A distributional approach to the geometry of $2D$ dislocations at the mesoscale

Part A: General theory and Volterra dislocations

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Abstract

We develop a mathematical theory to represent dislocations and disclinations in single crystals at the mesoscopic scale by considering concentrated effects, governed by the distribution theory, combined with multiple-valued kinematic fields. Our approach provides a new understanding of the continuum theory of defects as developed by Kröner (1980) and other authors. The fundamental identity relating the incompatibility tensor to the Frank and Burgers vectors is proved in the $2D$ case under appropriate assumptions on the strain curl behaviour in the vicinity of the assumed isolated defect lines. In general our theory provides a rigorous framework for the treatment of crystal line defects at mesoscopic scale. Eventually this work will represent a basis to strengthen the mathematical theory of homogenization from mesoscopic to macroscopic scale.

1 Introduction

Dislocations can be considered as the most complex class of defects for several kinds of single crystals (Völkl & Müller 1994; Jordan *et al.* 2000) and the development of a relevant and accurate physical model represents a key issue with a view to reducing the dislocation density in the crystal by acting on the temperature field and the solid-liquid interface shape during the growth process (Dupret and Van den Bogaert 1994).

However the dislocation models available in the literature, such as the model of Alexander and Haasen (1986), are often based on a rather crude extension of models initially developed for polycrystals (as usual metals and ceramics are). In this case, some particular features of single crystals, such as material anisotropy or the existence of preferential glide planes, can be taken into account up to some extent, but the fundamental physics of dislocations in single crystals cannot be captured. In fact, dislocations are lines that either form loops, or end at the single crystal boundary, or join together at some locations, while each dislocation segment has a constant Burgers vector which exhibits additive properties at dislocation junctions. These properties play a fundamental role in the modelling of line defects in single crystals and induce key conservation laws at the macro-scale (typically defined by the crystal diameter). On the contrary, no dislocation conservation law exists at the macro-scale for polycrystals since dislocations can abruptly end at grain boundaries inside the medium without any conservation law holding across these interfaces.

Aware of these principles and of the pioneer works of Volterra (1907) and Cosserat (1909), Burgers (1939), Eshelby (1956, 1966), Eshelby, Frank & Nabarro (1951), Kondo (1952), Nye (1953), and Kröner (1980) among other authors (Bilby 1960; Nabarro 1967; Mura 1987) consider a tensorial density to model dislocations in single crystals at the macro-scale, in order to take into account both the dislocation orientation and the associated Burgers vector (cf. the survey contributions of Kröner 1980, 1990, Kleinert 1989 and Maugin 2003). However, in these works, the relationship between the macro-scale crystal properties and the basic physics governing the nano-scale (defined by the inter-atomic distance) is not completely justified from a mathematical viewpoint. Therefore, to well define the concept of tensorial dislocation density, we here introduce the meso-scale as defined by some average distance between the dislocations. The laws governing the dislocation behaviour are modelled at the nano-scale, while the meso-scale (defined from the nano-scale by ensemble averaging or by averaging over a representative volume (Kröner 2001)) defines the "dislocated continuous medium", where each dislocation is viewed as a line and the interactions between dislocations can be modelled while the laws of linear elasticity govern the adjacent medium.

The present paper focuses on meso-scale modelling with a further view to clarifying the homogenization process from meso- to macro-scale. This latter issue is addressed in the companion work of Van Goethem & Dupret (2009*a*). Since dislocations are lines at the meso-scale, concentrated effects must be introduced in the mesoscopic model as governed by the distribution theory (Schwartz 1957). In addition, since integration around the dislocations generates a multiple-valued displacement field with the dislocations as branching lines, multivalued functions must be considered (cf, e.g., Almgren 1986). This combination of distributional effects and multivaluedness is a key feature of the dislocation theory at the meso-scale but unfortunately the difficulties resulting from this mathematical association have not well been addressed so far in the literature (see also Thom 1980). As an example, non-commuting differentiation operators are freely introduced without any justification by Kleinert (1989). Therefore, the principal objective of this paper is to provide a strong mathematical foundation to the meso-scale theory of dislocations, showing how the distribution and geometric measure theories can be correctly used with multiple-valued fields.

In fact, a key modelling issue arises from the fact that homogenization from meso- to macro-scale has no meaning for multiple-valued fields such as displacement and rotation, since this operation is exclusively allowed for additive (or extensive) fields such as stress, energy density or heat flux. This observation becomes obvious when homogenization is defined by an ensemble averaging procedure, since multiple-valued fields are mathematically defined as extended functions which cannot be added since their "domains" depend on the defect line locations. This consideration justifies the present analysis. For the sake of generality, disclinations, which represent a second but rarer kind of line defect, with in addition a multiple-valued rotation field, are here considered together with dislocations.

In the literature the macroscopic dislocation density is classically defined as the curl of the plastic distortion (Head *et al.* 1993; Cermelli & Gurtin 2001; Koslowski *et al.* 2002), following a postulated distortion decomposition into elastic and plastic parts. However, this decomposition cannot be rigorously justified (contrarily to the strain decomposition) since elastic and plastic rotations cannot be set apart without some hidden arbitrariness. In contrast, the present paper paves the way for a rigourous definition and treatment of the macroscopic dislocation density, as obtained from well-defined mesoscopic fields under precise geometric-measure model assumptions, and from which the distortion decomposition can be obtained together with its relationship with the dislocation density (Van Goethem & Dupret 2009*a*).

The present paper is restricted to the mesoscopic $2D$ theory for a set of assumed isolated dislocations and/or disclinations. This theory is extended to the case of countably many dislocations in Van Goethem & Dupret (2009*b*) where the appropriate mathematical objects and functional spaces are ultimately defined for homogenization to the macro-scale. This latter paper will be referred to as Part B in the sequel. Extension to the dynamic $3D$ case is under investigation. Eventually, the complete link between the mesoscopic and macroscopic behaviours of single crystals with line defects should be derived from these developments. In §2, the scaling analysis summarized in this introduction is detailed and the basic concepts used to represent the dislocated continuous medium are introduced. The general mathematical theory is developped in §3, while in §4, the $2D$ distributional theory of the dislocated continuous medium is established in the case of isolated parallel dislocations/disclinations. Conclusions are drawn in §5.

2 Multiscale analysis of dislocations

2.1 Nano-scale analysis: crystalline lattice

At the nano-scale the characteristic length is the interatomic distance and the reference body is a perfect lattice. Given a dislocation in the general sense (dislocation and/or disclination), the atomic arrangement at time t generaly differs from the reference arrangement, but however the atom displacements are not uniquely defined (Kleinert 1989). Indeed any atom of the reference configuration can in principle be selected to define the displacement of a given atom of the actual configuration which therefore is a multivalued discrete mapping. Moreover, in general, the dislocation position cannot be determined precisely at the atomic level since several dislocation locations in the actual crystal can be associated with the same picture of the atom positions. In fact the defect should be understood as located inside a nanoscopic lattice region.

2.2 Meso-scale analysis: dislocated continuous medium an associated reference configurations

At the meso-scale the characteristic length is some average distance between two neighbour dislocation lines. This scale is the one on which this paper focuses, in the framework of $2D$ linear elasticity. At time t, the body is referred to as $\mathcal{R}^{\star}(t)$ as corresponding a random sample corresponding to a given growth experiment.

A *reference configuration* $\mathcal{R}_0^\star$ with respect to the actual configuration $\mathcal{R}^\star(t)$ is any selected one-to-one transformation of $\mathcal{R}^\star(t)$. $\mathcal{R}_0^\star$ may be chosen as being the body at any given (past or future) time t_0 or in contrast be a fictitious transformation of $\mathcal{R}^\star(t)$, and the displacement and rotation fields on $\mathcal{R}^\star(t)$ ($u_i^\star$ and $\omega_k^\star$) are then defined with respect to the chosen $\mathcal{R}_0^\star$. In the present $\mathcal{R}_0^\star$ will always be defined as stress-free and without dislocations, but its selection will remain arbitrary up to this restriction and hence (and this is a keypoint) the defect governing laws must be invariant with respect to the choice of $\mathcal{R}_0^\star$.

