

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

N. Van Goethem¹, F. Dupret¹
¹ CESAME, Université catholique de Louvain,
 Louvain-la-Neuve, Belgium

Keywords: dislocations, single crystals, multi-scale analysis, homogenisation, distribution theory, multivalued functions

Abstract

We develop a theory to represent dislocated single crystals at the mesoscopic scale by considering concentrated effects, governed by the distribution theory combined with multiple-valued kinematic fields. Our approach gives a new understanding of the continuum theory of defects as developed by Kröner (1980) and other authors. Fundamental $2D$ identities relating the incompatibility tensor to the Frank and Burgers vectors are proved under global strain assumptions relying on the geometric measure theory, thereby giving rise to rigorous homogenisation from mesoscopic to macroscopic scale.

1 Introduction

Dislocations can be considered as the most undesirable and resistant class of defects for several kinds of single crystals (Maroudas and Brown, 1991; Jordan et al., 2000). Therefore, in order to improve crystal quality, 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 in an appropriate way on the temperature field and the solid-liquid interface shape during the growth process (Van den Bogaert and Dupret, 1997).

However the dislocation models available in the literature, such as the model of Alexander and Haasen (1968, 1986), are often based on a rather crude extension of models previously developed for polycrystals (such as usual metals and ceramics). 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, Frank and Nabarro (1951, 1956), Kondo (1952), Nye (1953), and Kröner (1980) among other authors (Bilby, 1960; 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) and Kleinert (1989)). However, in these works, the relationship between 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 an additional scale to the macro- and nano-scales, viz. the meso-scale as defined by the average distance between dislocations. The laws governing 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 view to clarifying the homogenisation process from meso- to macro-scale. Since dislocations are lines at the meso-scale, concentrated effects, as governed by the distribution theory (a key reference is here Schwartz (1957)), must be introduced in the mesoscopic model. In addition, since integration around the dislocations generates a multiple-valued displacement field with the dislocations as branching lines, multivalued functions must be considered (Almgren, 1986; Knopp, 1996; Remmert, 1996). 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 (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 particular, the application limits of Stokes' theorem are clarified. 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.

After homogenisation from meso- to macro-scale, no concentrated effects remain anymore present in the macroscopic model, which consists of a set of evolution PDE's governing scalar or tensorial defect density fields in the framework of elasto- or viscoplasticity (Kratochvil and Dillon, 1969). However, it should be pointed out that homogenisation 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 consideration becomes obvious when homogenisation 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 issue is clarified in the present paper. Moreover, since the macroscopic displacement and rotation fields are not defined as ensemble averages of their mesoscopic counterparts, no unique privileged reference configuration can be defined at the macro-scale for single crystals with dislocations. Having in mind that displacement and rotation fields are defined with respect to the selected reference configuration (which can be, or not, defect free), the invariance laws governing the behaviour of single crystals with line defects at the macro-scale are constructed in accordance with this observation.

In the literature the macroscopic dislocation density is classically defined as the curl of the plastic distortion (Head et al., 1993; Cermelli and Gurtin, 2001; Gurtin, 2002; Koslowski et al., 2002; Ariza and Ortiz, 2005), following a postulated distortion decom-

position into elastic and plastic parts. However, this approach cannot be rigorously justified (contrarily to the strain decomposition) since elastic and plastic rotations cannot be set apart. In contrast, the present paper introduces the macroscopic dislocation density by homogenisation of well-defined mesoscopic fields, under precise geometric-measure model assumptions, from which the distortion decomposition is obtained together with its relationship with the dislocation density. Since dislocations and disclinations represent body torsion and curvature, respectively, these concepts also appear as macroscopic counterparts of well-defined mesoscopic defect measures. The present paper is restricted to the $2D$ theory. Extension to the $3D$ case is under investigation. A complete link between the mesoscopic and macroscopic behaviours of single crystals with line defects should be derived from these developments. In Section 2, the scaling analysis summarised in this introduction is detailed and the basic concepts used to represent the dislocated continuous medium are introduced. Classical invariance theorems are recalled in Section 3. In Section 4, the $2D$ distributional theory of the dislocated continuous medium is established in the case of a single dislocation, while Section 5 treats the more general case of an ensemble of isolated dislocations. Finally, Section 6 introduces the non-Riemannian macroscopic body by homogenisation from the mesoscale, and conclusions are drawn in Section 7.

2 Multiscale analysis of dislocations

To address the modelling of elastic single crystals with line defects, the various scales relevant for matter description and their interrelations are briefly reviewed.

- At the nano-scale the characteristic length is the interatomic distance. At time t , the body is referred to as $\mathcal{R}^{**}(t)$ and the reference body is a perfect lattice \mathcal{R}_0^{**} .
- At the meso-scale the characteristic length is the average distance between two neighbour dislocation lines. At time t , the body is referred to as $\mathcal{R}^*(t)$, to be interpreted as a random sample corresponding to a given growth experiment. The reference body \mathcal{R}_0^* is a perfect crystal, i.e. a body without dislocations or disclinations.
- At the macro-scale the characteristic length is the diameter of the crystal and the body $\mathcal{R}(t)$ has a physical meaning related to $\mathcal{R}^*(t)$ and $\mathcal{R}^{**}(t)$ in terms of ensemble average; the reference body \mathcal{R}_0 can be, or not, a perfect crystal.

2.1 Nano-scale analysis: crystalline lattice

Given a dislocation in the general sense, the atomic arrangement $\mathcal{R}^{**}(t)$ differs from the reference lattice \mathcal{R}_0^{**} , but however the atom displacements are not uniquely defined (Kleinert, 1989). More exactly, a discrete multivalued mapping $x_i := \chi_i^{**}(X_i)$ where $i = 1, 2$ or 3 , is defined with $X_i \in \mathcal{R}_0^{**}$ and $x_i \in \mathcal{R}^{**}(t)$. 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. Let us insist on the fact that there is no way to uniquely define the displacement field. Indeed any atom of \mathcal{R}_0^{**} can in principle be selected to define the displacement of a given atom of $\mathcal{R}^{**}(t)$ which is therefore a multivalued discrete mapping. This remark also makes sense at higher scales.

2.2 Meso-scale analysis: dislocated continuous medium

This scale is the one on which this paper focuses, in the framework of $2D$ linear elasticity. Let us here describe some general and basic field properties at the meso-

scale level. Details are given in the forthcoming sections.

- The displacement field is a multivalued function such that for any point $X_l \in \mathcal{R}_0^*$ one has

$$u_i^*(X_l) = x_i - X_i, \quad \text{with} \quad x_i := \chi_i^*(X_l),$$

and where $\chi_i^*(X_l)$ is a multivalued mapping from \mathcal{R}_0^* to $\mathcal{R}^*(t)$. Displacement multivaluedness represents an important difficulty to address at the meso-scale in dislocation modelling. As opposed to multiple-valued fields, single-valued fields will also be called uniform.

- The strain will be denoted by \mathcal{E}_{ij}^* . In general, the Lagrange deformation tensor is given by

$$\mathcal{E}_{ij}^* := \frac{1}{2}(\partial_j u_i^* + \partial_i u_j^* + \partial_j u_m^* \partial_i u_m^*), \quad \text{with} \quad \partial_j u_i^* := \frac{\partial u_i^*}{\partial X_j},$$

with the classical indicial notations and summation convention used. In the sequel, linear elasticity will be assumed and hence the nonlinear terms are not taken into account at the meso-scale. This fundamental hypothesis relies on the assumption¹ that all nonlinear deformation effects take place around the dislocation in a nano-scale region whose diameter is small compared to the meso-scale characteristic distance. Therefore, using a singular perturbation asymptotic treatment, the nonlinear effects become concentrated inside the defect line at the meso-scale and hence the strain can be assumed to be the single-valued linear symmetric tensor given by

$$\mathcal{E}_{ij}^* := \frac{1}{2}(\partial_j u_i^* + \partial_i u_j^*)$$

outside the defect line and arbitrarily set to 0 on the defect line (noting that concentrated deformation effects inside this line do not play any role in displacement integration at the meso-scale).

