T \times \kappa, \qquad (1.1)$$

where $\left(\nabla^T \times \kappa\right)_{ij} := \epsilon_{imn}\partial_m\kappa_{jn}$ and where the superscript KR is to recall that this formula is due to Kröner [10]. It should be noted that the scale of matter description at which Kröner derives (1.1) is not the same as the scale considered in the present paper. In fact he considers a scale where the singularities due to the physical presence of the line have been erased and hence he uses tools from differential geometry on a smooth manifold. Moreover the defect quantities are identified with some geometrical objects, and this identification serves as a definition for these objects at this scale [4, 10, 14]. In the present approach the contortion tensor is a direct combination of the dislocation and disclination[2] density tensors which themselves are defined at the *mesoscale*, i.e., at a scale where the body is considered as a continuum with a finite number of line singularities called dislocations or disclinations. At the mesoscale a formula relating strain incompatibility and defect densities still needs to be proved. To provide specific assumptions with a view to the line singularities and to prove the counterpart of (1.1) is the object of the remaining of this paper.

Dislocations in single crystals are considered, where it is known that four classes of defects appear. Three classical defects are purely $2D$ rectilinear defects – that is, defects along the z-axis whose strain depends only on the planar coordinates. These are the screw and edge dislocations and the wedge disclination [7]. The fourth type of line defect is the $3D$ twist disclination which is here considered together with the three others. By conservation laws, rectilinear defects end at the crystal boundary, whereas dislocations as resulting from the saturation of point-defects form loops in $3D$.

The present paper deals with formula (1.1) for a set $\mathcal{L}$ of isolated skew defect lines in $3D$ elasticity. A simplified version of (1.1) is first found in Nye's work [13], but the formal derivation of (1.1) is ascribed to Kröner [10], as a simple consequence of the displacement gradient decomposition into an elastic and a plastic part. In the present approach we want to avoid any kind of a-priori decomposition of the deformation gradient. Another formal derivation of (1.1) can be found in [8] but there, field multi-valuedness is not rigorously addressed. Let us remark that in the present approach, no equilibrium condition is ever required, and so the results found here eventually apply to a dynamical (instead of purely kinematical) description of dislocation networks.

In this paper, considering the distribution [14] and geometric measure [1] theories and introducing single-valued objective fields[3], the following result will be proved:

$$inc\ \mathcal{E} = \left((inc\ \mathcal{E})^{KR} - \frac{I}{2}\operatorname{tr}(inc\ \mathcal{E})^{KR}\right)_{\mathcal{L}}, \qquad (1.2)$$

where for a second order tensor A the symmetric operator $A_{\mathcal{L}} := \sum_{L\in\mathcal{L}} \left(\Gamma^L A^L\right)^{sym}$ is defined, with $\Gamma^L := \tau^L \otimes \tau^L$, and τ^L the tangent vector of line L. It should be

[2] Let us remark that Θ is not a symmetric tensor at the mesoscale, whereas its macroscopic counterpart, sometimes called "linearized Einstein tensor", is in general symmetric [11].

[3] Here "objective" means independent of a reference configuration: displacement, deformation gradient and rotation are therefore not objective fields (this should not to be confused with the notion of "objectivity" as it is used in other areas of continuum mechanics.)

remarked that (1.2) coincide with (1.1) in $2D$ (detail of the $2D$ case is given in [17]).

The main contributions of this paper are the following:

- prove Kröner's formula (1.2) under precise strain singularity growth, i.e., under local assumptions, for a set of isolated skew lines
- provide equivalent distributional, i.e., global, assumptions on the Frank tensor (defined as the strain curl: cf. Definition 1) to prove (1.2)

The paper is organized as follows: in Section 2, preliminary results some of which are detailed in [17] are recalled. Section 3 provides singularity growth assumptions for a single line and equivalent distributional assumptions for a set of skew lines allowing us to prove Eq. (1.2) in a planar section of the crystal, while in Section 4, Eq. (1.2) is proved for a set of isolated skew defect lines in the entire crystal.

2 $3D$ elasticity in the dislocated crystal: preliminary results and main assumptions

In this paper, Einstein summation convention on repeated indices will always be assumed, with vectors designated by a single lower index, and tensor by the number of indices corresponding to their order. Moreover the upper $\star$-symbol appearing on all physical fields aims at recalling that the fields are considered at the meso-scale, that is, at a scale where the defect lines are viewed as isolated defect lines.

The crystal Ω is an open (bounded or not) connected set of $\mathbb{R}^3$ which contains either a single defect line L or a set $\mathcal{L}$ of isolated skew dislocations and/or disclinations, while $3D$ linear elasticity applies everywhere in the adjacent medium. The following notation is also adopted: $\Omega_L := \Omega \setminus L$ and $\Omega_{\mathcal{L}} := \Omega \setminus \mathcal{L}$. The notation ∂_i refers to partial derivation w.r.t. the ith coordinate of a $3D$ Cartesian frame $\{e_1, e_2, e_3\}$ attached to the origin with coordinates x_i. This derivation is intended, according to the context, either in the distribution, or in the classical pointwise sense. Moreover a Greek indice $\alpha, \beta \cdots$ will run from 1 to 2 while Roman indices $i, j, k \cdots$ run from 1 to 3.

The theory of distributions [15] will be considered in this approach. A distribution is a linear form defined as the dual of the space of smooth functions with compact support $\mathcal{C}_c^\infty(\Omega)$. A distribution defined on $\mathcal{C}_c^k(\Omega)$ with the integer $k \geq 1$ is said to be of order k. In the particular case where $k = 0$ the distribution is called a *Radon measure*. Let us recall that the Radon-Nikodým (or Lebesgue) decomposition theorem [1] states that a Radon measure can be decomposed into three parts: a regular L^1-part, a concentrated part (where the concentration sets are typically lines or surfaces) and a singular diffuse part (also called Cantor part) [1]. Note that the derivative of a distribution f is also a distribution defined by $< f', u >= - < f, u' >$ with $u \in \mathcal{C}_c^\infty(\Omega)$, while for every $\varphi \in \mathcal{C}_c^\infty(\Omega)$, φf is the distribution defined by $< \varphi f, u >=< f, \varphi u >$.

2.1 Single-valued strain: main assumption and decomposition property

In the following, the strain $\mathcal{E}^\star$ is considered as a distribution on Ω [14]. It is considered to be an objective, measurable field[4].

[4] For instance, as related to the stress σ by the relation $\sigma = C\mathcal{E}^\star$, where C is the Lamé tensor.

Assumption 1 (3D elastic strain) *The linear strain $\mathcal{E}^\star_{mn}$ is a given symmetric L^1_{loc} $(\Omega, \mathbb{R}^{3\times 3})$-tensor compatible on $\Omega_\mathcal{L}$. In other words, the incompatibility tensor, as defined by the distribution*

$$\eta^\star_{kl} := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathcal{E}^\star_{mn}, \tag{2.1}$$

vanishes everywhere on $\Omega_\mathcal{L}$.

In general 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 [6]).

Lemma 1 (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:*

$$\mathcal{E} = \mathcal{E}^c + \mathcal{E}^s, \tag{2.2}$$

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

Remark 1 *In particular we have for some distribution F:*

$$\mathcal{E}^s = \nabla \times F \times \nabla \quad \textit{with} \quad \Delta\Delta F = \nabla \times \mathcal{E} \times \nabla. \tag{2.3}$$

Remark 2 (Solenoidal strain) *In the sequel of the paper, $\mathcal{E}^\star$ (or $\mathcal{E}^\star_{ij}$) will always denote a solenoidal strain, since the compatible part of the strain has no impact on the sought representation theorem involving the strain incompatibility. Moreover, the strain component will in general be denoted by $\mathcal{E}^\star_{xx}, \mathcal{E}^\star_{xy}, \mathcal{E}^\star_{xz}$, etc. instead of $\mathcal{E}^\star_{11}, \mathcal{E}^\star_{12}, \mathcal{E}^\star_{13}$, etc.*

2.2 Frank and Burgers tensors: model governing assumptions

Besides the strain, the following tensors will appear crucial. Their role and physical sense will be made clear in the last section.