It will be precised later that displacement and rotation are multivalued fields at the mesoscale, and hence are defined on a set called a Riemann foliation F (and not of $\mathcal{R}_0^\star$). The set F can be univoquely associated to $\mathcal{R}^\star(t)$ if a cut is introduced in the foliation in order to select one particular branch of the displacement and rotation.

In view of multivaluedness and the existence of a family of acceptable reference configurations, the main field of our analysis is the assumed linear elastic strain which is clearly single valued and independent of the choice of $\mathcal{R}_0^\star$. The Burgers vector $B_i^\star$ and Frank vector $\Omega_i^\star$ are key invariant quantities related to the jump of the multivalued displacement and rotation fields, as directly derived from the linear strain. Their precise definition will be given in §3.

At this stage, some definitions and assumptions have to be introduced.

Notations 2.1 *In the following sections, the assumed open domain is denoted by Ω (in practice but not necessarily Ω is bounded), the defect line(s) are indicated by $\mathcal{L} \subset \Omega$, and $\Omega_{\mathcal{L}}$ is the chosen symbol for $\Omega \setminus \mathcal{L}$, which is also assumed to be open.*

Definition 2.1 ($3D$ mesoscopic defect lines) *At the meso-scale, a $3D$ set $\mathcal{L}$ of dislocations and/or disclinations is defined as a set of isolated rectifiable arcs $L^{(k)}$, $k \in \mathcal{I}$, without multiple points except possibly their extremities and on which the linear elastic strain is singular. Here a set of isolated arcs means a set of arcs: (i) whose extremeties form a set of isolated points of Ω in the classical sense and (ii) such that each point $\hat{x}$ of these arcs except their extremities can be located in a smooth surface $S(\hat{x})$ bounded by a loop $C(\hat{x})$ and such that $S(\hat{x}) \setminus \hat{x} \in \Omega_{\mathcal{L}}$.*

Assumption 2.1 ($3D$ mesoscopic elastic strain) *Henceforth we will assume that the linear strain $\mathcal{E}_{mn}^\star$ is a given symmetric $L^1(\Omega)$ tensor* [1] *prolonged by 0 on the dislocation set $\mathcal{L}$ and compatible on $\Omega_{\mathcal{L}}$. In other words, the incompatibility tensor, as defined by*

$$\eta_{kl}^\star := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathcal{E}_{mn}^\star, \tag{2.1}$$

where derivation is intended in the distribution sense, is assumed to vanish everywhere on $\Omega_{\mathcal{L}}$.

Let us now introduce the dislocation and disclination density tensors ($\Lambda_{ij}^\star$ and $\Theta_{ij}^\star$) which are the basic physical tools that will be used to model defect density at the meso-scale.

Definition 2.2 (defect densities)

DISCLINATION DENSITY: $$\Theta_{ij}^\star := \sum_{k\in\mathcal{I}\subset\mathbb{N}} \Omega_j^{\star(k)}\tau_i^{(k)}\delta_{L^{(k)}} \, (i,j = 1\cdots3), \tag{2.2}$$

DISLOCATION DENSITY: $$\Lambda_{ij}^\star := \sum_{k\in\mathcal{I}\subset\mathbb{N}} B_j^{\star(k)}\tau_i^{(k)}\delta_{L^{(k)}} \, (i,j = 1\cdots3), \tag{2.3}$$

[1]It should be noted that $L^q(\Omega)$ with any $1 \le q < 2$ would hold as well.

where symbol $\delta_{L^{(k)}}$ is used to represent the one-dimensional Hausdorff measure [2] density concentrated on the rectifiable arc $L^{(k)}$ with the tangent vector $\tau_i^{(k)}$ defined almost everywhere on $L^{(k)}$, while $\Omega_j^{\star(k)}$ and $B_j^{\star(k)}$ denote the Frank and Burgers vectors of $L^{(k)}$, respectively.

The present paper and Part B address the $2D$ problem only. Generalization of our theory to the $3D$ case will be considered in further publications.

Definition 2.3 **($2D$ mesoscopic defect lines)** *At the meso-scale, a $2D$ set $\mathcal{L}$ of dislocations and/or disclinations is defined as a set of isolated parallel lines $L^{(i)}$, $i \in \mathcal{I}$, on which the linear elastic strain is singular. In the sequel, these lines will be assumed as parallel to the z-axis.*

More complex sets of $2D$ defect lines are considered in Part B.

Remark 2.1 *The term $2D$ here refers to the structure of the countable union of points, denoted by l_0, located at the intersection between $\mathcal{L}$ and the $z = z_0$-plane. In this context, the strain is said $2D$ if it solely depends upon the coordinates $x_\alpha \in \Omega_{z_0}$ $(\alpha = 1, 2)$. In that case, the displacement and rotation fields will generaly depend on the three space variables.*

Notations 2.2 **($2D$ defect densities and incompatibility)** *In $2D$, the vectors $\eta_k^\star, \Theta_k^\star$ and $\Lambda_k^\star$ will denote the tensor components $\eta_{zk}^\star, \Theta_{zk}^\star$ and $\Lambda_{zk}^\star$. Greek indices will be used to denote the values $1, 2$ (instead of the Latin indices used in $3D$ to denote the values $1, 2$ or 3). Moreover, $\epsilon_{\alpha\beta}$ will denote the permutation symbol $\epsilon_{z\alpha\beta}$.*

The disclination and dislocation density tensors $\Theta_k^\star$ and $\Lambda_k^\star$ will be shown in this paper to be related by a fundamental distributional relation to the strain incompatibility $\eta_k^\star$. In fact, under suitable assumptions on the strain curl (the so-called Frank tensor), the following theorem will be proved in the $2D$ linear elastic case.

Main theorem:
incompatibility decomposition for $2D$ isolated defect lines.

The mesoscopic strain incompatibility for a set of isolated parallel rectilinear dislocations $\mathcal{L}$ writes as

$$\eta_k^\star = \Theta_k^\star + \epsilon_{\alpha\beta}\partial_\alpha\kappa_{k\beta}^\star, \tag{2.4}$$

where $\kappa_{k\beta}^\star$ denotes the contortion tensor,

$$\kappa_{k\beta}^\star = \delta_{kz}\alpha_\beta^\star - \frac{1}{2}\alpha_z^\star\delta_{k\beta}, \tag{2.5}$$

with $\alpha_k^\star$ standing for an auxiliary defect density vector,

$$\alpha_k^\star := \Lambda_k^\star - \delta_{k\alpha}\epsilon_{\alpha\beta}\Theta_z^\star(x_\beta - x_{0\beta}), \tag{2.6}$$

and where x_0 is a selected reference point in Ω.

[2]The reader is referred to Mattila (1995) for details on Hausdorff measures.

The latter result appears in Kröner's work (1981) under assumptions which are not compatible with our approach. In fact, in his work this result follows in a straightforward manner from an "elastic-plastic" displacement gradient (or distortion) decomposition postulate, which itself requires the selection of a particular reference configuration and does not properly handle the intrinsic multivaluedness of the mesoscopic problem. Moreover, in our result the link between the defect densities and the Frank and Burgers vectors is clearly made, and precise assumptions on the strain field and the admissible defect structures are provided in order to validate the result.

The above theorem will be generalized in Part B to the case of a countable union of parallel rectilinear dislocations. Eventually, the required "single-valued" distributional fields will be defined in the appropriate functional spaces for their homogenization to the macro-scale.