- The infinitesimal rotation tensor is a possibly multiple-valued field given by $\omega_{ij}^* := \frac{1}{2}(\partial_j u_i^* - \partial_i u_j^*)$ with the associated rotation vector given by

$$\omega_k^* = -\frac{1}{2}\epsilon_{ijk}\omega_{ij}^* = \frac{1}{2}\epsilon_{ijk}\partial_j u_i^*$$

and the identity $\omega_{ij}^* = -\epsilon_{ijk}\omega_k^*$. The Frank and Burgers vectors Ω_k^* and B_i^* associated with a defect line are commonly defined as functions of the jumps of ω_k^* and u_i^* around this line. From Weingarten's theorems, these vectors are shown as invariants of the defect line.

The following geometric tensors are also introduced:

Definition 2.1

$$\text{DISCLINATION DENSITY:} \quad \Theta_{ij}^* := \Omega_j^* \delta_{iL}, \quad (2.1)$$

$$\text{DISLOCATION DENSITY:} \quad \Lambda_{ij}^* := B_j^* \delta_{iL}, \quad (2.2)$$

$$\text{DISPLACEMENT JUMP DENSITY:} \quad \alpha_{ij}^* := \Lambda_{ij}^* + \epsilon_{jlm} \Theta_{il}^*(x_m - x_{0m}), \quad (2.3)$$

$$\text{CONTORTION:} \quad \kappa_{ij}^* := \alpha_{ij}^* - \frac{1}{2}\alpha_{mm}^* \delta_{ij}, \quad (2.4)$$

where x_{0m} is a reference point for rotation and displacement integration.

¹In practise this assumption is certainly valid in single crystal growth.

Here, the symbol δ_{iL} is used to represent the concentrated vectorial measure density on the defect region L . In particular, when L is a rectifiable curve, δ_{iL} is equal to $\tau_i \delta_L$ with τ_i the unit tangent vector to L and δ_L the one-dimensional Hausdorff measure density concentrated on L .

The disclination and dislocation density tensors Θ_{ij}^* and Λ_{ij}^* are measure densities (cf Evans and Gariépy, 1992; Mattila, 1995) related to the so-called strain incompatibility η_{ij}^* to be defined later. In general at the meso-scale a dislocation or a disclination is a defect line (i.e. a singular line for the strain) to which non-vanishing Burgers and/or Frank vectors are attached. The tensors Λ_{ij}^* and Θ_{ij}^* are basic physical tools to model defect density at the meso-scale while η_{ij}^* plays a key role to understand their behaviour. The displacement jump density and mesoscopic contortion (or lattice curvature) tensors α_{ij}^* and κ_{ij}^* are combinations of these basic density tensors, with $\alpha_{ij}^* = \Lambda_{ij}^*$ when the disclination density tensor vanishes.

2.3 Macro-scale analysis: continuous medium

At this level, a point x_i of the actual body $\mathcal{R}(t)$, $x_i = \chi_i(X_i)$ where $X \in \mathcal{R}_0$ will be called a material point to be understood as a certain volume of matter of mesoscopic size located around the point x_i . In order to define macroscopic concepts such as temperature or stress, one needs to give a meaning to the temperature and stress at any point. The rigorous definition is obtained from an ergodicity argument and hence, at the macroscopic level the fields on $\mathcal{R}(t)$ are defined as ensemble averages of the fields defined on $\mathcal{R}^*(t)$. By this operation these fields are smoothed, which means that concentration effects at the meso-scale level along the defect lines are erased. To this end, a weak limiting procedure (or homogenisation) is needed in order to define the dislocation and disclination densities Λ_{ij} and Θ_{ij} at the macro-scale level from the knowledge of the meso-scale fields Λ_{ij}^* and Θ_{ij}^* .

Remark 2.1 *In this context, the reference body \mathcal{R}_0 is basically arbitrary and can, or not, be a perfect crystal. Indeed, at the macro-scale, the displacement u_i must be a single-valued function, while the displacement field u_i^* is multivalued at the meso-scale. Therefore, u_i^* cannot be considered as belonging to a (linear) Banach space (single-valued functions can be added since they share the same domain, whereas a multivalued function is defined on its specific Riemann foliation and cannot be added to a multivalued function defined on another Riemann foliation). Consequently the ensemble averaging procedure is forbidden for multivalued fields such as u_i^* and hence u_i is not the ensemble average of u_i^* . It should also be observed that removing the field multivaluedness by performing appropriate cuts is of no use here, since by derivation these cuts introduce arbitrary distributional contributions without physical meaning. In general, it is important to make it clear that the only fields which can be obtained at the macro-scale by ensemble averaging from the meso-scale are the so-called extensive fields associated with additive physical properties (such as specific mass, stress, specific internal energy... and the dislocation and disclination densities).*

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

Notations 3.1 *In the following sections, the assumed open domain is denoted by Ω (in practise but not necessarily Ω is bounded), the defect line(s) are indicated by $L \in \Omega$, and Ω_L is the chosen symbol for $\Omega \setminus L$, which is also assumed to be open without loss of generality. Focussing on the meso-scale, symbol \hat{x} or \hat{x}_i denotes a generic point of the defect line(s), x or x_i is a generic point of Ω_L and x_0 or x_{0i} is a given fixed reference*

point of Ω_L . When x and \hat{x} are used together, \hat{x} denotes the projection of x onto the defect line(s) L in a appropriate sense and $\hat{\nu}_i := \nu_i(\hat{x}, x)$ is the unit vector joining \hat{x} to x . The symbol \odot_ϵ is intended for a set of diameter 2ϵ enclosing the region L . More precisely, \odot_ϵ is defined as the intersection with Ω of the union of all closed spheres of radius ϵ centred on L :

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

In case L is an isolated line, \odot_ϵ is a tube of radius ϵ enclosing L . In the sequel, considering a surface S of Ω crossed by 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 $\hat{\sigma}_j$ and τ_j the unit tangent vectors to C at x and to L at \hat{x} (when they exist). 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.

Assumption 3.1 (Mesoscopic elastic strain) Henceforth we will assume that the linear strain \mathcal{E}_{mn}^* is a given symmetric $C^\infty(\Omega_L, \mathbb{R}^{3 \times 3})$ -tensor prolonged by 0 on the line L , L^1 -integrable on Ω and compatible on Ω_L . In other words, the equality

$$\epsilon_{qlm} \epsilon_{kpn} \partial_l \partial_p \mathcal{E}_{mn}^* = 0 \quad (3.1)$$

is assumed everywhere on Ω_L .

3.1 Distributional analysis of the multiple-valued fields

In general, a multivalued function from Ω_L to \mathbb{R}^N consists of a pair of single-valued mappings with appropriate properties:

$$F \rightarrow \Omega_L \quad \text{and} \quad F \rightarrow \mathbb{R}^N,$$

where F is the associated Riemann foliation (Almgren, 1986; Knopp, 1996; Remmert, 1996). In the present case of meso-scale elasticity, we limit ourselves to multivalued functions obtained by recursive line integration of single-valued mappings defined on Ω_L . Reducing these multiple line integrals to simple line integrals, the Riemann foliation shows to be the set of equivalence path classes in Ω_L from a given $x_0 \in \Omega_L$ with the homotopy as equivalence relationship. Accordingly, a multivalued function will be called of index n on Ω_L if its n -th differential is single-valued on Ω_L . No other kinds of multifunctions are considered in this work, whether L is a single line or belongs to a more complex set of defect lines (with possible branchings, etc.).