Definition 1 (Frank and Burgers tensors) *The Frank tensor $\overline{\partial}_m\omega^\star_k$ is defined on the entire domain Ω as the following distribution:*

$$\overline{\partial}_m\omega^\star_k := \epsilon_{kpq}\partial_p\mathcal{E}^\star_{qm}, \tag{2.4}$$

in such a way that incompatibility is governed by $\eta^\star_{kl} = \eta^\star_{lk} := \epsilon_{lpm}\partial_p\overline{\partial}_m\omega^\star_k$. Moreover, for a selected $x_0 \in \Omega_\mathcal{L}$, the Burgers tensor is defined on the entire domain Ω as the distribution

$$\overline{\partial}_l b^\star_k(x) := \mathcal{E}^\star_{kl}(x) + \epsilon_{kpq}(x_p - x_{0p})\overline{\partial}_l\omega^\star_q(x). \tag{2.5}$$

Assumption 2 (Frank tensor projection on the defect set) *Let τ^L_k be the tangent vector of $L \in \mathcal{L}$. The Frank tensor, is such that its projection on $\mathcal{L}$,* [5]

$$p^\star_m = \sum_{L\in\mathcal{L}} \overline{\partial}_m\omega^\star_k\tau^L_k, \tag{2.6}$$

[5] As $\overline{\partial}_m\omega^\star_k$ is a measure, Eqs. (2.6) and (2.7) are written with an abuse notation. In fact, we implicitly consider that the – constant – vector τ^L_k is multiplied by a cut-off function $\varphi^L_1 \in \mathcal{C}^\infty_c(\Omega)$, i.e., $\varphi^L_1 \equiv 1$ on a compact subset U of its support and $L \subset U$. Also, in (2.7) τ^L_k is (implicitely) multiplied by a cut-off function φ^L_2 whose support is strictly included in U.

is a vector-valued Radon measure on Ω, with a singular part $c^\star_m$ and a $L^1(\Omega)-$ regular part $r^\star_m := p^\star_m - c^\star_m$ s.t. the following quantities are purely concentrated on $\mathcal{L}$:

$$c^\star_m \quad , \quad \sum_{L\in\mathcal{L}} \tau^L_k \epsilon_{klm}\partial_l r^\star_m \quad \text{and} \quad \sum_{L\in\mathcal{L}} \partial_\alpha \left(\tau^L_m r^\star_m\right). \tag{2.7}$$

2.3 Multiple-valued rotation, displacement and Burgers fields

Classical rotation and displacement fields in $\Omega_{\mathcal{L}}$. It is classically known that in $\Omega_{\mathcal{L}}$, the *infinitesimal rotation vector $\omega^\star_k$ and displacement vector $u^\star_i$* are given by

$$\omega^\star_k(x) = \omega^\star_{0k} + \int_{x_0}^{x} \epsilon_{klm}\partial_l \mathcal{E}^\star_{mn}(\xi)d\xi_n = \frac{1}{2}\epsilon_{ijk}\partial_i u^\star_j(x), \tag{2.8}$$

$$u^\star_i(x) = u^\star_{0i} + \int_{x_0}^{x} \left(\mathcal{E}^\star_{il}(\xi) - \epsilon_{ilk}\omega^\star_k(\xi)\right) d\xi_l, \tag{2.9}$$

respectively, where $x \in \Omega$ and $x_0 \in \Omega_{\mathcal{L}}$ is a point where the displacement $u^\star_{0i}$ and rotation $\omega^\star_{0k}$ are known. It immediately results that on $\Omega_{\mathcal{L}}$, $\partial_l u^\star_i = \mathcal{E}^\star_{il} + \omega^\star_{il}$. The key point to observe here is that because of the presence of the defects $\mathcal{L}$, the domain $\Omega_{\mathcal{L}}$ is not simply-connected, and hence rotation and displacement depend on the integration path between x_0 and x. Therefore these two fields are said to be *multiple-valued*.

Multiple-valued rotation and Burgers fields in Ω. As discussed in detail in [17], the displacement cannot be considered to describe the dislocated crystal without reference configuration. Indeed displacement should be replaced by the *Burgers field*[6]:

$$b^\star_i(x) := b^\star_{0i} + \int_{x_0}^{x} \left(\mathcal{E}^\star_{il}(\xi) + \epsilon_{ipk}(\xi_p - x_{0p})\overline{\partial}_l\omega^\star_k(\xi)\right) d\xi_l \tag{2.10}$$

since it is observed that in the absence of disclinations and by simple integration by parts, (2.10) and (2.9) coincide, while (2.10) is explicitly given in terms of single-valued objective fields. Moreover, the displacement gradient should be replaced by the Burgers tensor $\overline{\partial}_l b^\star_k$, which is defined according to (2.5) on the *entire crystal Ω* as a single-valued distribution coinciding *almost everywhere* on Ω with $\partial_l b^\star_k$. The rotation gradient is also given by the Frank tensor $\overline{\partial}_m\omega^\star_k$ as a first-order distribution on Ω. So, (2.10) should replace (2.9) and be considered as the (translational) counterpart of (2.8). The physical link between the displacement and the Burgers fields will appear clearer in Definition 3 and Remark 3.

Since (2.8)-(2.10) depend on the integration path, it is natural to introduce the following set:

Definition 2 (Riemann foliation)

$$F := \{(x, \#C) \text{ for every } x \in \Omega_{\mathcal{L}} \text{ and for every curve } C \text{ joining } x_0 \text{ to } x\},$$

where the equivalence class $\#C$ represents all regular loops homotopic to C in $\Omega_{\mathcal{L}}$, and where x_0 is a point where rotation and Burgers fields are known.

[6] Pointwise expressions of the strain and Frank tensors will be given in section 3.1.

Since the rotation and Burgers fields are multiple-valued they are associated with a Riemann foliation F in the sense that the following relations exist (with $\mathcal{P}$ the projection of F onto $\Omega_{\mathcal{L}}$):

$$\Omega_{\mathcal{L}} \overset{\mathcal{P}}{\longleftarrow} F \overset{\omega_k^\star, b_i^\star}{\longrightarrow} \mathbb{R}^3. \tag{2.11}$$

Single-valued rotation and Burgers fields in defect-free subsets of Ω. A defect-free subset of Ω is a subset $U \subset \Omega$ which does not contain any curve $C \subset U$ making one or more loops around $L \in \mathcal{L}$. The restriction on every defect-free subset U of the rotation and Burgers fields, together with all their derivatives at every order (as long as they exist) are single-valued fields denoted by an upper symbol (s):

$$\omega_k^{\star(s)}, b_i^{\star(s)} : U \subset \Omega_{\mathcal{L}} \rightleftarrows F \longrightarrow \mathbb{R}^3,$$

where the first relation of (2.11) has become one-to-one (as designated by the two arrow symbol). In practice, defect-free subsets are obtained by means of cuts in F.

Theorem 1 (Distortion decomposition) *From a symmetric smooth linear strain tensor $\mathcal{E}_{ij}^\star$ on $\Omega_{\mathcal{L}}$ and a point x_0 where the displacement is known, the single-valued displacement field $u_i^{\star(s)}$ as restricted to any defect-free subset U is given by expression (2.9) on U and is such that $\mathcal{E}_{ij}^\star := \frac{1}{2}\left(\partial_j u_i^{\star(s)} + \partial_i u_j^{\star(s)}\right)$ is the single-valued symmetric part of its gradient $\partial_j u_i^{\star(s)}$ (i.e. the distortion tensor), while its skew-symmetric part is the multiple-valued rotation tensor $\omega_{ij}^\star = -\epsilon_{ijk}\omega_k^\star := \frac{1}{2}\left(\partial_j u_i^{\star(s)} - \partial_i u_j^{\star(s)}\right)$.*

2.4 Defect invariants and density tensors

Definition 3 (Frank and Burgers vectors) *The Frank and Burgers vectors of the single isolated line L are defined as*

$$\begin{aligned} \Omega_k^{\star L} &:= [\omega_k^{\star L}] = \int_{C_L} \overline{\partial}_m \omega_k^{\star L} dx_m, \\ B_k^{\star L} &:= [b_k^{\star L}] = \int_{C_L} \overline{\partial}_m b_k^{\star L} dx_m = [u_k^{\star L}](x) + \epsilon_{klm}(x_l - x_{0l})\Omega_m^{\star L}, \end{aligned}$$

respectively, where the brackets mean the jump of the considered quantity along a curve C_L which makes one loop around L. Also, subscript L means that the quantity is related to the isolated line L (in the sequel, it will be omitted when there is no risk of confusion).