3 Multiple-valued fields and line invariants in the $3D$ case; distributions as a modelling tool at the meso-scale

Notations 3.1 *In the following sections, $\hat{x}$ or $\hat{x}_i$ will denote a generic point of the defect line(s), x or x_i a generic point of $\Omega_{\mathcal{L}}$, and x_0 or x_{0i} a given fixed reference point of $\Omega_{\mathcal{L}}$. When x and $\hat{x}$ are used together, $\hat{x}$ denotes the projection of x onto a given defect line in an appropriate sense and $\hat{\nu}_i := \nu_i(\hat{x}, x)$ is the unit vector joining $\hat{x}$ to x. The symbol $\odot_\epsilon$ is intended for a set of diameter 2ϵ enclosing the region $\mathcal{L}$. More precisely, $\odot_\epsilon$ is defined as the intersection with Ω of the union of all closed spheres of radius ϵ centred on $\mathcal{L}$:*

$$\odot_\epsilon := \Omega \cap \bigcup_{\hat{x} \in \mathcal{L}} B[\hat{x}, \epsilon].$$

If $\mathcal{L}$ consists of an single line L, $\odot_\epsilon$ is a tube of radius ϵ enclosing L.

Notations 3.2 *In the sequel, considering a surface S of Ω crossed by a dislocation L at $\hat{x}$ and bounded by the curve C, symbols dC, dL, and dS will denote the $1D$ Hausdorff measures on C and L, and the $2D$ Hausdorff measure on S, respectively, with τ_j standing for the unit tangent vector to L at $\hat{x}$ (when it exists). In some cases (having fractal curves in mind) the symbols dx_k and $dS_i := \epsilon_{ijk} dx_j^{(1)} dx_k^{(2)}$ will stand for infinitesimal vectors oriented along C and normal to S, respectively, with in addition $dC_l(x) := \epsilon_{lmn} dx_m \tau_n$ denoting an infinitesimal vector normal to C when $\tau_n = \tau_n(\hat{x})$ exists.*

In the present section, the strain is assumed to satisfy assumption 2.1 and to be smooth away from $\mathcal{L}$.

3.1 Distributional analysis of $3D$ multiple-valued fields

In general, a multivalued function from $\Omega_{\mathcal{L}}$ to $\mathbb{R}^N$ is defined as consisting of a pair of single-valued mappings with appropriate properties:

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

where F is the associated Riemann foliation (Almgren 1986). 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 path classes inside $\Omega_{\mathcal{L}}$ from a given $x_0 \in \Omega_{\mathcal{L}}$ with homotopy as equivalence relationship. Accordingly, a multivalued function will be called of index n on $\Omega_{\mathcal{L}}$ if its n-th differential is single-valued on $\Omega_{\mathcal{L}}$. No other kinds of multifunctions are considered in this work, whether $\mathcal{L}$ is a single line L or a more complex set of defect lines (with possible branchings, etc.).

Notations 3.3 *The symbol $\partial_j^{(s)}$ is used for partial derivation of a single- or multiple-valued function whose domain is restricted to $\Omega_{\mathcal{L}}$. Locally around $x \in \Omega_{\mathcal{L}}$, for smooth functions, the meanings of $\partial_j^{(s)}$ and the classical ∂_j are the same, whereas on the entire Ω the partial derivation operator ∂_j only applies to single-valued fields and must be understood in the distributive sense. A defect-free subset U of Ω is an open set such that $U \cap \mathcal{L} = \emptyset$, in such a way that $\partial_j^{(s)}$ and ∂_j coincide on U for every single- or multiple-valued index-*1 *function.*

In the following essential definition generalizing the concept of rotation gradient to dislocated media, the strain is considered as a distribution on Ω.

Definition 3.1 (Frank tensor) *The Frank tensor $\overline{\partial}_m \omega_k^\star$ is defined as the following distribution on Ω:*

$$\overline{\partial}_m \omega_k^\star := \epsilon_{kpq} \partial_p \mathcal{E}_{qm}^\star, \tag{3.1}$$

in such a way that

$$< \overline{\partial}_m \omega_k^\star, \varphi > := - \int_\Omega \epsilon_{kpq} \mathcal{E}_{qm}^\star \partial_p \varphi dV, \tag{3.2}$$

with φ a smooth test-function with compact support in Ω.

In fact, in the vicinity of a defect line the tensorial distribution $\overline{\partial}_m \omega_k^\star$ is the finite part of an integral when acting against test-functions. Indeed, since $\partial_p \mathcal{E}_{qm}^\star$ might be non $L^1(\Omega)$-integrable in view of its possibly too strong singularity near the defect lines, instead of being directly calculated as an integral, $< \epsilon_{kpq} \partial_p \mathcal{E}_{qm}^\star, \varphi >$ must be calculated on Ω as the limit

$$\lim_{\epsilon \longrightarrow 0} \left(\int_{\Omega \setminus \odot_\epsilon} \epsilon_{kpq} \partial_p \mathcal{E}_{qm}^\star \varphi dV + \int_{\partial \odot_\epsilon \cap \Omega} \epsilon_{kpq} \mathcal{E}_{qm}^\star \varphi dS_p \right), \tag{3.3}$$

where the second term inside the parenthesis is precisely added in order to achieve convergence. One readily sees after integration by parts that (3.3) is equal to (3.2) provided $\lim_{\epsilon \longrightarrow 0} \Omega \setminus \odot_\epsilon = \Omega_{\mathcal{L}}$ (which is a general hypothesis limiting the acceptable defect lines and certainly holds true for the lines satisfying definition 2.1).

Considering the possibly index-1 multivalued rotation vector $\omega_k^\star$, it should be observed from definition 3.1 that $\overline{\partial}_m \omega_k^\star = \partial_m^{(s)} \omega_k^\star$ on $\Omega_{\mathcal{L}}$ as a consequence of the classical relationship between infinitesimal rotation and deformation derivatives. However, $\overline{\partial}_m \omega_k^\star$ is defined by (3.1) as a distribution and therefore concentrated effects on $\mathcal{L}$ and its infinitesimal vicinity have to be added to $\partial_m^{(s)} \omega_k^\star$, justifying the use of the symbol

$\overline{\partial}_m\omega_k^\star$ instead of $\partial_m\omega_k^\star$ without giving to $\overline{\partial}_m$ the meaning of an exact derivation operator. In particular, it may be observed that the identical vanishing of $\partial_m^{(s)}\omega_k^\star$ on $\Omega_\mathcal{L}$ does not necessarily imply that the distribution $\overline{\partial}_m\omega_k^\star$ vanishes as well. In fact from (3.3), it can be shown in that case that

$$< \overline{\partial}_m\omega_k^\star, \varphi >= \lim_{\epsilon\to 0}\int_{\partial\odot_\epsilon\cap\Omega}\epsilon_{kpq}\mathcal{E}^\star_{qm}\varphi dS_p = -\int_\Omega \epsilon_{kpq}\mathcal{E}^\star_{qm}\partial_p\varphi dV, \tag{3.4}$$

which is generally non-vanishing. Finally, as soon as the definition of the tensor distribution $\overline{\partial}_m\omega_k^\star$ is given, so are the distributional derivatives of $\overline{\partial}_m\omega_k^\star$:

$$< \partial_l\overline{\partial}_m\omega_k^\star, \varphi >= - < \overline{\partial}_m\omega_k^\star, \partial_l\varphi >= \int_\Omega \epsilon_{kpn}\mathcal{E}^\star_{mn}\partial_p\partial_l\varphi dV. \tag{3.5}$$

3.2 $3D$ rotation and displacement vectors

The rotation vector is defined from the linear strain together with the rotation at a given point x_0. From this construction follows an invariance property of $\omega_k^\star$ as a multifunction (recalling that multivaluedness takes its origin from the existence of defect lines which render the strain incompatible on the entire Ω).