Notations 3.2 The notation $\partial_j^{(s)}$ is used for partial derivation of a single- or multiple-valued function whose domain is restricted to Ω_L . Locally around $x \in \Omega_L$, 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 $U \cap L = \emptyset$, in such a way that $\partial_j^{(s)}$ and ∂_j coincide on U for every single- or multiple-valued function of index 1.

In the following essential definition the strain is considered as a distribution on Ω :

Definition 3.1 [Frank tensor] The Frank tensor $\bar{\partial}_m \omega_k^*$ is defined on the entire domain Ω as the following distribution:

$$\bar{\partial}_m \omega_k^* := \epsilon_{kpq} \partial_p \mathcal{E}_{qm}^*, \quad (3.2)$$

in such a way that

$$\langle \bar{\partial}_m \omega_k^*, \varphi \rangle := - \int_{\Omega} \epsilon_{kpq} \mathcal{E}_{qm}^* \partial_p \varphi dV, \quad (3.3)$$

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

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

$$\lim_{\epsilon \rightarrow 0} \left(\int_{\Omega \setminus \odot_{\epsilon}} \epsilon_{kpq} \partial_p \mathcal{E}_{qm}^* \varphi dV + \int_{\partial \odot_{\epsilon} \cap \Omega} \epsilon_{kpq} \mathcal{E}_{qm}^* \varphi dS_p \right), \quad (3.4)$$

where the second term inside the parenthesis is precisely added in order to achieve convergence. One readily sees after integration by parts that expression (3.4) is equal to Eq. (3.3) provided $\lim_{\epsilon \rightarrow 0} \Omega \setminus \odot_{\epsilon} = \Omega_L$ (which is a general hypothesis limiting the acceptable defect lines together with the assumption that L is of vanishing $2D$ Hausdorff measure). Considering the possibly multivalued (with index 1) rotation vector ω_k^* , it should be observed from Definition 3.1 that $\bar{\partial}_m \omega_k^* = \partial_m^{(s)} \omega_k^*$ on Ω_L . This results from the classical relationship provided by elasticity theory between infinitesimal rotation and deformation derivatives. However, $\bar{\partial}_m \omega_k^*$ is defined by Eq. (3.2) as a distribution on Ω and therefore concentrated effects on L and its infinitesimal vicinity are added to $\partial_m^{(s)} \omega_k^*$, justifying the use of the symbol $\bar{\partial}_m \omega_k^*$ instead of $\partial_m \omega_k^*$ without giving to $\bar{\partial}_m$ the meaning of a derivation operator. In particular, it may be observed that the identical vanishing of $\partial_m^{(s)} \omega_k^*$ on Ω_L does not necessarily imply that the distribution $\bar{\partial}_m \omega_k^*$ vanishes as well. In fact from Eq. (3.4), it can be shown in this particular case that

$$\langle \bar{\partial}_m \omega_k^*, \varphi \rangle = \lim_{\epsilon \rightarrow 0} \int_{\partial \odot_{\epsilon} \cap \Omega} \epsilon_{kpq} \mathcal{E}_{qm}^* \varphi dS_p = - \int_{\Omega} \epsilon_{kpq} \mathcal{E}_{qm}^* \partial_p \varphi dV, \quad (3.5)$$

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

$$\langle \partial_l \bar{\partial}_m \omega_k^*, \varphi \rangle = - \langle \bar{\partial}_m \omega_k^*, \partial_l \varphi \rangle = \int_{\Omega} \epsilon_{kpn} \mathcal{E}_{mn}^* \partial_p \partial_l \varphi dV. \quad (3.6)$$

3.2 Rotation and displacement vectors

The rotation vector is defined from the knowledge of the linear strain together with the rotation at a given reference point x_0 . From this construction follows an invariance property of ω_k^* as a multifunction (recalling that multivaluedness takes its origin from the existence of a defect line which renders the strain incompatible on the entire Ω). Starting from the distributive Definition 3.1 of $\bar{\partial}_m \omega_k^*$, the differential form $\bar{\partial}_m \omega_k^* d\xi_m$ is integrated along a regular parametric curve $\Gamma \subset \Omega_L$ with endpoints $x_0, x \in \Omega_L$. For selected x_0 and ω_{0k}^* , the multivalued rotation vector is defined as

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

where $\#\Gamma$ is the equivalence class of all regular curves homotopic to Γ in Ω_L . Indeed, from strain compatibility in Ω_L , i.e. from relation (3.1), it is clear that ω_k^* is a function of $\#\Gamma$ only. Consider now a regular parametric loop C (in case C is a planar loop, it is called Jordan curve) and the equivalence class $\#C$ of all regular loops homotopic to C in Ω_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 Ω_L . The jump of the rotation vector ω_k^* along $\#C$ depends on $\#C$ only and is defined as²

$$[\omega_k^*] = [\omega_k^*](\#C) = \int_C \bar{\partial}_m \omega_k^* d\xi_m. \quad (3.7)$$

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 $\bar{\partial}_m \omega_k^*$ in the construction of the rotation field:

Definition 3.2 [Burgers tensor] *For a selected reference point $x_0 \in \Omega_L$, the Burgers tensor is defined on the entire domain Ω as the distribution*

$$\bar{\partial}_l b_k^*(x; x_0) := \mathcal{E}_{kl}^*(x) + \epsilon_{kpq}(x_p - x_{0p}) \bar{\partial}_l \omega_q^*(x). \quad (3.8)$$

The Burgers tensor can be integrated in the same way as the Frank tensor along any parametric curve Γ , providing for selected x_0 , ω_{0k}^* and u_{0k}^* the multivalued displacement vector u_k^* of index 2:

$$u_k^* = u_k^*(\#\Gamma, \omega_0^*, u_0^*) = u_{0k}^* + \epsilon_{klm} \omega_l^*(x; \Gamma)(x_m - x_{0m}) + \int_\Gamma \bar{\partial}_l b_k^*(\xi) d\xi_l,$$

which is a function of $\#\Gamma$ only. It may be observed that $\bar{\partial}_l b_k^*$ and the vector $b_k^* = u_k^* - \epsilon_{klm} \omega_l^*(x_m - x_{0m})$ are related in the same way as $\bar{\partial}_m \omega_k^*$ and ω_k^* , including the fact that $\bar{\partial}_l b_k^* = \partial_l^{(s)} b_k^*$ on Ω_L . The jumps of b_k^* along $\#C$ and of u_k^* at x along $\#C$ (which depends on $\#C$ only) are defined as

$$[b_k^*](\#C; x_0) = [u_k^*](x; \#C; x_0) - \epsilon_{klm} [\omega_l^*](\#C)(x_m - x_{0m}) = \int_C \bar{\partial}_l b_k^* d\xi_l. \quad (3.9)$$

Let us now, for the sake of simplicity, focus on the case of a defect line L which (i) can itself be represented as a single \mathcal{C}^0 , closed or not, parametric line without multiple points except possibly its extremities and (ii) is isolated in the sense that each of its points \hat{x} is located inside a smooth surface $S(\hat{x})$ bounded by a loop $C(\hat{x})$ and such that $S(\hat{x}) \setminus \{\hat{x}\} \subset \Omega_L$. Such a defect line L will be called an isolated dislocation or disclination. The jump $[\omega_k^*]$ of the rotation vector ω_k^* around L is defined as the jump of ω_k^* along $\#C(\hat{x})$ and hence is the same for any \hat{x} and suitable $C(\hat{x})$. Similarly, the jump $[b_k^*]$ of the vector b_k^* around L is defined as the jump of b_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] *The rotation vector ω_k^* is a multifunction of index 1 on Ω_L whose jump $\Omega_k^* := [\omega_k^*]$ around L is an invariant of the defect-line L . Moreover, for a given x_0 , the vector b_k^* is a multifunction of index 1 on Ω_L whose jump $B_k^* := [b_k^*]$ around L is an invariant of the defect-line.*

Proposition 3.1 [Multiple-valued displacement field] *From a symmetric smooth linear strain tensor \mathcal{E}_{ij}^* on Ω_L and a point x_0 where the displacement and rotation are given, a multivalued displacement field u_i^* of index 2 can be constructed on Ω_L such that the symmetric part of the deformation gradient $\partial_j^{(s)} u_i^*$ is the single-valued strain tensor \mathcal{E}_{ij}^* on Ω_L while its skew-symmetric part is the multivalued tensor $\omega_{ij}^* := -\epsilon_{ijk} \omega_k^*$.*

²We note that the curve C could be non rectifiable, i.e. of infinite length. In fact, integrals on fractal curves and the related Stokes' and Gauss-Green's theorems are analysed by Harrison and Norton (1992), where it is shown, by the \mathcal{C}^∞ -smoothness of the differential form $\bar{\partial}_m \omega_k^* dx_m$ on Ω_L that Eq. (3.7) still holds even when the Hausdorff dimension of C is higher than 1.