Theorem 2 (Weingarten) *The rotation $\omega_k^\star$ and Burgers field $b_i^\star$ are multiple-valued fields on Ω, whose jumps $\Omega_k^\star$ and $B_k^\star$ around an isolated line L are constant vectors.*

Let τ_i denote the tangent vector of an isolated line L, and δ_{iL} denote the line measure concentrated on L, as multiplied by τ_i. The defect density tensors on the set $\Omega_{\mathcal{L}}$ of isolated defect lines are defined as:

Definition 4 (Defect densities)

DISCLINATION DENSITY: $$\Theta^{\star}_{ij} := \sum_{L\in\mathcal{L}} \Theta^{\star L}_{ij} \quad \textit{with} \quad \Theta^{\star L}_{ij} := \Omega^{\star L}_j \delta_{iL}, \tag{2.12}$$

PURE DISLOCATION DENSITY: $$\Lambda^{\star}_{ij} := \sum_{L\in\mathcal{L}} \Lambda^{\star L}_{ij} \quad \textit{with} \quad \Lambda^{\star L}_{ij} := B^{\star L}_j \delta_{iL}, \tag{2.13}$$

CONTORTION: $$\kappa^{\star L}_{ij} := \alpha^{\star L}_{ij} - \frac{1}{2}\alpha^{\star L}_{mm}\delta_{ij}, \tag{2.14}$$

with the auxiliary defect density measure:

$$\alpha^{\star L}_{ij} := \Lambda^{\star L}_{ij} - \epsilon_{jlm}(x_l - x_{0l})\Theta^{\star L}_{im}, \tag{2.15}$$

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

Remark 3 (Burgers and displacement fields) *For an isolated defect line L, it follows from Definition 3, Theorem 2, and Eq. (2.12), that the invariant Burgers vector of L is equal to the displacement jump iff the disclination density vanishes.*

Moreover, from Weingarten's theorem, the following crucial conservation laws hold[7]:

Theorem 3 (Conservation laws) *Isolated defect lines are always closed or end at the boundary of Ω. Moreover, $\partial_i\Theta^{\star L}_{ij} = \partial_i\Lambda^{\star L}_{ij} = 0$ while $\partial_i\alpha^{\star L}_{ij} = \epsilon_{jmn}\Theta^{\star L}_{mn}$.*

2.5 Preliminary 2D result

The following result has been proved in [17] in the framework of $2D$ elasticity for a single isolated line, meaning that the defect line coincides with the z-axis (and is hence reductible to a point: the origin) and that the strain is independent of z. Under suitable singularity growth assumptions (explictly given by Assumption 4 in section 3.1, which is a direct consequence of Assumption 2), the strain incompatibility for a single isolated defect line L reduces to a vector $\eta^{\star}_{zk}$ whose components may be expressed as

$$\eta^{\star}_{zz} = \Omega^{\star}_z\delta_L + \epsilon_{\alpha\gamma}\left(B^{\star}_\gamma - \epsilon_{\beta\gamma}x_{0\beta}\Omega^{\star}_z\right)\partial_\alpha\delta_L, \tag{2.16}$$

$$\eta^{\star}_{z\kappa} = \frac{1}{2}\epsilon_{\kappa\alpha}B^{\star}_z\partial_\alpha\delta_L, \tag{2.17}$$

where $\epsilon_{\alpha\beta} := \epsilon_{z\alpha\beta}$. One aim of this paper is to generalize Eqs. (2.16) & (2.17) to the case of $3D$ elasticity for a set $\mathcal{L}$ of skew isolated defect lines. In order to proceed, one step will be to work on planar sections and to make use of this $2D$ result.

3 Local analysis of one isolated defect line

Let us now consider one isolated defect line L parallel to the z-axis, whose points are denoted by $\hat{x} = (\hat{x}^z, z)$ with z the coordinate along L and tangent vector $\tau(\hat{x})$ at $\hat{x}$.

Notations 1 (Planar sections) *The planar sections of Ω are introduced by fixing $\hat{x}$ (that is, z) on the line L and defining $\Omega^z := \{x \in \Omega \text{ such that } (x_i - \hat{x}_i)\,\tau_i(\hat{x}) = 0\}$, while for $\epsilon \geq 0$, $\Omega^z_\epsilon := \{x \in \Omega^z \text{ such that } r_z := \sqrt{(x_\alpha - \hat{x}_\alpha)^2} > \epsilon\}$. A point of Ω^z_ϵ will be denoted $x^z_p = (x^z_\alpha, z)$. Moreover, $\theta_z := \arctan(x^z_2/x^z_1)$.*

[7] For a proof of Theorems 2 and 3 we refer to [8].

Notations 2 (Defect-free subset on a planar section) *On a planar section Ω_0^z, let us define a defect-free set as $\Lambda_z := \{x^z = (r_z \cos\theta_z, r_z \sin\theta_z) : \theta_z \in [\theta_1, \theta_2]$ with $\theta_2 - \theta_1 < 2\pi$ and $r_z > 0\} \cap \Omega_0^z$.*

3.1 Asymptotic analysis near the defect line

According to Assumption 2 we have the following assumption on a planar section Ω^z:

Assumption 3 (Global behaviour) *On Ω^z, $\overline{\partial}_m \omega_z^\star =$ is a vector-valued Radon measure with singular part $c_m^\star$ and regular part $r_m^\star := \overline{\partial}_m \omega_z^\star - c_m^\star$ s.t. $c_m^\star, \epsilon_{\alpha\beta}\partial_\alpha r_\beta^\star$ and $\partial_\alpha r_z^\star$ are purely concentrated on L, i.e., there are vectors c_m, and a scalar d such that $c_m^\star = c_m \delta_{\hat{x}^z}, \epsilon_{\alpha\beta}\partial_\alpha r_\beta^\star = d\delta_{\hat{x}^z}$ and $\partial_\alpha r_z^\star = d_\alpha \delta_{\hat{x}^z}$, where $\delta_{\hat{x}}$ is the Dirac mass at $\hat{x}$.*

Lemma 2 *Under Assumptions 1 and 3, the (solenoidal) strain has the following growth near the defect line:*

$$\mathcal{E}_{\alpha m}^\star = \frac{e_{\alpha m}}{r} + o_{\alpha m}(r^{-1}), \tag{3.1}$$

where $e_{\alpha m}$ is a smooth tensor depending on θ_z and z only, and $o_{\alpha m}$ is the tensor Landau symbol[8]*.*