Starting from the distributive definition 3.1 of $\overline{\partial}_m\omega_k^\star$, the form $\overline{\partial}_m\omega_k^\star\, d\xi_m$ is integrated along a regular parametric curve $\Gamma\subset\Omega_\mathcal{L}$ with endpoints $x_0, x\in\Omega_\mathcal{L}$. For selected x_0 and $\omega_{0k}^\star$, the multivalued rotation vector is defined as [3]

$$\omega_k^\star = \omega_k^\star(\#\Gamma;\omega_0^\star) = \omega_{0k}^\star + \int_\Gamma \overline{\partial}_m\omega_k^\star d\xi_m,$$

where $\#\Gamma$ is the equivalence class of all regular curves homotopic to Γ in $\Omega_\mathcal{L}$. Indeed, from strain compatibility in $\Omega_\mathcal{L}$, i.e. from relation (2.1), it is clear that $\omega_k^\star$ is a function of $\#\Gamma$ only. Consider now a regular parametric loop C (in case C is a planar loop, it is a Jordan curve) and the equivalence class $\#C$ of all regular loops homotopic to C in $\Omega_\mathcal{L}$. Here, the extremity points play no role anymore and two loops are equivalent if and only if they can be continuously transformed into each other in $\Omega_\mathcal{L}$. The jump of the rotation vector $\omega_k^\star$ along $\#C$ depends on $\#C$ only and is calculated as [4]

$$[\omega_k^\star] = [\omega_k^\star](\#C) = \int_C \overline{\partial}_m\omega_k^\star d\xi_m. \tag{3.6}$$

The following developments address the displacement field multivaluedness as a mere consequence of strain incompatibility. The procedure defining the displacement vector from the rotation vector by means of line integrals is classical in linear elasticity. The following tensor plays in the construction of the displacement field a role analogous to $\overline{\partial}_m\omega_k^\star$ in the construction of the rotation field.

Definition 3.2 (Burgers tensor) *For a selected reference point $x_0\in\Omega_\mathcal{L}$, the Burgers tensor is defined on the entire domain Ω as the distribution*

$$\overline{\partial}_l b_k^\star(x;x_0) := \mathcal{E}^\star_{kl}(x) + \epsilon_{kpq}(x_p - x_{0p})\overline{\partial}_l\omega_q^\star(x). \tag{3.7}$$

[3] For a non-smooth strain, integration is to be understood in the distribution sense.

[4] We note that C could be non rectifiable, i.e. of infinite length. Integrals on fractal curves and the related Stokes' and Gauss-Green's theorems are analysed by Harrison & Norton (1992), where it is shown by the $\mathcal{C}^\infty$ smoothness of the differential form $\overline{\partial}_m\omega_k^\star dx_m$ on $\Omega_\mathcal{L}$ that (3.6) still holds even when the Hausdorff dimension of C is higher than 1.

The Burgers tensor can be integrated in the same way as the Frank tensor along any parametric curve Γ, providing for selected $\omega^\star_{0k}$ and $u^\star_{0k}$ the index 2-multivalued displacement vector $u^\star_k$:

$$u^\star_k = u^\star_k(x, \#\Gamma; \omega^\star_0, u^\star_0) = u^\star_{0k} + \epsilon_{klm}\omega^\star_l(\#\Gamma; \omega^\star_0)(x_m - x_{0m}) + \int_\Gamma \overline{\partial}_l b^\star_k(\xi) d\xi_l,$$

which is a function of x and $\#\Gamma$ only (this following from (2.1) and (3.7)). It may be observed that $\overline{\partial}_l b^\star_k$ and the vector

$$b^\star_k = b^\star_k(\#\Gamma; u^\star_0) = u^\star_k - \epsilon_{klm}\omega^\star_l(x_m - x_{0m}) \tag{3.8}$$

are related in the same way as $\overline{\partial}_m\omega^\star_k$ and $\omega^\star_k$, including the fact that $\overline{\partial}_l b^\star_k = \partial^{(s)}_l b^\star_k$ on $\Omega_{\mathcal{L}}$. The jumps of $b^\star_k$ along $\#C$ and of $u^\star_k$ at x along $\#C$ (which depend on $\#C$ only) are calculated as

$$[b^\star_k](\#C; x_0) = [u^\star_k](x; \#C; x_0) - \epsilon_{klm}[\omega^\star_l](\#C)(x_m - x_{0m}) = \int_C \overline{\partial}_l b^\star_k d\xi_l. \tag{3.9}$$

Let us now focus on the case of a given isolated defect line $L^{(i)}$, $i \in \mathcal{I}$. The jump $[\omega^\star_k]$ of the rotation vector $\omega^\star_k$ around $L^{(i)}$ is defined as the jump of $\omega^\star_k$ along $\#C(\hat{x})$, with $\hat{x}$ a point of $L^{(i)}$ and $C(\hat{x})$ a loop enclosing once the defect line $L^{(i)}$ and no other defect line as specified in definition 2.1. It turns out that this jump is the same for any $\hat{x}$ and suitable $C(\hat{x})$. Similarly, the jump $[b^\star_k]$ of the vector $b^\star_k$ around $L^{(i)}$ is defined as the jump of $b^\star_k$ along $\#C(\hat{x})$ and is also the same for any $\hat{x}$ and suitable $C(\hat{x})$, given x_0. In fact, the following result is well-known (Kleinert 1989).

Theorem 3.1 (Weingarten's theorem) *The rotation vector $\omega^\star_k$ is an index-1 multifunction on $\Omega_{\mathcal{L}}$ whose jump $\Omega^\star_k := [\omega^\star_k]$ around the isolated defect line $L^{(i)}$, $i \in \mathcal{I}$, is an invariant of this line. Moreover, for a given x_0, the vector $b^\star_k$ is a multifunction of index 1 on $\Omega_{\mathcal{L}}$ whose jump $B^\star_k := [b^\star_k]$ around $L^{(i)}$ is an invariant of this line.*

From this result, the Frank and Burgers vectors are defined as invariants of $L^{(i)}$.

Definition 3.3 (Frank and Burgers vectors) *The Frank vector of an isolated defect line $L^{(i)}$, $i \in \mathcal{I}$, is the invariant*

$$\Omega^\star_k := [\omega^\star_k], \tag{3.10}$$

while for a given reference point x_0 its Burgers vector is the invariant

$$B^\star_k := [b^\star_k] = [u^\star_k](x) - \epsilon_{klm}\Omega^\star_l(x_m - x_{0m}). \tag{3.11}$$

A defect line with non-vanishing Frank vector is called a disclination while a defect line with non-vanishing Burgers vector is called a dislocation. Clearly a disclination should always be considered as a dislocation by appropriate choice of x_0 while the reverse statement is false since $\Omega^\star_k$ might vanish. In fact, two distinct reference points x_0 and x'_0 define two distinct Burgers vectors, obeying the relation $B^\star_k - B'^\star_k = \epsilon_{klm}(x_{0m} - x'_{0m})\Omega^\star_l$ (noting that $B^\star_k\Omega^\star_k$ is an invariant independent of the arbitrary choice of x_0). Therefore, for a non-zero Frank vector, the vanishing of the Burgers vector depends on the arbitrary choice of x_0. This is why in the present paper, the word "dislocation" means in the general sense a dislocation and/or a disclination. A pure dislocation is a dislocation with vanishing Frank vector.

Remark 3.1 *It should be emphasized that the assumption of isolated defect lines is required to construct appropriate enclosing loops in order to define their Frank and Burgers vectors. In Part B this assumption will be removed for a countable set of parallel defect lines under appropriate assumptions on the Frank tensor.*

In general, every defect line will contribute to the rotation and displacement multivaluedness, and hence these latter fields are defined over $\Omega_{\mathcal{L}}$ and do not share the structure of a vector space. In other words, the displacement and rotation fields cannot be added since their domains depend on the defect line locations.

Therefore, besides the strain field which is the seminal ingredient of the present theory, the Burgers and Frank tensors appear as fundamental quantities able to characterize the amount of defects on each single line or in the whole dislocated crystal. Together with the geometry of the defect set, these vectors provide the key defect measures called the dislocation and disclination density tensors (which now belong to a vector space). Accordingly, the following well-known result can be readily shown and is fundamental in the framework of our investigations since it implies conservation laws at the meso- and macro-scales.

Theorem 3.2 (conservation laws) *Single disclination and dislocation lines are always closed or end at the boundary of Ω. Moreover, in all cases,*

$$\partial_i \Theta^\star_{ij} = \partial_i \Lambda^\star_{ij} = 0.$$

4 Distributional analysis of incompatibility for a single rectilinear dislocation

4.1 The $2D$ model for rectilinear dislocations

$2D$ elasticity means that the strain $\mathcal{E}^\star_{ij}$ is independent of the "vertical" coordinate z. However this assumption introduces no restriction on the dependence of the multiple-valued displacement and rotation fields upon z.