From this result, the Frank and Burgers vectors can be defined as invariants of the single isolated line L .

Definition 3.3 [Frank and Burgers vectors] *The Frank vector of the line L is the invariant*

$$\Omega_k^* := [\omega_k^*], \quad (3.10)$$

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

$$B_k^* := [b_k^*] = [u_k^*](x) - \epsilon_{klm} \Omega_l^* (x_m - x_{0m}). \quad (3.11)$$

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 Ω_k^* might vanish. 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 *Two distinct reference points x_0 and x'_0 define two distinct Burgers vectors, related by*

$$B_k^* - B_k'^* = \epsilon_{klm} (x_{0m} - x'_{0m}) \Omega_l^*,$$

in such a way that $B_k^* \Omega_k$ 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 .

The following 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 *Single disclination and dislocation lines are always closed or end at the boundary of Ω . Moreover,*

$$\begin{aligned} \partial_i \Theta_{ij}^* &= 0 \\ \partial_i \alpha_{ij}^* &= -\epsilon_{jmn} \Theta_{mn}^*. \end{aligned}$$

Definition 3.4 (Mesoscopic strain incompatibility) *According to Eq. (3.1) combined with Eq. (3.3), the incompatibility tensor is defined by*

$$\eta_{ik}^* := \epsilon_{lmn} \partial_m \bar{\partial}_n \omega_k^*.$$

The strain field is called compatible on the set U if the associated incompatibility tensor vanishes on U .

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}_{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 Henceforth the single defect line will be assumed to be located along the z -axis. The two planar coordinates will be denoted by x and y or x_α . The projection of $x = (x_\alpha, z)$ on L is $\hat{x} = (0, 0, z)$. By convention, Latin indices i, j, k, l, \dots take their values from 1 to 3 and are basically used for 3D elasticity, while Greek indices $\alpha, \beta, \gamma, \delta, \dots$ take the values 1 or 2 and are used for 2D elasticity. 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 $dC_\alpha(x) = \epsilon_{\alpha\beta} dx_\beta$ will be used for 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:

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

The following propositions can be readily proved from Assumption 3.1:

Proposition 4.1 [2D compatibility] In Ω_L , from 2D strain compatibility, there are real numbers K, a_α and b such that

$$\begin{cases} \epsilon_{\alpha\gamma} \epsilon_{\beta\delta} \partial_\alpha \partial_\beta \mathcal{E}_{\gamma\delta}^* = 0, \\ \epsilon_{\alpha\beta} \partial_\alpha \mathcal{E}_{\beta z}^* = K, \\ \mathcal{E}_{zz}^* = a_\alpha x_\alpha + b. \end{cases} \quad (4.1)$$

Lemma 4.1 Let $C(\hat{x})$ denote a family of 2D closed rectifiable curves. Then, in 2D elasticity, the Frank tensor and the strain verify the relation

$$\lim_{C(\hat{x}) \rightarrow \hat{x}} \int_{C(\hat{x})} x_\alpha \bar{\partial}_\beta \omega_\kappa^* dx_\beta + \epsilon_{\kappa\beta} \mathcal{E}_{\beta z}^* dx_\alpha = 0,$$

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

$$\max\{\|x - \hat{x}\|, x \in C(\hat{x})\} \rightarrow 0.$$

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

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

from which, so far as 2D elasticity is concerned,

$$\bar{\partial}_\beta \omega_\kappa^* := \epsilon_{\kappa\gamma} \partial_\gamma \mathcal{E}_{\beta z}^* = \epsilon_{\kappa\gamma} \partial_\beta \mathcal{E}_{\gamma z}^* - K \delta_{\kappa\beta},$$

and

$$(x_\alpha \bar{\partial}_\beta \omega_\kappa^* + \delta_{\alpha\beta} \epsilon_{\kappa\gamma} \mathcal{E}_{\gamma z}^*) = \partial_\beta (x_\alpha \epsilon_{\kappa\gamma} \mathcal{E}_{\gamma z}^*) - x_\alpha K \delta_{\kappa\beta}.$$

Since, under the limit assumptions of this lemma,

$$\lim_{C(\hat{x}) \rightarrow \hat{x}} \int_{C(\hat{x})} x_\alpha dx_\alpha = 0,$$

and since the strain is a single-valued tensor, the proof is achieved. \square

Lemma 4.2 In 2D elasticity the planar Frank vector Ω_α^* vanishes.

Proof. Since

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

the planar Burgers vector simply writes as

$$B_\tau^* = \int_C (\mathcal{E}_{\beta\tau}^* + \epsilon_{\tau\gamma}(x_\gamma - x_{0\gamma})\delta_\beta\omega_z^*) dx_\beta - \epsilon_{\tau\gamma}(z - z_0)\Omega_\gamma^*,$$

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. \square

In general, the present theory does not make any use of the linear elasticity constitutive laws and of the momentum and energy conservation laws, since in the framework of Continuum Mechanics arbitrary body forces and heat supply could be applied. However 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 body force free and isothermal (detailed computations are given in Appendix A).

- *Pure screw dislocation.* From Eq. (A.7), (A.9), and Proposition A.1, the displacement and rotation vectors write as

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

in such a way that the jump $[\omega_i^*]$ vanishes identically, while from Eq. (A.8) the Cartesian strain writes as

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

Moreover, in Ω_L , appealing to Eq. (4.3), the Frank tensor writes as

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

- *Pure edge dislocation.* From Eq. (A.6), (A.7), and Proposition A.1, the displacement is the vector

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

while the rotation ω_i^* vanishes together with its jump. The Cartesian strain writes from Eq. (A.5) as

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

noting that the tensor $\overline{\partial}_m \omega_k^* = \nabla \omega$ vanishes identically in Ω_L .

- *Wedge disclination.* From Eqs. (A.7), (A.6), and Proposition A.1, the rotation vector is

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

with the multiple-valued planar displacement field given by

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

and a vanishing Burgers vector:

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

The Cartesian strain writes from Eq. (A.5) as

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

and hence

$$[\bar{\partial}_m \omega_k^*] - \frac{\Omega_z^*}{2\pi r} \begin{bmatrix} 0 & 0 & \sin \theta \\ 0 & 0 & -\cos \theta \\ 0 & 0 & 0 \end{bmatrix}. \quad (4.8)$$

Remark 4.1 *It should be noted that the energy density (or compliance) $\mathcal{E}^* = \frac{1}{2} \sigma_{ij}^* \mathcal{E}_{ij}^*$ is not L^1 -integrable for both kinds of dislocations, while it is finite for the wedge disclination. Therefore, a Hadamard finite part distribution (Schwartz, 1957; Estrada and 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.*

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 *In the 2D case, the mesoscopic incompatibility vector is defined by*

$$\eta_k^* := \epsilon_{\alpha\beta} \partial_\alpha \bar{\partial}_\beta \omega_k^*. \quad (4.9)$$

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 *Recalling Notations 4.1, Ω_z and Ω_z^0 stand for the sets $\Omega_z := \{x \in \Omega \text{ such that } x = (x_\alpha, z)\}$ 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 concentrated on L is denoted by δ_L (cf Ambrosio et al. (2000), Evans and Gariepy (1992) and Mattila (1995) for general definitions and properties on the geometric measure theory).*

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 $O(\ln r)$ and by the screw and edge dislocations whose strains are $O(r^{-1})$.³ For a straight defect-line L , according to these examples, the hypotheses on the strain and Frank tensors read as follows:

³A function $f(\epsilon)$ is said to be $O(g(\epsilon))$ ($\epsilon \rightarrow 0^+$) 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 $o(g(\epsilon))$ ($\epsilon \rightarrow 0^+$) if $\lim_{\epsilon \rightarrow 0^+} \frac{f(\epsilon)}{g(\epsilon)} = 0$.