Proof. Let us consider the planar section Ω^z. By (2.3) and Assumption 3 we have $\Delta\Delta F_{zz} = \nabla \times (c_z^\star + r^\star) = \nabla \times (c_z \delta_{\hat{x}}) + d\delta_{\hat{x}}$ which has a solution (recall that $2\pi\delta_{\hat{x}^z} = \Delta \log r_z$): $F_{zz} = (d + \epsilon_{\alpha\beta}\partial_\alpha c_\beta)(\frac{r_z^2}{8\pi}(\log r_z - 1))$. It follows that (3.1) holds (recall (2.3)) on Ω^z for $m = \beta$. Since r has the same meaning as r_z, the result is proved on Ω_L. By (2.3) and Assumption 3 we have $F_{\alpha z} = F_{\alpha z}^1 + F_{\alpha z}^2$ with $\Delta\Delta F_{\alpha z}^1 = \epsilon_{\alpha\beta}\partial_\beta r_z^\star = \epsilon_{\alpha\beta} d_\beta \delta_{\hat{x}}$ and $\Delta\Delta F_{\alpha z}^2 = \epsilon_{\alpha\beta}\partial_\beta c_z^\star = \epsilon_{\alpha\beta}\partial_\beta (c_z \delta_{\hat{x}})$ with a solution of the form

$$F_{\alpha z}^1 = \epsilon_{\alpha\beta} d_\beta (\frac{r_z^2}{8\pi}(\log r_z - 1)) \quad \text{and} \quad \begin{cases} \partial_x F_{yz}^2 - \partial_y F_{xz}^2 = -\frac{c_z}{2\pi}\log r_z, \\ \partial_x F_{xz}^2 + \partial_y F_{yz}^2 = \quad 0, \end{cases}$$

in such a way that by (2.3), $\mathcal{E}_{\alpha z}^\star = \mathcal{E}_{\alpha z}^{\star 1} + \mathcal{E}_{\alpha z}^{\star 2}$ with $\mathcal{E}_{\alpha z}^{\star 1} = \epsilon_{\alpha\beta}\partial_\beta \left(\epsilon_{\gamma\kappa}\partial_\gamma F_{\kappa z}^1\right)$ and $\mathcal{E}_{\alpha z}^{\star 2} = -\epsilon_{\alpha\beta}\partial_\beta \left(\frac{c_z}{2\pi}\log r_z\right)$ yields the required form (3.1) for $m = z$. □

Remark 4 (Twist Disclinations) *Accordingly, the strain $\mathcal{E}_{\alpha z}^{\star 1}$ has the form*

$$\mathcal{E}_{xz}^{\star 1} = -\frac{d_x}{4\pi}\frac{xy}{r^2} - \frac{d_y}{4\pi}\left(\log r + \frac{y^2}{r^2} - \frac{1}{2}\right) \text{ and } \mathcal{E}_{yz}^{\star 1} = \frac{d_y}{4\pi}\frac{xy}{r^2} + \frac{d_x}{4\pi}\left(\log r + \frac{y^2}{r^2} - \frac{1}{2}\right).$$

By letting $d_x = -\Omega_y^\star$ and $d_y = \Omega_x^\star$, the above equations are recognized as the αz-components of the so-called twist disclinations [3]. Let us mention that the other components are given by replacing $B_x^\star$ by $\Omega_y^\star z/2$ and $B_y^\star$ by $-\Omega_x^\star z/2$ in the edge dislocation expression [17], i.e.,

$$[\mathcal{E}_{\alpha\beta}^\star] = \frac{(\Omega_x^\star + \Omega_y^\star)z}{4\pi r^2}\begin{bmatrix} x & y \\ y & -x \end{bmatrix}_{\alpha\beta}.$$

[8] A function $f(\epsilon)$ is said to be $O(g(\epsilon))\,(\epsilon \to 0^+)$ if there exists $K, \epsilon_0 > 0$ s.t. $0 < \epsilon < \epsilon_0 \Rightarrow |f(\epsilon)| \le K|g(\epsilon)|$. A function $f(\epsilon)$ is said to be $o(g(\epsilon))\,(\epsilon \to 0^+)$ if $\lim_{\epsilon \to 0^+} \frac{f(\epsilon)}{g(\epsilon)} = 0$.

Remark 5 *The third statement of Assumption (2.7) states that $\overline{\partial}_z \omega^\star_z$ is a constant K on Ω_L. It can be verified that $K = 0$ for all four types of line defects in $3D$.*

According to Lemma 2 and Definition 1 the *global* Assumption 3 implies the following *local* assumption:

Assumption 4 (Local behaviour) *The strain tensor $\mathcal{E}^\star_{ij}$ is $o(r^{-2})$ $(r \to 0^+)$ while the Frank tensor is $o(r^{-3})(r \to 0^+)$.*

However, the above result can be made more precise:

Lemma 3 *Under Assumptions 1 and 3, the following estimates hold near the line L:*

$$u^{\star(s)}_i = O_i(\log r), \quad \mathcal{E}^\star_{zz} = O(\log r), \quad \overline{\partial}_z \omega^\star_i = O_i(1/r), \tag{3.2}$$

where O and O_i are the scalar and vector Landau symbols, respectively.

Proof. Let us consider a defect-free subset Λ_z and let $u^{\star(s)}_r, u^{\star(s)}_\theta, u^{\star(s)}_z$ denote the single-valued displacement components as expressed in the polar coordinate system with coordinates r_z, θ_z (with fixed z) and as restricted to Λ_z. By Theorem 1 and Lemma 2, the radial component $\mathcal{E}^\star_{rr} = \partial_r u^{\star(s)}_r$ is $e_{rr}/r_z + o(r_z^{-1})$ with e_{rr} independent of r_z, showing by integration that $u^{\star(s)}_r = O(\log r_z)$. Eqs. (3.2)-a- and (3.2)-b- follow on Λ_z from the formulas $2\mathcal{E}^\star_{\theta r} = 1/r_z \partial_\theta u^{\star(s)}_r - u^{\star(s)}_\theta / r_z$, $2\mathcal{E}^\star_{rz} = \partial_r u^{\star(s)}_z + \partial_z u^{\star(s)}_r$ and $\mathcal{E}^\star_{zz} = \partial_z u^{\star(s)}_z$. By arbitrary rigid rotations of Λ_z around L, (3.2)-a- and (3.2)-b- are proved at every point of Ω_L. Observe that (3.2)-c- with $i = \kappa$ follows from (3.2)-b- and Lemma 2, while for $i = z$, it follows from Assumption 3 and Remark 5. □

Notations 3 *In the sequel, we consider a surface S of Ω perforated by L at $\hat{x}_i$ and bounded by the curve C, and let σ_j and τ_j denote the unit tangent vectors to C at x_i and to L at $\hat{x}_i$, respectively. Moreover, dx_α (resp. $dC_\gamma = \epsilon_{\gamma\alpha} dx_\alpha$) denotes the infinitesimal line element tangent (resp. externaly normal) to C.*

Lemma 4 *Let $\hat{x} = (\hat{x}^z, z)$ be a point on the line L and consider $\mathcal{C}(\hat{x})$, a family of $2D$ closed curves around $\hat{x}$ in Ω^z. From Assumptions 1 and 2 it follows that*

$$\lim_{C(\hat{x}) \to \{\hat{x}^z\}} \int_{C(\hat{x}^z)} \left(x^z_\alpha \overline{\partial}_\beta \omega^\star_\kappa dx_\beta + \epsilon_{\kappa\beta} \mathcal{E}^\star_{\beta z} dx_\alpha \right) = 0,$$

provided the length of $C(\hat{x}) \in \mathcal{C}(\hat{x})$ is uniformly bounded. Here the convergence is understood in the Hausdorff sense, i.e., $\max\{\| x - \hat{x} \|,\ x \in \mathcal{C}(\hat{x})\} \to 0$.

Corollary 1 *Let $\hat{x}$ be a point on the line L. From Assumptions 1 and 2, we see that*

$$\int_{C^z_\epsilon} \mathcal{E}^\star_{\beta\xi} dx_\beta = B^\star_\xi - \epsilon_{\xi pq}(x_{0p} - \hat{x}_p)\Omega^\star_q + o_\xi(1), \tag{3.3}$$

$$\int_{C^z_\epsilon} \mathcal{E}^\star_{\beta z} dx_\beta = \frac{1}{2}\left(B^\star_z + \epsilon_{\alpha\beta} x_{0\alpha} \Omega^\star_\beta \right) + o(1), \tag{3.4}$$

where C^z_ϵ is the circle of radius ϵ centered at $\hat{x}$ in Ω^z, x_0 is a point where the displacement and rotation are known, and $o(1), o_\xi(1)$ represent the scalar and vector Landau symbols, respectively.