Notations 4.1 *In this §4.1, the single defect line L is assumed to be located along the z-axis. The two planar coordinates will be denoted by (x, y) or x_α. The projection of $x = (x_\alpha, z)$ on L is $\hat{x} = (0, 0, z)$ and $(\nu_\alpha, 0)$ stands for the unit vector from $\hat{x}$ to x. Symbols (e_x, e_y, e_z) or (e_α, e_z) denote the Cartesian base vectors, while (e_r, e_θ, e_z) denote the local cylindrical base vectors. For a planar curve C, the notation $dC_\alpha(x) = \epsilon_{\alpha\beta} dx_\beta$ is used for an infinitesimal vector parallel to the curve normal.*

Let us observe that many fields are singular at the origin and that Ω_L is in fact the domain where the laws of linear elasticity apply. Moreover, the strain can be decomposed into three tensors:

$$\mathcal{E}^\star_{ij} = \underbrace{\delta_{\alpha i}\delta_{\beta j}\mathcal{E}^\star_{\alpha\beta}}_{planar\ strain} + \underbrace{\left(\delta_{iz}\delta_{j\gamma}\mathcal{E}^\star_{\gamma z} + \delta_{jz}\delta_{i\gamma}\mathcal{E}^\star_{\gamma z}\right)}_{3D\ shear} \underbrace{+\delta_{iz}\delta_{jz}\mathcal{E}^\star_{zz}.}_{pure\ vertical\ compression/dilation}$$

Lemma 4.1 ($2D$ compatibility) *In Ω_L, from $2D$ strain compatibility, there are real numbers K, a_α and b such that*

$$\left\{ \begin{array}{l} \epsilon_{\alpha\gamma}\epsilon_{\beta\delta}\partial_\alpha\partial_\beta\mathcal{E}^\star_{\gamma\delta} = 0, \\ \epsilon_{\alpha\beta}\partial_\alpha\mathcal{E}^\star_{\beta z} = K, \\ \mathcal{E}^\star_{zz} = a_\alpha x_\alpha + b. \end{array} \right. \tag{4.1}$$

This lemma is easily proved from assumption 2.1. □

Remark 4.1 *The present theory does not make use of the linear elasticity constitutive laws and the momentum and energy conservation laws, since in the framework of Continuum Mechanics arbitrary body forces and heat supply can always be applied to the medium. Moreover, the sum of these two body contributions and the unsteady terms governing the medium dynamics can generally be nonsmooth, and hence the stress and heat flux derivatives have to be treated as mathematical distributions thereby providing a physical justification to our approach.*

The remaining of this section will be devoted to present the three classical examples of $2D$ line-defects for which the medium is assumed to be steady, body force free and isothermal (detail is given in Van Goethem 2007).

- *Pure screw dislocation.* The displacement and rotation vectors write as

$$u_i^\star e_i = \frac{B_z^\star \theta}{2\pi} e_z \quad \text{and} \quad \omega_i^\star e_i = \frac{1}{2}\nabla \times u_i^\star e_i = \frac{B_z^\star}{4\pi r} e_r, \tag{4.2}$$

in such a way that the jump $[\omega_i^\star]$ vanishes identically, while the Cartesian strain is divergence-free on Ω and writes as

$$[\mathcal{E}_{ij}^\star] = \frac{-B_z^\star}{4\pi r^2} \begin{bmatrix} 0 & 0 & y \\ 0 & 0 & -x \\ y & -x & 0 \end{bmatrix}. \tag{4.3}$$

Moreover, inside Ω_L, the Frank tensor writes as

$$[\overline{\partial}_m \omega_k^\star] = \frac{-B_z^\star}{4\pi r^2} \begin{bmatrix} \cos 2\theta & \sin 2\theta & 0 \\ \sin 2\theta & -\cos 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{4.4}$$

- *Pure edge dislocation.* The displacement vector is

$$u_i^\star e_i = \frac{-B_y^\star(\log \frac{r}{R} + 1)}{2\pi} e_x + \frac{B_y^\star \theta}{2\pi} e_y,$$

while the rotation $\omega_i^\star$ vanishes together with its jump. The Cartesian strain (which requires additional regular terms to correspond to balanced stresses) writes as

$$[\mathcal{E}_{ij}^\star] = \frac{-B_y^\star}{2\pi r^2} \begin{bmatrix} x & y & 0 \\ y & -x & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{4.5}$$

noting that the tensor $\overline{\partial}_m \omega_k^\star$ vanishes identically inside Ω_L.

- *Wedge disclination.* The rotation vector is

$$\omega_i^\star e_i = \frac{\Omega_z^\star \theta}{2\pi} e_z,$$

with the multiple-valued planar displacement field given by

$$\begin{aligned} u_x^\star - i u_y^\star = {} & \tfrac{\Omega_z^\star}{4\pi}(1-\nu^*) x \ln(\tfrac{r}{R}) - \tfrac{\Omega_z^\star}{8\pi}(1+\nu^*) x - \tfrac{\Omega_z^\star}{2\pi} y\theta \\ & -i\left[\tfrac{\Omega_z^\star}{4\pi}(1-\nu^*) y \ln(\tfrac{r}{R}) - \tfrac{\Omega_z^\star}{8\pi}(1+\nu^*) x + \tfrac{\Omega_z^\star}{2\pi} x\theta\right] \end{aligned} \tag{4.6}$$

(where ν^* stands for the $2D$ Poisson coefficient, to be considered as an arbitrary constant together with R) and with a vanishing Burgers vector:

$$B_x^\star - iB_y^\star = [u_x^\star] - i[u_y^\star] + \Omega_z^\star(y + ix) = 0.$$

The Cartesian strain writes as

$$[\mathcal{E}_{ij}^\star] = \frac{\Omega_z(1-\nu^\star)}{4\pi}\begin{bmatrix} (\log\frac{r}{R}+1) & 0 & 0 \\ 0 & (\log\frac{r}{R}+1) & 0 \\ 0 & 0 & 0 \end{bmatrix}$$
$$-\frac{\Omega_z^\star(1+\nu^*)}{8\pi}\begin{bmatrix} \cos 2\theta & \sin 2\theta & 0 \\ \sin 2\theta & -\cos 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{4.7}$$

and hence

$$[\overline{\partial}_m\omega_k^\star] = -\frac{\Omega_z^\star}{2\pi r}\begin{bmatrix} 0 & 0 & \sin\theta \\ 0 & 0 & -\cos\theta \\ 0 & 0 & 0 \end{bmatrix}. \tag{4.8}$$

Remark 4.2 *The energy density $\mathcal{E}^\star = \frac{1}{2}\sigma_{ij}^\star\mathcal{E}_{ij}^\star$ is not L^1-integrable for both kinds of dislocations, while it is finite for the wedge disclination. Therefore, a Hadamard finite part (Schwartz 1957; Estrada & Kanwal 1989) is needed to represent the compliance at the meso-scale (another approach makes use of strain mollification by a so-called core tensor (Koslowski et al. 2002)). This issue, whose solution requires to develop matched asymptotic expansions around the singular line in accordance with the infinitesimal displacement hypothesis, will not be addressed further in the present paper which only focuses on the geometry of dislocations.*

Remark 4.3 *The above expressions of dislocations and disclinations do not necessarily provide balanced stresses. The present theory is fully independent of any dynamical assumption and only focuses on the geometrical concentrated properties of the defect lines.*

4.2 Mesoscopic incompatibility for a single defect line

For $2D$ problems the incompatibility vector contains all the information provided by the general incompatibility tensor. The latter expresses on the one hand the non-commutative action of the defect line over the second derivatives of the rotation vector and on the other hand is related to concentrated effects of the Frank and Burgers vectors along the defect line.

Definition 4.1 ($2D$ incompatibility tensor) *In the $2D$ case, the mesoscopic incompatibility vector is defined by*

$$\eta_k^\star := \epsilon_{\alpha\beta}\partial_\alpha\overline{\partial}_\beta\omega_k^\star. \tag{4.9}$$

A strain field is compatible if the associated incompatibility vector vanishes.