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

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

Theorem 4.1 [Main result for a single line] Under Assumption 4.1 and 4.2, for a dislocation located along the z -axis, incompatibility as defined by Eq. (4.9) is the vectorial first order distribution

$$\eta_k^* = \delta_{kz}\eta_z^* + \delta_{k\kappa}\eta_\kappa^*,$$

where its vertical component is

$$\eta_z^* = \Omega_z^* \delta_L + \epsilon_{\alpha\gamma} (B_\gamma^* - \epsilon_{\beta\gamma} x_{0\beta} \Omega_z^*) \partial_\alpha \delta_L, \quad (4.10)$$

while its planar components are

$$\eta_\kappa^* = \frac{1}{2} \epsilon_{\kappa\alpha} B_z^* \partial_\alpha \delta_L. \quad (4.11)$$

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

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

while the boundary circle of $\Omega_{\epsilon,z}$ is designated by $C_{\epsilon,z}$.

▲ Let us firstly treat the left-hand side of Eq. (4.10). Indeed, from Definition 4.1 with Eq. (3.2), Definition 3.1, and Eqs. (3.3) and (3.4), it follows that

$$\langle \eta_k^*, \varphi \rangle = \int_L dz \lim_{\epsilon \rightarrow 0^+} \Pi_k(z, \varphi, \epsilon),$$

where

$$\Pi_k(z, \varphi, \epsilon) := - \int_{\Omega_{\epsilon,z}} \epsilon_{\alpha\beta} \bar{\partial}_\beta \omega_k^* \partial_\alpha \varphi dS - \int_{C_{\epsilon,z}} \epsilon_{\alpha\beta} \epsilon_{k\gamma n} \mathcal{E}_{\beta n}^* \partial_\alpha \varphi dC_\gamma.$$

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

$$\varphi(x) = \varphi(\hat{x}) + r \hat{\nu}_\alpha \partial_\alpha \varphi(\hat{x}) + \frac{r^2}{2} \hat{\nu}_\tau \hat{\nu}_\delta \partial_\tau \partial_\delta \varphi(\hat{x} + \gamma_1(x - \hat{x})), \quad (4.12)$$

$$\partial_\alpha \varphi(x) = \partial_\alpha \varphi(\hat{x}) + r \hat{\nu}_\tau \partial_\tau \partial_\alpha \varphi(\hat{x} + \gamma_2(x - \hat{x})), \quad (4.13)$$

with $0 < \gamma_1(x - \hat{x}), \gamma_2(x - \hat{x}) \leq 1$.

▲ Consider the first term of Eq. (4.12), noted $\hat{\Pi}_k$. By virtue of strain compatibility on Ω_L and Gauss-Green's theorem, this term writes as

$$\hat{\Pi}_k(z, \varphi, \epsilon) := - \int_{\Omega_{\epsilon,z}} \partial_\gamma (\epsilon_{\gamma\beta} \bar{\partial}_\beta \omega_k^* \varphi) dS = \int_{C_\epsilon} \epsilon_{\gamma\beta} \bar{\partial}_\beta \omega_k^* \varphi dC_\gamma.$$

Since by Notations 4.1 $r \hat{\nu}_\alpha := x_\alpha - \hat{x}_\alpha = x_\alpha$, then Eq. (4.12) and Assumption 4.2 show that, for $\epsilon \rightarrow 0^+$,

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

▲ Consider the second term of Eq. (4.12), noted Π_k^* . On account of Assumption 4.2 and by expansion (4.13), this term may be rewritten as

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

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

$$\begin{aligned}\Pi_k &= \partial_\alpha \varphi(\hat{x}) \int_{C_{\epsilon, z}} (x_\alpha \bar{\partial}_\tau \omega_k^* - \epsilon_{\alpha\beta} \epsilon_{k\gamma n} \epsilon_{\gamma\tau} \mathcal{E}_{\beta n}^*) dx_\tau \\ &+ \Omega_k^* \varphi(\hat{x}) + o(1).\end{aligned}\tag{4.14}$$

▲ Consider the first term of Eq. (4.14), noted Π'_k , and take $\delta = \gamma$ in the identity

$$\epsilon_{k\delta n} \epsilon_{\gamma\tau} = \delta_{kz} (\delta_{\gamma\delta} \delta_{n\tau} - \delta_{n\gamma} \delta_{\tau\delta}) - \delta_{nz} (\delta_{\gamma\delta} \delta_{k\tau} - \delta_{k\gamma} \delta_{\tau\delta})\tag{4.15}$$

in such a way that

$$\Pi'_k \partial_\alpha \varphi(\hat{x}) \int_{C_{\epsilon, z}} (x_\alpha \bar{\partial}_\tau \omega_k^* - \delta_{kz} \epsilon_{\alpha\beta} \mathcal{E}_{\beta\tau}^* + \delta_{k\tau} \epsilon_{\alpha\beta} \mathcal{E}_{\beta z}^*) dx_\tau.\tag{4.16}$$

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

- When $k = z$, Definition 3.2 shows that

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

which, after multiplication by $\epsilon_{\tau\alpha}$ and using Eq. (4.15) with τ, α and z substituted for k, δ and n , is inserted into Eq. (4.16), thence yielding:

$$\Pi'_z = \partial_\alpha \varphi(\hat{x}) \int_{C_{\epsilon, z}} (\epsilon_{\tau\alpha} \bar{\partial}_\beta b_\tau^* + x_{0\alpha} \bar{\partial}_\beta \omega_z^* + (z - z_0) \bar{\partial}_\beta \omega_\alpha^*) dx_\beta,\tag{4.17}$$

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

$$\lim_{\epsilon \rightarrow 0^+} \Pi'_z = \ll \{ \epsilon_{\alpha\tau} B_\tau^* - (z - z_0) \Omega_\alpha^* - x_{0\alpha} \Omega_z^* \} \partial_\alpha \delta_0, \varphi_z \gg,\tag{4.18}$$

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

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

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

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

Then, by Lemma 4.1 with a permutation of indices κ and α , Eq. (4.16) also writes as

$$\begin{aligned}\Pi'_\kappa &= \partial_\alpha \varphi(\hat{x}) \int_{C_{\epsilon, z}} (-\epsilon_{\kappa\alpha} \bar{\partial}_\beta b_z^* + \epsilon_{\kappa\alpha} \mathcal{E}_{\beta z}^* + x_{0\alpha} \bar{\partial}_\beta \omega_\kappa^* - x_{0\kappa} \bar{\partial}_\beta \omega_\alpha^*) dx_\beta \\ &+ o(1).\end{aligned}$$