Proof. Let us observe that $x^z_\gamma = \hat{x}^z_\gamma + \epsilon(e_r)_\gamma$, where e_r is the radial base vector at $\hat{x}^z$, in such a way that (2.5) with $x_i \in C^z_\epsilon$ has the form

$$\mathcal{E}^\star_{\xi\beta}(x_i) = \overline{\partial}_\beta b^\star_\xi(x_i) - \epsilon\overline{\partial}_\beta \omega^\star_z(x_i)\epsilon_{\xi\gamma}(e_r)_\gamma + \epsilon_{\xi pq}(x_{0p} - \hat{x}_p)\overline{\partial}_\beta \omega^\star_q(x_i),$$

immediately yielding (3.3) by integration over C_ϵ, Definition 3 and Theorem 2.
From the Burgers tensor definition (2.5), it follows that $x_\alpha\overline{\partial}_\beta\omega^\star_k - x_k\overline{\partial}_\beta\omega^\star_\alpha = \epsilon_{kn\alpha}\overline{\partial}_\beta b^\star_n$ $-\epsilon_{kn\alpha}\mathcal{E}^\star_{\beta n} + x_{0\alpha}\overline{\partial}_\beta\omega^\star_k - x_{0k}\overline{\partial}_\beta\omega^\star_\alpha$, so that by Lemma 4 and $k = \kappa$,

$$\begin{aligned}
&\epsilon_{\alpha\kappa}B^\star_z + x_{0\alpha}\Omega^\star_\kappa - x_{0\kappa}\Omega^\star_\alpha - \int_{C^z_\epsilon} \epsilon_{\alpha\kappa}\mathcal{E}^\star_{\beta z}dx_\beta + o(1)\\
&= \int_{C^z_\epsilon} \left(\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta z}dx_\kappa - \epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha\right) = \int_{C^z_\epsilon} \epsilon_{\gamma\tau}\epsilon_{\alpha\kappa}\epsilon_{\gamma\beta}\mathcal{E}^\star_{\beta z}dx_\tau = \int_{C^z_\epsilon} \epsilon_{\alpha\kappa}\mathcal{E}^\star_{\beta z}dx_\beta,
\end{aligned}$$

thereby proving (3.4) since: $2\int_{C^z_\epsilon} \epsilon_{\alpha\kappa}\mathcal{E}^\star_{\beta z}dx_\beta = \epsilon_{\alpha\kappa}B^\star_z + x_{0\alpha}\Omega^\star_\kappa - x_{0\kappa}\Omega^\star_\alpha + o_{\alpha\kappa}(1)$. □

3.2 Strain incompatibility of an isolated defect line

Notations 4 *Let φ be a test-function on Ω, $\varphi^z = \varphi(\cdot, z)$ a test-function on Ω^z, and d^z_{mn} a 2D distribution tensor in Ω^z such that $< d^z_{mn}, \varphi^z >$, as a function of z, is integrable on a line L parallel to the z-axis. Then,*

$$d^z_{mn} \quad \text{is said} \quad o^L_{mn} \quad \text{iff} \quad < d^z_{mn}, \varphi > := \int_L < d^z_{mn}, \varphi^z > (z)dz = 0. \tag{3.5}$$

Lemma 5 (Preliminary result on a planar section) *Let the (solenoidal) strain and the Frank tensors as restricted to Ω^z satisfy Assumptions 1 and 3, respectively. Then,*

$$\eta^\star_{\alpha\beta}(\hat{x}^z) = o^L_{\alpha\beta}, \tag{3.6}$$

$$\eta^\star_{zz}(\hat{x}^z) = \Omega^\star_z\delta_{\hat{x}^z} + \epsilon_{\alpha\gamma}\left(B^\star_\gamma - \epsilon_{\gamma pq}(\hat{x}_p - x_{0p})\Omega^\star_q\right)\partial_\alpha\delta_{\hat{x}^z}, \tag{3.7}$$

$$\eta^\star_{z\kappa}(\hat{x}^z) = \Omega^\star_\kappa\delta_{\hat{x}^z} + \frac{1}{2}\epsilon_{\kappa\alpha}\left(B^\star_z - \epsilon_{\beta\gamma}(\hat{x}_\beta - x_{0\beta})\Omega^\star_\gamma\right)\partial_\alpha\delta_{\hat{x}^z} + o^L_{z\kappa}, \tag{3.8}$$

$$\eta^\star_{\kappa z}(\hat{x}^z) = \eta^\star_{z\kappa}(\hat{x}^z), \tag{3.9}$$

with x_0 a point where the displacement and rotation are known, and o^L_{ij} is defined by (3.5).

Proof. By Lemmas 2 and 3, the strain is $o(r_z^{-2})$ near the line L and smooth away from it. Moreover, the test-function φ^z on Ω^z depends on (x^z_1, x^z_2) with prescribed z.
First part: proof of (3.6). By definition of incompatibility on Ω^z and Definition 1, integration by parts shows that

$$< \eta^\star_{\alpha\kappa}(\hat{x}^z), \varphi^z > := \lim_{\epsilon \to 0}\left(-\int_{\Omega^z_\epsilon} \epsilon_{\alpha lm}\overline{\partial}_m\omega^\star_\kappa\partial_l\varphi^z dS - \int_{C^z_\epsilon} \epsilon_{\alpha lm}\epsilon_{\kappa pn}\overline{\mathcal{E}}^\star_{mn}\partial_l\varphi^z dC_p\right),$$

where the first and second terms inside the parenthesis are denoted by $\overline{\pi}_\epsilon(\alpha, \kappa)$ and $\pi^\star_\epsilon(\alpha, \kappa)$, respectively. After integration by parts of $\overline{\pi}_\epsilon$ and from strain compatibility on Ω^z_0, we find that

$$\overline{\pi}_\epsilon(\alpha, \kappa) = \int_{C^z_\epsilon} \epsilon_{\alpha\beta}\overline{\partial}_z\omega^\star_\kappa\varphi^z dC_\beta \quad \text{and} \quad \pi^\star_\epsilon(\alpha, \kappa) = -\int_{C^z_\epsilon} \epsilon_{\alpha li}\epsilon_{\kappa\gamma}\mathcal{E}^\star_{iz}\partial_l\varphi^z dC_\gamma. \tag{3.10}$$

Computation of $\overline{\pi}_\epsilon(\alpha,\kappa)$ and $\pi^\star_\epsilon(\alpha,k)$. The term $\overline{\pi}_\epsilon(\alpha,\kappa)$ may be written, using Notation 3, as $\overline{\pi}_\epsilon(\alpha,\kappa) := \int_{C^z_\epsilon} \epsilon_{\alpha\beta}\overline{\partial}_z\omega^\star_\kappa\varphi^z\epsilon_{\beta\tau}dx_\tau$, which by the Taylor expansion of φ^z at $\hat{x}^z$ at the first order, and Lemma 3 becomes $\overline{\pi}_\epsilon(\alpha,\kappa) := \overline{\Pi}_\epsilon(\alpha,\kappa) + o_{\alpha\kappa}(1)$, with

$$\overline{\Pi}_\epsilon(\alpha,\kappa) = \varphi^z(\hat{x}^z)\int_{C^z_\epsilon}\left(\epsilon_{\kappa\beta}\partial_z\mathcal{E}^\star_{\beta z} - \epsilon_{\kappa\beta}\partial_\beta\mathcal{E}^\star_{zz}\right)dx_\alpha \tag{3.11}$$

$$= \partial_z\left(\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha\right) + \hat{\Pi}_\epsilon(\alpha,\kappa) + \tilde{\Pi}_\epsilon(\alpha,\kappa), \tag{3.12}$$

where we recall that $\hat{x} = (\hat{x}^z, z)$ and where

- $\hat{\Pi}_\epsilon(\alpha,\kappa) := -\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha$ (3.13)
- $\tilde{\Pi}_\epsilon(\alpha,\kappa) := -\varphi^z(\hat{x}^z)\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\partial_\beta\mathcal{E}^\star_{zz}dx_\alpha.$ (3.14)