As shown in the following sections, concentration effects will be represented by means of first- and second-order distributions.

Notations 4.2 *Let, with use of notation 4.1,* $\Omega_z := \{x \in \Omega$ *with a prescribed* $z\}$ *and* $\Omega_z^0 := \Omega_z \setminus L$ *while the radius* $r = \|x - \hat{x}\|$ *is the distance from a point* x *inside* Ω *to* L*. Then, the* $1D$ *Hausdorff measure density concentrated on* L *will be denoted by* δ_L*.*

In what follows the hypothesis consists in assuming that the strain radial dependence in the vicinity of L is less singular than a critical threshold. This is verified for instance by the wedge disclination whose strain radial behaviour is $O(\ln r)$ [5] and by the screw and edge dislocations whose strains are $O(r^{-1})$.

For a straight defect line L, according to these examples, the hypotheses on the strain and Frank tensors read as follows.

Assumption 4.1 ($2D$ **strain for line defects)** *The strain tensor* $\mathcal{E}^\star_{ij}$ *is independent of the coordinate* z*, compatible on* $\Omega_L = \Omega \setminus L$ *in the sense that conditions (4.1) hold, smooth on* Ω_L*, and* L^1*-integrable on* Ω*.*

Assumption 4.2 (local behaviour) *The strain tensor* $\mathcal{E}^\star_{ij}$ *is assumed to be* $o(r^{-2})$ $(\epsilon \to 0^+)$ *while the Frank tensor is assumed to be* $o(r^{-3})(\epsilon \to 0^+)$*.*

The two following lemmas are needed for the proof of our main result for a single isolated defect line.

Lemma 4.2 *Let* $C_\epsilon(\hat{x})$*,* $\epsilon > 0$*, denote a family of* $2D$ *closed rectifiable curves. Then, in* $2D$ *elasticity, the Frank tensor and the strain verify the relation*

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

provided the length of C_ϵ *is uniformly bounded and as long as the convergence* $C_\epsilon(\hat{x}) \to \hat{x}$ *is understood in the Hausdorff sense, i.e. in such a way that*

$$\max\{\|x - \hat{x}\|, x \in C_\epsilon(\hat{x})\} \to 0.$$

Proof. The second compatibility condition of (4.1) is equivalent to

$$\partial_\gamma \mathcal{E}^\star_{\beta z} - \partial_\beta \mathcal{E}^\star_{\gamma z} = K \epsilon_{\gamma\beta},$$

from which, in $2D$ elasticity:

$$\overline{\partial}_\beta \omega^\star_\kappa := \epsilon_{\kappa\gamma} \partial_\gamma \mathcal{E}^\star_{\beta z} = \epsilon_{\kappa\gamma} \partial_\beta \mathcal{E}^\star_{\gamma z} - K \delta_{\kappa\beta},$$

and

$$\left(x_\alpha \overline{\partial}_\beta \omega^\star_\kappa + \delta_{\alpha\beta} \epsilon_{\kappa\gamma} \mathcal{E}^\star_{\gamma z} \right) = \partial_\beta \Big(x_\alpha \epsilon_{\kappa\gamma} \mathcal{E}^\star_{\gamma z} \Big) - x_\alpha K \delta_{\kappa\beta}.$$

Since, under the assumptions of this lemma,

$$\lim_{C_\epsilon(\hat{x}) \to \hat{x}} \int_{C_\epsilon(\hat{x})} x_\alpha dx_\kappa = 0,$$

while the strain is a single-valued tensor, the proof is achieved. □

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

Lemma 4.3 *In 2D elasticity the planar Frank vector $\Omega^\star_\alpha$ vanishes.*

Proof. Since

$$\overline{\partial}_\beta b^\star_\tau = \mathcal{E}^\star_{\beta\tau} + \epsilon_{\tau\gamma}(x_\gamma - x_{0\gamma})\delta_\beta\omega^\star_z - \epsilon_{\tau\gamma}(z - z_0)\delta_\beta\omega^\star_\gamma,$$

the planar Burgers vector simply writes as

$$B^\star_\tau = \int_C \left(\mathcal{E}^\star_{\beta\tau} + \epsilon_{\tau\gamma}(x_\gamma - x_{0\gamma})\delta_\beta\omega^\star_z\right) dx_\beta - \epsilon_{\tau\gamma}(z - z_0)\Omega^\star_\gamma,$$

where C is any planar loop. By Weingarten's theorems the Burgers vector is a constant while the integrand is independent of z, from which the result obviously follows. □

Theorem 4.1 (main result for a single defect line) *Under assumptions 4.1 and 4.2, for a dislocation located along the z-axis, incompatibility as defined by equation (4.9) is the vectorial first order distribution*

$$\eta^\star_k = \delta_{kz}\eta^\star_z + \delta_{k\kappa}\eta^\star_\kappa, \tag{4.10}$$

with

$$\eta^\star_z = \Omega^\star_z\delta_L + \epsilon_{\alpha\gamma}\left(B^\star_\gamma - \epsilon_{\beta\gamma}x_{0\beta}\Omega^\star_z\right)\partial_\alpha\delta_L, \tag{4.11}$$

$$\eta^\star_\kappa = \frac{1}{2}\epsilon_{\kappa\alpha}B^\star_z\partial_\alpha\delta_L. \tag{4.12}$$

Proof. For some small enough $\epsilon > 0$ and using notations 3.1, a tube $\odot_\epsilon$ can be constructed around L and inside Ω. Assuming that the smooth $3D$ test-function φ has its compact support containing a part of L, $\Omega_{\epsilon,z}$ denotes the slice of the open $\Omega \setminus \odot_\epsilon$ obtained for a given $\hat{x} \in L$, i.e.

$$\Omega_{\epsilon,z} := \{x \in \Omega_z \quad \text{such that} \quad ||x_\alpha|| > \epsilon\},$$

while the boundary circle of $\Omega_{\epsilon,z}$ is designated by $C_{\epsilon,z}$.
▲ Let us firstly treat the left-hand side of (4.10). From definitions 4.1 and 3.1, and equations (3.1), (3.2) and (3.3), it follows that

$$< \eta^\star_k, \varphi > = \int_L dz \lim_{\epsilon\to 0^+} \Pi_k(z, \varphi, \epsilon), \tag{4.13}$$

where

$$\Pi_k(z, \varphi, \epsilon) := -\int_{\Omega_{\epsilon,z}} \epsilon_{\alpha\beta}\overline{\partial}_\beta\omega^\star_k\partial_\alpha\varphi dS - \int_{C_{\epsilon,z}} \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\mathcal{E}^\star_{\beta n}\partial_\alpha\varphi dC_\gamma. \tag{4.14}$$

From notation 4.1, the boundedness of $|\partial_\tau\partial_\delta\varphi|$ on Ω_L provides the following Taylor expansions of φ and $\partial_\alpha\varphi$ around $\hat{x}$:

$$\varphi(x) = \varphi(\hat{x}) + r\nu_\alpha\partial_\alpha\varphi(\hat{x}) + \frac{r^2}{2}\nu_\tau\nu_\delta\partial_\tau\partial_\delta\varphi\left(\hat{x} + \gamma_1(x - \hat{x})\right), \tag{4.15}$$

$$\partial_\alpha\varphi(x) = \partial_\alpha\varphi(\hat{x}) + r\nu_\tau\partial_\tau\partial_\alpha\varphi\left(\hat{x} + \gamma_2(x - \hat{x})\right), \tag{4.16}$$

with $0 < \gamma_1(x - \hat{x}), \gamma_2(x - \hat{x}) \leq 1$.
▲ Consider the first term of the right-hand side of (4.14), noted $\hat{\Pi}_k$. By virtue of the strain compatibility on Ω_L and Gauss-Green's theorem, this term writes as

$$\hat{\Pi}_k(z, \varphi, \epsilon) := -\int_{\Omega_{\epsilon,z}} \partial_\gamma\left(\epsilon_{\gamma\beta}\overline{\partial}_\beta\omega^\star_k\varphi\right) dS = \int_{C_\epsilon} \epsilon_{\gamma\beta}\overline{\partial}_\beta\omega^\star_k\varphi dC_\gamma.$$