On the other hand, from Eq. (4.16) and Lemma 4.1 (i.e. from strain compatibility) it follows that:

$$\begin{aligned}\Pi'_\kappa &= \partial_\alpha \varphi(\hat{x}) \int_{C_{\epsilon,z}} (-\epsilon_{\kappa\beta} \mathcal{E}_{\beta z}^* dx_\alpha + \epsilon_{\alpha\beta} \mathcal{E}_{\beta z}^* dx_\kappa) + o(1) \\ &= \partial_\alpha \varphi(\hat{x}) \int_{C_{\epsilon,z}} \epsilon_{\alpha\kappa} \mathcal{E}_{\beta z}^* dx_\beta + o(1).\end{aligned}\quad (4.19)$$

By summing this latter expression of Π'_κ with Eq. (4.19), from the definitions of the Frank and Burgers vector it follows that

$$\Pi'_\kappa = \frac{1}{2} \partial_\alpha \varphi(\hat{x}) \epsilon_{\alpha\kappa} (B_z^* - \epsilon_{\gamma\beta} \Omega_\gamma^* x_{0\beta}) + o(1). \quad (4.20)$$

Hence, in the limit $\epsilon \rightarrow 0^+$ Eq. (4.20) writes as

$$\lim_{\epsilon \rightarrow 0^+} \Pi'_\kappa = \ll \left\{ \frac{1}{2} \epsilon_{\kappa\alpha} B_z^* - \frac{1}{2} \epsilon_{\kappa\alpha} \epsilon_{\gamma\beta} \Omega_\gamma^* x_{0\beta} \right\} \partial_\alpha \delta_0, \varphi_z \gg. \quad (4.21)$$

Therefore, the result is proved on Ω_z^0 , since

$$\lim_{\epsilon \rightarrow 0^+} \Pi_\kappa(z, \varphi, \epsilon) = \lim_{\epsilon \rightarrow 0^+} \Pi'_\kappa(z, \varphi, \epsilon) + \ll \Omega_\kappa^* \delta_0, \varphi_z \gg. \quad (4.22)$$

▲ As suggested by Eq. (4.12), to obtain the result for the entire domain Ω it suffices to integrate Eqs. (4.17) and (4.20) and expression $\Omega_\kappa^* \varphi(\hat{x})$ over L , in order to replace δ_0 by the line measure δ_L in Eqs. (4.18), (4.21) and (4.22). By Eqs. (4.12), (4.18), (4.21) and (4.22), the proof is achieved. \square

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 dislocation.* Since $B_\gamma^* = \Omega_z^* = 0$, Eq. (4.11) yields

$$[\eta_k^*] = \frac{B_z^*}{2} \begin{bmatrix} \partial_y \delta_L \\ -\partial_x \delta_L \\ 0 \end{bmatrix}.$$

This result is easily verified with use of Eq. (3.6). One needs to compute $\int_\Omega \epsilon_{kpn} \epsilon_{\alpha\beta} \mathcal{E}_{\beta n}^* \partial_p \partial_\alpha \varphi dV$, that is to calculate the integral of

$$\frac{B_z^*}{4\pi} \begin{bmatrix} \partial_y \partial_x \varphi \frac{\cos \theta}{r} + \partial_y^2 \varphi \frac{\sin \theta}{r} \\ -\partial_x^2 \varphi \frac{\cos \theta}{r} - \partial_x \partial_y \varphi \frac{\sin \theta}{r} \\ 0 \end{bmatrix}.$$

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

$$-\frac{B_z^*}{4\pi} \int_\Omega \begin{bmatrix} \partial_y \varphi \left(\partial_x \frac{\cos \theta}{r} + \partial_y \frac{\sin \theta}{r} \right) \\ -\partial_x \varphi \left(\partial_x \frac{\cos \theta}{r} + \partial_y \frac{\sin \theta}{r} \right) \\ 0 \end{bmatrix} dV \frac{B_z^*}{4\pi} \int_\Omega \begin{bmatrix} -\partial_y \varphi \partial_m^2 \log r \\ \partial_x \varphi \partial_m^2 \log r \\ 0 \end{bmatrix} dV.$$

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

- *Edge dislocation.* Whereas $\bar{\partial}_m \omega_k^*$ identically vanishes on Ω_L , it is easily seen that Eqs. (4.10) and (4.11) with $B_z^* = \Omega_z^* = 0$ yield

$$[\eta_k^*] = B_y^* \begin{bmatrix} 0 \\ 0 \\ \partial_x \delta_L \end{bmatrix}.$$

We must compute $[\eta_k^*] = \int_{\Omega} \epsilon_{pnk} \epsilon_{\alpha\beta} \mathcal{E}_{\beta n}^* \partial_p \partial_{\alpha} \varphi dV$. For $k = 1$ and 2 and with $n \neq 3$, the tensor $\epsilon_{\alpha\beta} \mathcal{E}_{\beta n}^* \partial_p \partial_{\alpha} \varphi$ equals $\mathcal{E}_{yx}^* \partial_z \partial_y \varphi - \mathcal{E}_{yy}^* \partial_z \partial_x \varphi$ and $\mathcal{E}_{xy}^* \partial_z \partial_x \varphi - \mathcal{E}_{xx}^* \partial_z \partial_y \varphi$ respectively. By integration by parts, the related integrals vanish. For $k = 3$, the integrand is

$$\epsilon_{pnz} \epsilon_{\alpha\beta} \mathcal{E}_{\beta n}^* \partial_p \partial_{\alpha} \varphi \mathcal{E}_{xx}^* \partial_y \partial_y \varphi + \mathcal{E}_{yy}^* \partial_x \partial_x \varphi - 2\mathcal{E}_{xy}^* \partial_y \partial_x \varphi.$$

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

$$[\eta_k^*] = \Omega_z^* \begin{bmatrix} 0 \\ 0 \\ \delta_L \end{bmatrix}.$$

We must calculate $\langle \eta_k^*, \varphi \rangle$. For $k = 1, k = 2, n \neq 0$ and $p = 3$ the integrand vanishes. For $k = 3$, one computes

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

achieving the third verification.

5 Distributional analysis of incompatibility for a set of isolated dislocations

In the previous section, a single defect line was considered. However, to address the macro-scale physics, homogenisation must be performed on a set of dislocation lines whose number tends to infinity in order to define regular defect density tensors. Therefore, our goal is to introduce appropriate hypotheses that can easily be applied to a set of defect lines and to a regular defect density as well.

5.1 Governing assumptions for the strain and Frank tensors

Besides the strain Assumptions 4.1 two measure hypotheses on the strain derivatives are introduced to replace the local Assumption 4.2 in order to validate Theorem 4.1 in a global framework.

Assumption 5.1 *The strain divergence and trace gradient $\partial_{\alpha} \mathcal{E}_{\alpha i}^*$ and $\partial_{\gamma} \mathcal{E}_{\kappa \kappa}^*$ are finite Radon measures on Ω .⁴*

⁴A finite Radon measure on Ω is a measure bounded on compact subsets of Ω .

Remark 5.1 No assumption could be made on the complete Lebesgue integrable strain gradient without contradicting the 2D examples of Appendix A. On the other hand, it can be shown that the sharp Assumption 5.1 are required to demonstrate Proposition 5.4.

Remark 5.2 Assumption 5.1 is natural in infinitesimal elasticity if one considers the strain-stress constitutive law and the equilibrium laws. As a consequence, the stress divergence must be a measure on Ω .

The following Lemmas are needed for the proof of Proposition 5.4.

Lemma 5.1 • A solenoidal distributional vector field a_α on Ω_z writes as

$$a_\alpha = \epsilon_{\alpha\gamma} \partial_\gamma \phi, \quad (5.1)$$

with $\phi \in \mathcal{D}'(\Omega_z)$.

• A symmetric solenoidal distribution tensor $a_{\alpha\beta}$ on Ω_z writes as

$$a_{\alpha\beta} = \epsilon_{\alpha\gamma} \epsilon_{\beta\tau} \partial_\gamma \partial_\tau \psi, \quad (5.2)$$

with $\psi \in \mathcal{D}'(\Omega_z)$.

Proof.