By Lemma 3 and a Taylor expansion at $\hat{x}^z$ the term $\pi^\star_\epsilon(\alpha,k)$ becomes $\pi^\star_\epsilon(\alpha,\kappa) = \Pi^\star_\epsilon(\alpha,\kappa) + o_{\alpha\kappa}(1)$, where

- $\Pi^\star_\epsilon(\alpha,\kappa) := -\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta z}dx_\kappa.$ (3.15)

Computation of $\tilde{\Pi}_\epsilon(\alpha,\kappa)$. By integration and Theorem 1, it follows that

$$\tilde{\Pi}_\epsilon(\alpha,\kappa) = -\partial_z\left(\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\partial_\beta u^{\star(s)}_z dx_\alpha\right) + \partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\partial_\beta u^{\star(s)}_z dx_\alpha, \tag{3.16}$$

whose last term may be rewritten as

$$2\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha - \partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\partial_z u^{\star(s)}_\beta dx_\alpha. \tag{3.17}$$

By Lemma 3, the last term of (3.17) is $o(1)$, and hence by (3.16):

- $\tilde{\Pi}_\epsilon(\alpha,\kappa) = -\partial_z\left(\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\partial_\beta u^{\star(s)}_z dx_\alpha\right) + \tilde{\tilde{\Pi}}_\epsilon(\alpha,\kappa) + o(1),$ (3.18)

where

- $\tilde{\tilde{\Pi}}_\epsilon(\alpha,\kappa) = 2\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha.$ (3.19)

Computation of $\Pi_\epsilon(\alpha,\kappa) := \hat{\Pi}_\epsilon(\alpha,\kappa) + \Pi^\star_\epsilon(\alpha,\kappa) + \tilde{\tilde{\Pi}}_\epsilon(\alpha,\kappa)$. By equations (3.14)-(3.19), let us observe that the diagonal components of the skew-symmetric tensor

$$\Pi_\epsilon(\alpha,\kappa) = -\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\left(\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta z}dx_\kappa - \epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha\right)$$

identically vanish, while the $1-2$ and $2-1$ components are given by

$$\Pi_\epsilon(1,2) = -\Pi_\epsilon(2,1) = -\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\left(\mathcal{E}^\star_{yz}dy + \mathcal{E}^\star_{xz}dx\right) = -\partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\mathcal{E}^\star_{\beta z}dx_\beta,$$

which by Corollary 1 (Eq. (3.4)) becomes

$$\Pi_\epsilon(1,2) = -\partial_z\varphi(\hat{x})\frac{1}{2}\left(B^\star_z + \epsilon_{\alpha\beta}x_{0\alpha}\Omega^\star_\beta + o(1)\right). \tag{3.20}$$

Computation of $\overline{\pi}_\epsilon(\alpha,\kappa)+\pi^\star_\epsilon(\alpha,\kappa)$**.** Since the first term on the RHS of (3.12) and of (3.18), together with all remaining terms as collected in (3.20), are $o^L_{\alpha\kappa}$ according to Notation 4 (because the test-function vanishes at the boundary), then equation (3.6) is obtained by integration of (3.13)-(3.15) over L and letting $\epsilon\to 0$.

Second part: proof of (3.7)-(3.9). By Assumption 1 and Definition 1, integration by parts shows that

$$\eta^\star_{zk} = \lim_{\epsilon\to 0}\left(-\int_{\Omega^z_\epsilon}\epsilon_{\alpha\beta}\overline{\partial}_\beta\omega^\star_k\partial_\alpha\varphi^z dS - \int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{kpn}\mathcal{E}^\star_{\beta n}\partial_\alpha\varphi^z dC_p\right) = \eta^{\star(1)}_{zk} + \eta^{\star(2)}_{zk},$$

where, integrating by parts and by strain compatibility, we see that

$$\begin{aligned}\eta^{\star(1)}_{zk} &:= -\lim_{\epsilon\to 0}\left(\int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{\kappa\xi}\partial_\xi\mathcal{E}^\star_{\beta z}\varphi^z dC_\alpha + \int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{\kappa\gamma}\mathcal{E}^\star_{\beta z}\partial_\alpha\varphi^z dC_\gamma\right)\delta_{k\kappa}\\ &\quad + \lim_{\epsilon\to 0}\left(\int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{\zeta\xi}\partial_\xi\mathcal{E}^\star_{\beta\zeta}\varphi^z dC_\alpha + \int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{\zeta\gamma}\mathcal{E}^\star_{\beta\zeta}\partial_\alpha\varphi^z dC_\gamma\right)\delta_{kz}, \quad (3.21)\\ \eta^{\star(2)}_{zk} &:= \lim_{\epsilon\to 0}\left(\int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{\kappa\xi}\partial_z\mathcal{E}^\star_{\beta\xi}\varphi^z dC_\alpha\right)\delta_{k\kappa}. \quad (3.22)\end{aligned}$$

By slightly adapting the proof [17] of the $2D$ result for a dislocation located at the origin (cf., Eqs. (2.16) & (2.17)), the term $\eta^{\star(1)}_{zk}$ can be easily treated taking into account the non-vanishing of $\Omega^\star_\alpha$ and the translation of the $2D$ formulas by $(\hat{x}_\gamma, 0)$):

$$\begin{aligned}\eta^{\star(1)}_{zz} &= \Omega^\star_z\delta_{\hat{x}^z} + \epsilon_{\alpha\gamma}\left(B^\star_\gamma - \epsilon_{\gamma pq}(\hat{x}_p - x_{0p})\Omega^\star_q\right)\partial_\alpha\delta_{\hat{x}^z}, \quad (3.23)\\ \eta^{\star(1)}_{z\kappa} &= \Omega^\star_\kappa\delta_{\hat{x}^z} + \frac{1}{2}\epsilon_{\kappa\alpha}\left(B^\star_z - \epsilon_{\beta\gamma}(\hat{x}_\beta - x_{0\beta})\Omega^\star_\gamma\right)\partial_\alpha\delta_{\hat{x}^z}, \quad (3.24)\end{aligned}$$

hence proving (3.7).

Concerning the $\eta^{\star(2)}_{zk}$ term, we see by a Taylor expansion of φ^z around $\hat{x}^z$, by Proposition 2, by part integration in z and by $dx_\beta = \epsilon_{\alpha\beta}dC_\alpha$ that

$$\eta^{\star(2)}_{zk} = \lim_{\epsilon\to 0}\left(\partial_z\left(\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\alpha\beta}\epsilon_{\kappa\xi}\mathcal{E}^\star_{\beta\xi}dx_\beta\right) - \partial_z\varphi(\hat{x})\int_{C^z_\epsilon}\epsilon_{\kappa\xi}\mathcal{E}^\star_{\beta\xi}dx_\beta\right), \tag{3.25}$$

where the second term on the RHS may be replaced by $\partial_z\varphi(\hat{x})\epsilon_{\kappa\xi}\Big(B^\star_\xi + \epsilon_{\xi pq}(x_{0p} - \hat{x}_p)$ $\Omega^\star_q\Big)$ because of Corollary 1. This yields a vanishing integral over L due to the invariance property of $B^\star_\xi$ and $\Omega^\star_q$ over L. Therefore, Eq. (3.8) follows because the first term on the RHS of (3.25) identically satisfies (3.5). Eq. (3.9) follows from the symmetry of the incompatibility tensor (2.1). □

4 Main result: strain incompatibility of a set of isolated skew defect lines

Kröner's formula (1.1) is revisited according to the assumptions and preliminary results of previous sections. In particular, Eq. (1.2) will be proved, and discussed. We recall that the crystal is an elastic continuum containing a set $\mathcal{L}$ of isolated skew defect lines.