Since by notations 4.1 and 4.2, $r\nu_\alpha := x_\alpha - \hat{x}_\alpha = x_\alpha$, then equation (4.15) and assumption 4.2 show that, for $\epsilon \to 0^+$,

$$\hat{\Pi}_k = \int_{C_{\epsilon,z}} \epsilon_{\gamma\beta}\overline{\partial}_\beta\omega_k^\star\Big(\varphi(\hat{x}) + x_\alpha\partial_\alpha\varphi(\hat{x})\Big)dC_\gamma + o(1).$$

▲ Consider the second term of the right-hand side of (4.14), noted $\Pi_k^\star$. On account of assumption 4.2 and from expansion (4.16), this term may be rewritten as

$$\begin{aligned}\Pi_k^\star(z,\varphi,\epsilon) \quad &:= \quad -\int_{C_{\epsilon,z}} \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\mathcal{E}_{\beta n}^\star\partial_\alpha\varphi dC_\gamma \\ &= \quad -\partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\mathcal{E}_{\beta n}^\star dC_\gamma + o(1).\end{aligned}$$

▲ From Weingarten's theorem and recalling that $dC_\gamma = \epsilon_{\gamma\tau}dx_\tau$, the expression $\Pi_k = \hat{\Pi}_k + \Pi_k^\star$ then writes as

$$\begin{aligned}\Pi_k = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} \left(x_\alpha\overline{\partial}_\tau\omega_k^\star - \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\epsilon_{\gamma\tau}\mathcal{E}_{\beta n}^\star\right)dx_\tau \\ +\Omega_k^\star\varphi(\hat{x}) + o(1).\end{aligned} \tag{4.17}$$

▲ Consider the first term of the right-hand side of (4.17), noted Π_k', and take $\xi = \gamma$ in the identity

$$\epsilon_{k\xi n}\epsilon_{\gamma\tau} = \delta_{kz}\left(\delta_{\gamma\xi}\delta_{n\tau} - \delta_{n\gamma}\delta_{\tau\xi}\right) - \delta_{nz}\left(\delta_{\gamma\xi}\delta_{k\tau} - \delta_{k\gamma}\delta_{\tau\xi}\right) \tag{4.18}$$

in such a way that

$$\Pi_k' = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} \left(x_\alpha\overline{\partial}_\tau\omega_k^\star - \delta_{kz}\epsilon_{\alpha\beta}\mathcal{E}_{\beta\tau}^\star + \delta_{k\tau}\epsilon_{\alpha\beta}\mathcal{E}_{\beta z}^\star\right)dx_\tau. \tag{4.19}$$

▲ The cases $k = z$ and $k = \kappa$ are now treated separately.

• When $k = z$, definition 3.2 shows that

$$\overline{\partial}_\beta b_\tau^\star := \mathcal{E}_{\beta\tau}^\star + \epsilon_{\tau\gamma}(x_\gamma - x_{0\gamma})\overline{\partial}_\beta\omega_z^\star - \epsilon_{\tau\gamma}(z - z_0)\overline{\partial}_\beta\omega_\gamma^\star$$

which, after multiplication by $\epsilon_{\tau\alpha}$ and using (4.18) with τ, α and z substituted for k, ξ and n, is inserted into (4.19), thence yielding:

$$\Pi_z' = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} \left(\epsilon_{\tau\alpha}\overline{\partial}_\beta b_\tau^\star + x_{0\alpha}\overline{\partial}_\beta\omega_z^\star + (z - z_0)\overline{\partial}_\beta\omega_\alpha^\star\right)dx_\beta, \tag{4.20}$$

and consequently, from the definitions of the Frank and Burgers vectors,

$$\lim_{\epsilon\to 0^+}\Pi_z' = \ll \{\epsilon_{\alpha\tau}B_\tau^\star - (z - z_0)\Omega_\alpha^\star - x_{0\alpha}\Omega_z^\star\}\,\partial_\alpha\delta_0, \varphi_z \gg, \tag{4.21}$$

where δ_0 is the $2D$ Dirac measure located at 0 and $\varphi_z(x_\alpha) := \varphi(x_\alpha, z)$, while symbol $\ll \cdot,\cdot \gg$ denotes the $2D$ distribution by test-function product.

• When $k = \kappa$, definition 3.2 shows that

$$\overline{\partial}_\beta b_z^\star := \mathcal{E}_{\beta z}^\star + \epsilon_{\gamma\tau}(x_\gamma - x_{0\gamma})\overline{\partial}_\beta\omega_\tau^\star,$$

from which, after multiplication by $\epsilon_{\kappa\alpha}$, it results that:

$$x_\alpha\overline{\partial}_\tau\omega_\kappa^\star = -\epsilon_{\kappa\alpha}\overline{\partial}_\tau b_z^\star + \epsilon_{\kappa\alpha}\mathcal{E}_{\tau z}^\star + x_{0\alpha}\overline{\partial}_\tau\omega_\kappa^\star + (x_\kappa - x_{0\kappa})\overline{\partial}_\tau\omega_\alpha^\star.$$

Then, by lemma 4.2 with a permutation of κ and α, (4.19) also writes as

$$\Pi'_\kappa = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}}\left(-\epsilon_{\kappa\alpha}\overline{\partial}_\beta b^\star_z + \epsilon_{\kappa\alpha}\mathcal{E}^\star_{\beta z} + x_{0\alpha}\overline{\partial}_\beta\omega^\star_\kappa - x_{0\kappa}\overline{\partial}_\beta\omega^\star_\alpha\right)dx_\beta + o(1).$$

On the other hand, from equation (4.19) and lemma 4.2 (i.e. from strain compatibility) it follows that:

$$\begin{aligned}\Pi'_\kappa &= \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}}\left(-\epsilon_{\kappa\beta}\mathcal{E}^\star_{\beta z}dx_\alpha + \epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta z}dx_\kappa\right) + o(1)\\ &= \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}}\epsilon_{\alpha\kappa}\mathcal{E}^\star_{\beta z}dx_\beta + o(1). \qquad (4.22)\end{aligned}$$

By summing this latter expression of Π'_κ with (4.22), from the definitions of the Frank and Burgers vector it follows that

$$\Pi'_\kappa = \frac{1}{2}\partial_\alpha\varphi(\hat{x})\epsilon_{\alpha\kappa}\left(B^\star_z - \epsilon_{\gamma\beta}\Omega^\star_\gamma x_{0\beta}\right) + o(1). \qquad (4.23)$$

Hence, in the limit $\epsilon \to 0^+$ (4.23) writes as

$$\lim_{\epsilon\to 0^+}\Pi'_\kappa = \ll \left\{\frac{1}{2}\epsilon_{\kappa\alpha}B^\star_z - \frac{1}{2}\epsilon_{\kappa\alpha}\epsilon_{\gamma\beta}\Omega^\star_\gamma x_{0\beta}\right\}\partial_\alpha\delta_0, \varphi_z \gg . \qquad (4.24)$$

▲ Therefore, the result is proved on Ω^0_z, since

$$\lim_{\epsilon\to 0^+}\Pi_k(z,\varphi,\epsilon) = \lim_{\epsilon\to 0^+}\Pi'_k(z,\varphi,\epsilon) + \ll \Omega^\star_k\delta_0, \varphi_z \gg . \qquad (4.25)$$

As suggested by equation (4.13), to obtain the result for the entire domain Ω it suffices to integrate equations (4.20) and (4.23) and the expression $\Omega^\star_k\varphi(\hat{x})$ over L, in order to replace δ_0 by the line measure δ_L in (4.21), (4.24) and (4.25). By (4.13) the proof is then achieved. □