- *First statement.* Let ϕ_0 be any x_2 -primitive distribution of a_1 (Schwartz, 1957). Then $\partial_2 \phi_0 = a_1$ and, from the solenoidal property of a_α , there exists a distribution $G(x_1)$ s.t. $\partial_1 \phi_0 + a_2 = G(x_1)$. By x_1 -primitivation of $G(x_1)$, it is easy to find $F(x_1)$ s.t. $\partial_1 F = G(x_1)$, and to verify that $\phi = \phi_0 + F(x_1)$ solves the problem.
- *Second statement.* From $\partial_\alpha a_{\alpha\beta} = 0$, there is a distribution ϕ_β s.t. $a_{\alpha\beta} = \epsilon_{\alpha\gamma} \partial_\gamma \phi_\beta$. Then $\epsilon_{\alpha\gamma} \partial_\gamma (\partial_\beta \phi_\beta) \partial_\beta a_{\alpha\beta} = 0$ and hence $\partial_\beta \phi_\beta$ is a constant C or equivalently $\partial_\beta (\phi_\beta - \frac{1}{2} C x_\beta) = 0$. From Eq. (5.1), there exists a distribution ψ such that $\phi_\beta - \frac{1}{2} C x_\beta = \epsilon_{\beta\tau} \partial_\tau \psi$, and hence $a_{\alpha\beta} = \epsilon_{\alpha\gamma} \epsilon_{\beta\tau} \partial_\gamma \partial_\tau \psi + \frac{1}{2} \epsilon_{\alpha\beta} C$. The symmetry of $a_{\alpha\beta}$ implies that $C = 0$. \square

Lemma 5.2 • For a given $L^1(\Omega_z)$ -scalar function f , there exists an irrotational distribution field g_β such that

$$\partial_\beta g_\beta = f. \quad (5.3)$$

• For a given $L^1(\Omega_z)$ -vector function f_β such that $\partial_\beta f_\beta = \Delta g$ where g is a $L^1(\Omega_z)$ function, there exists a symmetric compatible tensor $g_{\alpha\beta}$ on Ω_z such that

$$\partial_\alpha g_{\alpha\beta} = f_\beta. \quad (5.4)$$

Proof.

- *First statement.* It is sufficient to consider an ultra-weak solution (Brezis, 1983) of $\Delta H = f$ and to define $g_\beta = \partial_\beta H$.
- *Second statement.* By primitivation, there is a non-compatible $L^1(\Omega_z)$ -field $g_{\alpha\beta}^*$ such that $f_1 = \partial_1 g_{11}^*, f_2 = \partial_2 g_{22}^*$ and $0 = g_{21}^* = g_{12}^*$. A necessary condition for $g_{\alpha\beta}$ to exist is that $\hat{g}_{\alpha\beta} = g_{\alpha\beta} - g_{\alpha\beta}^*$ verifies $\partial_\alpha \hat{g}_{\alpha\beta} = 0$, or by Lemma 5.1 that $\hat{g}_{\alpha\beta} = \epsilon_{\alpha\gamma} \epsilon_{\beta\tau} \partial_\gamma \partial_\tau \phi$ for some gauge distribution ϕ . In order that $g_{\alpha\beta}$ be compatible on Ω_z , ϕ must satisfy the following equation, equivalent to the 2D compatibility of $g_{\alpha\beta}$ on Ω_z :

$$\Delta \Delta \phi = \Delta g_{\kappa\kappa}^* - \partial_\beta \partial_\alpha g_{\alpha\beta} = \Delta (g_{\kappa\kappa}^* - g). \quad (5.5)$$

Up to a harmonic and hence smooth function on Ω_z , the solution of Eq. (5.5) is the solution of $\Delta\phi = g_{\kappa\kappa}^* - g$. Since the right-hand side is $L^1(\Omega_z)$, a solution ϕ exists in the ultra-weak sense and hence the existence of a symmetric compatible distribution field $g_{\alpha\beta}$ on Ω_z verifying Eq. (5.4) follows. \square

Lemma 5.3 *For constant C and C_β , there are a vector g_κ and a symmetric, compatible tensor $G_{\alpha\beta}$ on Ω_z such that*

$$\partial_\kappa g_\kappa = C\delta_0, \quad (5.6)$$

$$\partial_\alpha G_{\alpha\beta} = C_\beta\delta_0. \quad (5.7)$$

Proof. The solutions are given by $g_\kappa = (2\pi)^{-1}\partial_\kappa \log r$ and $G_{\alpha\beta} = \frac{1}{2}(\partial_\alpha H_\beta + \partial_\beta H_\alpha)$, where

$$H_1 = \frac{C_1}{2\pi} \left(\frac{3}{2} \log r - \frac{x_1^2}{2r^2} \right) - C_2 \frac{x_1 x_2}{4\pi r^2},$$

$$H_2 = \frac{C_2}{2\pi} \left(\frac{3}{2} \log r - \frac{x_2^2}{2r^2} \right) - C_1 \frac{x_1 x_2}{4\pi r^2}.$$

\square

Lemma 5.4 *Under Assumptions 4.1 and 5.1, the strain components can be put in the form:*

$$\mathcal{E}_{\kappa z}^* = E_\kappa + e_\kappa, \quad (5.8)$$

$$\mathcal{E}_{\alpha\beta}^* = E_{\alpha\beta} + e_{\alpha\beta}, \quad (5.9)$$

where vector E_κ has a vanishing curl on Ω_z for any given z while vector e_κ is $o(r^{-2})$ as $r \rightarrow 0^+$, and where tensor $E_{\alpha\beta}$ is compatible on Ω_z for any given z while tensor $e_{\alpha\beta}$ is $o(r^{-2})$ as $r \rightarrow 0^+$.

Proof. By Assumption 5.1, $\partial_\kappa \mathcal{E}_{\kappa i}^*$ is a Radon measure on Ω_z , and hence writes by Radon-Nykodým's decomposition theorem as

$$\partial_\kappa \mathcal{E}_{\kappa i}^* = f_i + \phi_i, \quad (5.10)$$

where $f_i \in L^1(\Omega_z)$ and where ϕ_i is a Radon measure on Ω_z singular with respect to Lebesgue's measure. As a mere consequence of the smoothness of $\partial_\kappa \mathcal{E}_{\kappa i}^*$ on Ω_z^0 , ϕ_i is a concentrated measure on Ω_z and hence is proportional to the Dirac mass δ_0 ,

$$\phi_i = C_i \delta_0 = (2\pi)^{-1} C_i \partial_\kappa^2 \log r. \quad (5.11)$$

▲ *First statement.*

- By Eqs. (5.10), (5.11) with $i = z$, and Lemma 5.2, there exists an irrotational g_κ such that

$$\partial_\kappa (\mathcal{E}_{\kappa z}^* - g_\kappa - (2\pi)^{-1} C_z \partial_\kappa \log r) = 0,$$

in such a way that, by Lemma 5.1,

$$\mathcal{E}_{\kappa z}^* - g_\kappa - (2\pi)^{-1} C_z \partial_\kappa \log r = \epsilon_{\kappa\gamma} \partial_\gamma \psi, \quad (5.12)$$

where ψ is a distribution. Apply the curl operator to Eq. (5.12) and take into account the irrotational property of g_κ in such a way that $\Delta\psi = \epsilon_{\kappa\beta} \partial_\beta \mathcal{E}_{\kappa z}^*$. Since $\mathcal{E}_{\kappa z}^*$ is a L^1 -vector, its curl is a first-order distribution⁵ and hence, by the strain compatibility which ensures the curl of $\mathcal{E}_{\kappa z}^*$ to be a constant K on Ω_z^0 and a combination of the Dirac mass and its first-order derivatives at the origin (Schwartz, 1957), writes as $K + c\delta + c_\gamma \partial_\gamma \delta$.