4.1 Proof of Kröner's formula

Notations 5 *The concentrated measure on the isolated line $L \in \mathcal{L}$ is denoted by δ_{iL} and defined for any test-function $\varphi \in \mathcal{D}(\Omega)$ as*

$$< \delta_{iL}, \varphi >= \int_L \varphi(\hat{x})\tau_i(\hat{x})dL(\hat{x}). \tag{4.1}$$

Theorem 4 (Main result) *Under Assumptions 1 and 2, for a set of isolated skew defect lines $\mathcal{L}$, incompatibility as defined by (2.1) is the following first-order symmetric tensor distribution*

$$\eta^\star_{mn} = \sum_{L\in\mathcal{L}} \left[\tau^L_m \tau^L_k \left(\left(\Theta^{\star L}_{kn} + \epsilon_{kij}\partial_i \kappa^{\star L}_{nj} \right) - \frac{1}{2}\delta_{kn} \left(\Theta^{\star L}_{pp} + \epsilon_{pij}\partial_i \kappa^{\star L}_{pj} \right) \right) \right]_{m\leftrightarrow n} \tag{4.2}$$

where the defect densities are given by Definition 4, where the symbol $A_{m\leftrightarrow n}$ denotes that the sum of A_{mn} and its transposed A_{nm} is taken, and where superscript L indicates a concentrated quantitity on the line L.

Proof. ***First part: preliminary computations.*** Let us consider first that $\mathcal{L}$ consists of a single line L identified with the z-axis and define $\odot_\epsilon$ as an ϵ-neighbourhood of L. By definition of incompatibility, integration by parts shows that

$$< \eta^\star_{mn}, \varphi >= -\lim_{\epsilon\to 0} \left(\int_{\Omega\setminus\odot_\epsilon} \epsilon_{mlq}\overline{\partial}_q \omega^\star_n \partial_l \varphi dV - \int_{\partial\odot_\epsilon} \epsilon_{mlq}\epsilon_{npk}\mathcal{E}^\star_{qk}\partial_l\varphi dS_p \right). \tag{4.3}$$

We denote the 1^{st} and 2^{nd} terms inside the parenthesis as $\overline{\pi}_\epsilon(m,n)$ and $\pi^\star_\epsilon(m,n)$ and their sum by $\pi_\epsilon(m,n)$. Integration by parts of $\overline{\pi}_\epsilon$ and strain compatibility in $\Omega_{\mathcal{L}}$ yield

$$\overline{\pi}_\epsilon(m,n) = \int_{\partial\odot_\epsilon} \epsilon_{mlq}\overline{\partial}_q\omega^\star_n\varphi dS_l \quad \text{and} \quad \pi^\star_\epsilon(m,n) = -\int_{\partial\odot_\epsilon} \epsilon_{mlq}\epsilon_{npk}\mathcal{E}^\star_{qk}\partial_l\varphi dS_p \tag{4.4}$$

Let us fix a $\hat{x} \in L$ and consider the circle $C^z_\epsilon \subset \partial\odot_\epsilon$ centered at $\hat{x}$, such that $\int_{\partial\odot_\epsilon} dS_l(x) = \int_L \int_{C^z_\epsilon} dL(\hat{x})dC_l(x)$. Let us introduce $\varphi^z := \varphi(\cdot, z)$, and the planar incompatibility in Ω^z as expressed by

$$< \eta^\star_{mn}(\hat{x}^z), \varphi^z > := \lim_{\epsilon\to 0} \int_{C^z_\epsilon} \left(\epsilon_{mpq}\overline{\partial}_q\omega^\star_n\varphi^z - \epsilon_{mlq}\epsilon_{npk}\mathcal{E}^\star_{qk}\partial_l\varphi^z \right) dC_p. \tag{4.5}$$

Hence, by (4.3)-(4.5), $3D$ incompatibility may be expressed as $< \eta^\star_{mn}, \varphi >= \int_L < \eta^\star_{mn}(\hat{x}^z), \varphi^z > dL$. We now consider that $\mathcal{L}$ is a set of isolated skew lines. By considering a small enough ϵ-neigbourhood of each line of $\mathcal{L}$, the same computation as above could be done for each $L \in \mathcal{L}$ separately and then summed since every line is isolated from the others:

$$< \eta^\star_{mn}, \varphi >= \sum_{L\in\mathcal{L}} \int_L < \eta^\star_{mn}(\hat{x}^L), \varphi^L > dL, \tag{4.6}$$

where symbols $\hat{x}^L, C^L_\epsilon$ and φ^L are the counterparts of $\hat{x}^z, C^z_\epsilon$ and φ^z for a line L of arbitrary orientation (recall, superscript z denoted a defect along the z-axis).

Second part: planar incompatibility components. Let us rewrite the result of Lemma 5 for an individual line L of $\mathcal{L}$ with arbitrary orientation. One can disregard all o^L_{ij}-terms for the evaluation of Eq. (4.6), since each line $L \in \mathcal{L}$ ends at the boundary (by Theorem 3). Then, from Lemma 5 the relevant (i.e., not-o^L_{ij}) components of the incompatibility in any section of $\Omega_{\mathcal{L}}$ orthogonal to L reduce to

$$\eta^\star_{mn}(\hat{x}^L)\tau_m\tau_n = \tau_i\Omega^\star_i\delta_{\hat{x}^L} + \tau_k\epsilon_{klj}\left(B^\star_j - \epsilon_{jpq}(\hat{x}^L_p - x_{0p})\Omega^\star_q\right)\partial_l\delta_{\hat{x}^L}, \tag{4.7}$$

$$\eta^\star_{mn}(\hat{x}^L)\tau_m\sigma_n = \sigma_i\Omega^\star_i\delta_{\hat{x}^L} + \frac{1}{2}\left(B^\star_j - \epsilon_{jpq}(\hat{x}^L_p - x_{0p})\Omega^\star_q\right)\tau_j\nu_i\partial_i\delta_{\hat{x}^L}, \tag{4.8}$$

$$\eta^\star_{mn}(\hat{x}^L)\tau_m\nu_n = \nu_i\Omega^\star_i\delta_{\hat{x}^L} - \frac{1}{2}\left(B^\star_j - \epsilon_{jpq}(\hat{x}^L_p - x_{0p})\Omega^\star_q\right)\tau_j\sigma_i\partial_i\delta_{\hat{x}^L}, \tag{4.9}$$

where τ_m is the unit tangent vector to L at $\hat{x}^L$ and σ_n, ν_n are two orthogonal unit vectors to τ_m in such a way that these three vectors form a right-handed orthonormal base – i.e., with ν_m an inner normal to C^L_ϵ (for the sake of notation simplicity the subscript L of $\tau_k, \sigma_k, \nu_k, \Omega^\star_j$ and $B^\star_i$ will be omitted for the proof).

From Definition 4, $\alpha^\star_{kj}(\hat{x}^L) := \left(B^\star_j\tau_k\delta_{\hat{x}^L} - \epsilon_{jpq}(\hat{x}_p - x_{0p})\Omega^\star_q\tau_k\right)\delta_{\hat{x}^L}$, and since $\partial_i\hat{x}^L_p = \tau_i\tau_p$ and $\tau_k\epsilon_{kij}\tau_i = 0$, we have

$$\epsilon_{kij}\partial_i\alpha^\star_{kj}(\hat{x}^L) = \tau_k\epsilon_{kij}\left(B^\star_j - \epsilon_{jpq}(\hat{x}^L_p - x_{0p})\Omega^\star_q\right)\partial_i\delta_{\hat{x}^L},$$

$$\partial_i\left(\frac{1}{2}\alpha^\star_{ll}\right)(\hat{x}^L) = \frac{1}{2}\tau_l\left(B^\star_l - \epsilon_{lpq}(\hat{x}^L_p - x_{0p})\Omega^\star_q\right)\partial_i\delta_{\hat{x}^L},$$

and hence, recalling that $\tau_k\epsilon_{kni} = \sigma_n\nu_i - \nu_n\sigma_i$, (4.7)-(4.9), we have