Theorem 4.2 (main result for a set of isolated defect lines) *Let in the 2D case $L^{(i)}$, $i \in \mathcal{I} \subset \mathbb{N}$ stand for a set of isolated parallel dislocations and/or disclinations passing by $(\hat{x}^{(i)}_\beta, z)$ and $\Omega^{\star(i)}_z, B^{\star(i)}_k$ and $\delta_{L^{(i)}}$ denote the associated Frank and Burgers vectors, and the concentrated 1D Hausdorff measure density on $L^{(i)}$. Then under assumptions 4.1 and 4.2 in the vicinity of each defect line, incompatibility develops as the distribution*

$$\eta^\star_k = \delta_{kz}\eta^\star_z + \delta_{k\kappa}\eta^\star_\kappa, \qquad (4.26)$$

with

$$\begin{aligned}\eta^\star_z &= \sum_{i\in\mathcal{I}}\left(\Omega^{\star(i)}_z\delta_{L^{(i)}} + \epsilon_{\alpha\gamma}\left(B^{\star(i)}_\gamma + \epsilon_{\beta\gamma}(\hat{x}^{(i)}_\beta - x_{0\beta})\Omega^{\star(i)}_z\right)\partial_\alpha\delta_{L^{(i)}}\right), \qquad (4.27)\\ \eta^\star_\kappa &= \frac{1}{2}\epsilon_{\kappa\alpha}\sum_{i\in\mathcal{I}}B^{\star(i)}_z\partial_\alpha\delta_{L^{(i)}}. \qquad (4.28)\end{aligned}$$

Proof. the proof is straightforward from theorem 4.1. An alternative formulation is provided by (2.4)-(2.6). □

4.3 Applications of the main result

Throughout this section, (x, y, z) denotes a generic point of Ω_L and all tensors are written in matrix form in the Cartesian base (e_x, e_y, e_z).

• *Screw disclocation.* Since $B^\star_\gamma = \Omega^\star_z = 0$, (4.11) and (4.12) yield

$$[\eta^\star_k] = \frac{B^\star_z}{2}\begin{bmatrix} \partial_y \delta_L \\ -\partial_x \delta_L \\ 0 \end{bmatrix}.$$

This result is easily verified with use of equation (3.5). One needs to compute $< \eta^\star_k, \varphi >= \int_\Omega \epsilon_{kpn}\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta n}\partial_p\partial_\alpha\varphi dV$, that is to calculate the integral of

$$\frac{B^\star_z}{4\pi}\begin{bmatrix} \partial_y\partial_x\varphi\frac{\cos\theta}{r} + \partial^2_y\varphi\frac{\sin\theta}{r} \\ -\partial^2_x\varphi\frac{\cos\theta}{r} - \partial_x\partial_y\varphi\frac{\sin\theta}{r} \\ 0 \end{bmatrix}.$$

By integration by parts, using Gauss-Green's theorem on Ω, and recalling that test-functions have compact supports and that $\partial_m \log r = \frac{x_m}{r^2}$, this integral becomes

$$-\frac{B^\star_z}{4\pi}\int_\Omega \begin{bmatrix} \partial_y\varphi\left(\partial_x\frac{\cos\theta}{r} + \partial_y\frac{\sin\theta}{r}\right) \\ -\partial_x\varphi\left(\partial_x\frac{\cos\theta}{r} + \partial_y\frac{\sin\theta}{r}\right) \\ 0 \end{bmatrix} dV = \frac{B^\star_z}{4\pi}\int_\Omega \begin{bmatrix} -\partial_y\varphi\partial^2_m \log r \\ \partial_x\varphi\partial^2_m \log r \\ 0 \end{bmatrix} dV.$$

Hence, from the relation $\Delta(\log r) = 2\pi\delta_L$, the first statement is verified.

• *Edge dislocation.* Whereas $\overline{\partial}_m\omega^\star_k$ identically vanishes on Ω_L, it is easily seen that (4.11) and (4.12) with $B^\star_z = \Omega^\star_z = 0$ yield

$$[\eta^\star_k] = B^\star_y\begin{bmatrix} 0 \\ 0 \\ \partial_x\delta_L \end{bmatrix}.$$

We must compute $< \eta^\star_k, \varphi >= \int_\Omega \epsilon_{kpn}\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta n}\partial_p\partial_\alpha\varphi dV$. For $n \neq 3$, the strain components do not identically vanish and, for $k = 1$ and $k = 2$, we must have $p = 3$ and hence the only non-vanishing component of the expression $\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta n}\partial_p\partial_\alpha\varphi$ are $\mathcal{E}^\star_{yx}\partial_z\partial_y\varphi - \mathcal{E}^\star_{yy}\partial_z\partial_x\varphi$ and $\mathcal{E}^\star_{xy}\partial_z\partial_x\varphi - \mathcal{E}^\star_{xx}\partial_z\partial_y\varphi$. By integration by parts, recalling that the strain does not depend on z, the related integrals vanish. For $k = 3$, the integrand is

$$\epsilon_{pnz}\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta n}\partial_p\partial_\alpha\varphi = \left(\partial_y\mathcal{E}^\star_{xx} - \partial_x\mathcal{E}^\star_{xy}\right)\partial_y\varphi + \left(\partial_y\mathcal{E}^\star_{xy} - \partial_x\mathcal{E}^\star_{yy}\right)\partial_x\varphi.$$

By inserting the expression of the strain tensor into the right-hand side of this equation, integration by parts provides the expression $\int_\Omega -\frac{B_y}{2\pi}\partial_x\varphi\Delta(\log r)dV$, achieving the second verification.

• *Wedge disclination.* Incompatibility reads

$$[\eta^\star_k] = \Omega^\star_z\begin{bmatrix} 0 \\ 0 \\ \delta_L \end{bmatrix}.$$

We must calculate $< \eta_k^\star, \varphi >= \int_\Omega \epsilon_{kpn}\epsilon_{\alpha\beta}\mathcal{E}^\star_{\beta n}\partial_p\partial_\alpha\varphi dV$. For $k=1$ and $k=2$, we must have $n \neq 3$ and $p=3$, but then the integrand vanishes. For $k=3$, we compute

$$\begin{aligned}\epsilon_{pn}\epsilon_{lm}\mathcal{E}^\star_{mn}\partial_p\partial_l\varphi &= \frac{\Omega_z^\star(1-\nu^\star)}{4\pi}\varphi\Delta(\log\frac{r}{R}) + \frac{\Omega_z^\star(1+\nu^\star)}{4\pi}\varphi\Delta(\log\frac{r}{R}) \\ &= 2\frac{\Omega_z^\star}{4\pi}\varphi(2\pi\delta_L),\end{aligned}$$

achieving the third verification.

5 Conclusive remarks

In this paper a general theory revisiting the work of Kröner (1980) has been developed to model line defects in single crystals at the mesoscopic scale. A rigorous definition of the dislocation and disclination density tensors as concentrated effects on the defect lines has been provided in the framework of the distribution theory. The main difficulty resulting from the multivaluedness of the displacement and rotation vector fields in defective crystals has been addressed by defining the single-valued Burgers and Frank tensors from the distributional strain gradient. Whereas outside the defective lines both tensors are regular functions directly related to the displacement and rotation gradients, in addition they exhibit concentrated properties within the defect lines which may be linked to the displacement and rotation jumps around these lines.

Moreover, defining the incompatibility tensor as the distributional curl of the Frank tensor, the principal result of our work has been to express in the two-dimensional case incompatibility as a function of the dislocation and disclination density tensors and their distributional gradients, and to demonstrate this relationship under precise assumptions on the regularity of the strain tensor in the vicinity of the assumed isolated defect lines. In a subsequent paper (Van Goethem & Dupret, 2009*b*), our theory is extended to the case of a countable number of defect lines under specific hypotheses based on the geometric measure theory.

In general our work is devoted to provide a rigorous distributional definition and a new understanding of the different mathematical objects (dislocation and disclination densities, contortion, incompatibility, Burgers and Frank tensors, elastic strain, etc.) that can be added at the mesoscopic scale in order to well-define the associated homogenized objects at the macroscopic scale. Further work will deal with the general three-dimensional dynamic theory.

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