$$\eta^\star_{mn}(\hat{x}^L) = \tau_m\tau_n\left(\tau_i\Omega^\star_i\delta_{\hat{x}^L} + \epsilon_{kij}\partial_i\alpha^\star_{kj}(\hat{x}^L)\right) + \left[\tau_m\tau_k\epsilon_{kni}\partial_i\left(\frac{1}{2}\alpha^\star_{ll}(\hat{x}^L)\right)\right]_{m\leftrightarrow n}$$
$$+ \left[\tau_m\sigma_n(\Omega^\star_i\sigma_i) + \tau_m\nu_n(\Omega^\star_i\nu_i)\delta_{\hat{x}^L}\right]_{m\leftrightarrow n},$$

where symbol $A_{m\leftrightarrow n}$ denotes the sum of tensor A_{mn} with its transposed A_{nm}. By identity[9]

$$\tau_n\partial_i\alpha^\star_{kj} = \tau_k\partial_i\alpha^\star_{nj} \tag{4.10}$$

and by (2.15), we find that

$$\eta^\star_{mn}(\hat{x}^L) = \tau_m\tau_k\epsilon_{kij}\partial_i\alpha^\star_{nj}(\hat{x}^L) + \left[\tau_m\tau_k\epsilon_{kni}\partial_i\left(\frac{1}{2}\alpha^\star_{ll}(\hat{x}^L)\right)\right]_{m\leftrightarrow n}$$
$$+ \left[\delta_{mi}\left(\frac{1}{2}\tau_n\tau_j + \sigma_n\sigma_j + \nu_n\nu_j\right)\right]_{m\leftrightarrow n}\Theta^\star_{ij}(\hat{x}^L).$$

[9] Since $\alpha^\star$ is a concentrated measure it can be indifferently multiplied by any smooth function with compact support and unit values on L. Here, τ is implicitly multiplied by a cut-off function φ – see footnote by Assumption 2. Moreover since $\varphi\tau$ is constant in a neigbourhood of L, its derivative identically vanishes, from which the identity follows.

By Definition 4, since $\kappa^\star_{ll} = -\alpha^\star_{ll}/2$, and since $\delta_{nj} = \tau_n\tau_j + \sigma_n\sigma_j + \nu_n\nu_j$, we have

$$\begin{aligned}\eta^\star_{mn}(\hat{x}^L) = \quad & \tau_m\tau_k\epsilon_{kij}\partial_i\kappa^\star_{nj}(\hat{x}^L) + \tau_n\tau_k\epsilon_{kim}\partial_i\kappa^\star_{ll}(\hat{x}^L) \\ & + \left[\delta_{mi}\delta_{nj} - \frac{1}{2}\delta_{mi}\tau_n\tau_j\right]_{m\leftrightarrow n} \Theta^\star_{ij}(\hat{x}^L). \end{aligned} \tag{4.11}$$

Since $\tau_n\tau_k\epsilon_{kim}\partial_i\kappa^\star_{ll} = \tau_n\tau_k\epsilon_{kij}\partial_i\left(\kappa^\star_{mj} - \alpha^\star_{mj}\right)$, from $\Theta^\star_{mn} = \tau_m\tau_k\Theta^\star_{kn}$ and $\Theta^\star_{mj}\tau_j\tau_n = \tau_m\tau_n\Theta^\star_{jj}$ and by (4.10), Eq. (4.11) may be rewritten as

$$\begin{aligned}\eta^\star_{mn}(\hat{x}^L) = \quad & \left[\tau_m\tau_k\Theta^\star_{kn}(\hat{x}^L) + \tau_m\tau_k\epsilon_{kij}\partial_i\kappa^\star_{nj}(\hat{x}^L)\right]_{m\leftrightarrow n} \\ & - \left[\tau_m\tau_n\frac{1}{2}\left(\Theta^\star_{jj}(\hat{x}^L) + \epsilon_{kij}\partial_i\alpha^\star_{kj}\right)\right]_{m\leftrightarrow n}, \end{aligned} \tag{4.12}$$

proving Eq. (4.2) by the identity $\epsilon_{kij}\alpha^\star_{kj} = \epsilon_{kij}\kappa^\star_{kj}$, by line integration along L, by (4.6), Notation 5 and Definition 4. □

5 Summary and conclusion

In this paper, a formula (Eq. (4.2)) relating line-defect densities and elastic strain incompatibility in $3D$ has been proved at a scale of matter description where the defects are viewed as line singularities in a continuum. A similar formula (Eq. (1.1)), here named after Kröner's major accomplishments on the topic, had been derived formally in [10] using an elastic-plastic strain decomposition. Such a decomposition is here avoided on purpose. Instead, a global (i.e., valid on the entire domain, including its singularities) assumption (Assumption 2) is sought in order to validade the result. Let us define Kröner's expression of incompatibility [8, 10] by

$$inc\ \mathcal{E}^\star := \nabla \times \mathcal{E}^\star \times \nabla = \tilde{\eta}^\star := \Theta + \nabla^T \times \kappa \tag{5.1}$$

where Θ is the disclination density and κ the contortion tensor (see Definition 4). We have proved (Theorem 4) the following identity for a set $\mathcal{L}$ of skew defect lines:

$$inc\ \mathcal{E}^\star = \eta^\star := \left(\tilde{\eta}^\star - \frac{I}{2}\,\mathrm{tr}\ \tilde{\eta}^\star\right)_{\mathcal{L}}. \tag{5.2}$$

So, expression (5.2) should be considered as a relation to be satisfied by the elastic strain $\mathcal{E}^\star$ given a distribution of defects. Moreover, this formula shows that the only relevant components of the incompatibility tensor are those projected on the defect lines. This result has been proved in two steps: the main Theorem 4 relies on Lemma 5. The proof of this Lemma relies on a precise *pointwise* singularity growth assumption (namely Assumption 4 and Lemma 3) which themselves can be deduced from the *global* Assumption 2. Let us remark that such a global assumption, as formulated in terms of Radon measures defined on the whole domain, is a crucial step towards a general picture of dislocations and disclinations *across scales* since it allows us to work in a definite functional space (with appropriate topology, convergence, etc.).

It is interesting to note that the right-hand side of (5.2) shows the quantity inside the parenthesis as bearing the same form with respect to $\tilde{\eta}^\star$ as the form shown by the contortion $\kappa^\star$ with respect to $\alpha^\star$ (see Definition 4). Let us remark that in $2D$, the specific forms (5.2) and (2.15) are the deviatoric part of $\tilde{\eta}^\star$ and $\alpha^\star$, respectively. However, the general form $T = R - \frac{I}{2}\,\mathrm{tr}R$ is to be compared with the *Einstein field equations*[10] [4], where R is the (symmetric) Ricci tensor and T the (symmetric and solenoidal) "energy-momentum" tensor. Let us also observe that T may also be found written [11] as $T_{ij} = \epsilon_{ikm}\epsilon_{jln}K_{kmln}$ with K the curvature tensor associated to the Riemannian metric $g = I + 2\mathcal{E}^\star$. In the present case[11] we make the following identifications: $R = \tilde{\eta}^\star = \Theta + \nabla^T \times \kappa$ is a defect quantity and $T = \eta^\star = \nabla \times \mathcal{E}^\star \times \nabla$ is the strain incompatibility.

It should however be pointed out that with the formalism of differential geometry, relations such as (5.1) are classically *infered* [10–12]. The main difference with the present approach is that there the defect quantities are identified with geometrical quantities (i.e., chosen by definition), whereas here the defect tensors and the incompatibility tensor have a-priori their autonomous definition, and the identification is made by a proof under specific mathematical assumptions.

The work presented herein will be pursued to consider complex (and more realistic) sets of defects in $3D$. For instance dislocation and disclination loops and clusters can be described by means of sets of countably many defect segments, and hence appropriate extensions of the present theory should permit their complete treatment (including homogenization results).

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[10] Although Einstein equation is expressed in four dimensions, we mention this analogy to highlight the remarkable link pointed out by Kröner (among others) between dislocation theory and the field theory of General relativity (see [8]).

[11] The identifications hold on the set $\Omega_{\mathcal{L}}$ where the strain is smooth.

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