⁵Following Schwartz (1957), a distribution is of order 1 if it defines a linear continuous map on $C_c^1(\Omega)$.

- Now in the resulting equation

$$\partial_\beta \left(\epsilon_{\kappa\beta} \mathcal{E}_{\kappa z}^* - (2\pi)^{-1} c \partial_\beta \log r - \frac{K}{2} x_\beta \right) = c_\gamma \partial_\gamma \delta, \quad (5.13)$$

the term on the left-hand side is the divergence of a L^1 -vector, and hence Eq. (5.13) has no distributional solution unless $c_\gamma = 0$.

- It results that $\Delta\psi = K + (2\pi)^{-1} c \Delta(\log r)$ provides a gauge field ψ which writes as

$$\psi = h + (2\pi)^{-1} c \log r, \quad (5.14)$$

where h is a solution of $\Delta h = K$ on Ω_z . It is easily verified that the curl of ψ is $o(r^{-2})$ as $r \rightarrow 0^+$.

- Defining $E_\kappa = g_\kappa + (2\pi)^{-1} C_z \partial_\kappa \log r$ and $e_\kappa = \epsilon_{\kappa\gamma} \partial_\gamma \psi$ in Eq. (5.12) achieves the first statement proof.

▲ *Second statement.*

- Let us prove that the divergence of f_i is the Laplacian of an $L^1(\Omega_z)$ function. In fact, since η_z^* writes as

$$\eta_z^* = \partial_\alpha (\partial_\alpha \mathcal{E}_{\kappa\kappa}^* - \partial_\beta \mathcal{E}_{\alpha\beta}^*), \quad (5.15)$$

it is from Assumption 5.1 a concentrated first-order distribution writing as a combination of the Dirac mass and its first-order derivatives. Hence:

$$\begin{aligned} \partial_\beta f_\beta &= \partial_\alpha \partial_\beta \mathcal{E}_{\alpha\beta}^* - \partial_\beta \phi_\beta = \Delta \mathcal{E}_{\kappa\kappa}^* - \eta_z^* - \partial_\beta \phi_\beta = \Delta \mathcal{E}_{\kappa\kappa}^* - \hat{c} \delta_0 - \hat{c}_\gamma \partial_\gamma \delta_0 \\ &= \Delta (\mathcal{E}_{\kappa\kappa}^* - \bar{c} \log r - \bar{c}_\gamma \partial_\gamma \log r), \end{aligned} \quad (5.16)$$

where $\hat{c}, \hat{c}_\gamma, \bar{c}, \bar{c}_\gamma$ are constants.

- From Eqs. (5.10), (5.7), (5.4) and Lemma 5.2, there exists a compatible $g_{\kappa\beta}$ such that

$$\partial_\kappa (\mathcal{E}_{\kappa\beta}^* - g_{\kappa\beta} - G_{\kappa\beta}) = 0, \quad (5.17)$$

in such a way that, by Lemma 5.1,

$$\mathcal{E}_{\kappa\beta}^* - g_{\kappa\beta} - G_{\kappa\beta} = \epsilon_{\kappa\gamma} \epsilon_{\beta\tau} \partial_\gamma \partial_\tau A, \quad (5.18)$$

for some gauge field $A \in \mathcal{D}'(\Omega_z)$ verifying, by the compatibility of $g_{\kappa\beta}$ and $G_{\kappa\beta}$ on Ω_z , the relation

$$\eta_z^* = \Delta \Delta A \quad \text{on } \Omega_z. \quad (5.19)$$

Hence, since the left-hand side writes as a combination of derivatives of δ_0 of order lower or equal to 1, the field A is the solution of $\Delta A = (a + a_\gamma \partial_\gamma) \log r$ with constant a, a_γ , up to a smooth harmonic function on Ω_z . It follows that $A = (a + a_\gamma \partial_\gamma) \left(\frac{r^2}{4} (\log r - 1) \right)$ is a $C^0(\Omega_z)$ solution of Eq. (5.19) such that:

$$\partial_\kappa \partial_\beta A \quad \text{is } o(r^{-2}) \quad \text{as } r \rightarrow 0^+. \quad (5.20)$$

- The proof is complete with the definitions $E_{\kappa\beta} = G_{\kappa\beta} + g_{\kappa\beta}$ and $e_{\kappa\beta} = \epsilon_{\kappa\gamma} \epsilon_{\beta\tau} \partial_\gamma \partial_\tau A$ in Eqs. (5.18) and (5.20). \square

5.2 Mesoscopic incompatibility for a set of isolated defect lines

Theorem 5.1 [Main 2D result] Under Assumptions 4.1 and 5.1, for a set \mathcal{L} of isolated dislocations parallel to the z -axis and located at the positions x_β^L , $L \in \mathcal{L}$, incompatibility as defined by Eq. (4.9) is the vectorial first order distribution

$$\eta_k^* = \delta_{kz}\eta_z^* + \delta_{k\kappa}\eta_\kappa^*, \quad (5.21)$$

where

- its vertical component is

$$\eta_z^* = \sum_{L \in \mathcal{L}} \left(\Omega_z^* \delta_L + \epsilon_{\alpha\gamma} \left(B_\gamma^* + \epsilon_{\beta\gamma} (x_\beta^L - x_{0\beta}) \Omega_z^* \right) \partial_\alpha \delta_L \right), \quad (5.22)$$

- its planar components are

$$\eta_\kappa^* = \sum_{L \in \mathcal{L}} \frac{1}{2} \epsilon_{\kappa\alpha} B_z^* \partial_\alpha \delta_L. \quad (5.23)$$

Proof. From Lemma 5.4 the strain $\mathcal{E}_{\beta n}^*$ ($n = \alpha$ or z) is decomposed in compatible parts (E_β and $E_{\alpha\beta}$) and $o(r^{-2})$ parts (e_β and $e_{\alpha\beta}$) to which the demonstration may be limited by linearity. Since from Eqs. (5.14) and (5.20) the gradients $\partial_\gamma e_\beta$, $\partial_\gamma e_{\alpha\beta}$ are $o(r^{-3})$ for $r \rightarrow 0^+$, the proof of Theorem 4.1 can be followed for every $L \in \mathcal{L}$ as soon as $\mathcal{E}_{\beta z}^*$ is replaced by e_β and $\mathcal{E}_{\beta\tau}^*$ by $e_{\beta\tau}$. However, since the dislocations are located at positions x_β^L instead of 0, an additional shift x_β^L is required in Eq. (5.22). \square

5.3 Mesoscopic defect densities in 2D incompatible elasticity

Since the tensors Θ_{ik}^* , Λ_{ik}^* , α_{ik}^* vanish for $i \neq z$, the 2D densities for an ensemble \mathcal{L} of rectilinear dislocations write as follows⁶:

Definition 5.1

$$\Theta_k^* := \sum_{L \in \mathcal{L}} \delta_{kz} \Omega_z^* \delta_L \quad (5.24)$$

$$\Lambda_k^* := \sum_{L \in \mathcal{L}} B_k^* \delta_L, \quad (5.25)$$

$$\alpha_k^* := \alpha_{zk}^* = \Lambda_k^* - \delta_{k\alpha} \epsilon_{\alpha\beta} \Theta_z^* (x_\beta - x_{0\beta}). \quad (5.26)$$

Moreover, in the 2D case, the contortion tensor writes as:

$$\kappa_{ij}^* = \delta_{iz} \alpha_j^* - \frac{1}{2} \alpha_z^* \delta_{ij}. \quad (5.27)$$

The following result expresses the incompatibility in terms of κ_{ij}^* :

Theorem 5.2 Under Assumptions 4.1 and 5.1, the mesoscopic strain incompatibility for a set \mathcal{L} of rectilinear dislocations writes as

$$\eta_k^* = \Theta_k^* + \epsilon_{\alpha\beta} \partial_\alpha \kappa_{k\beta}^*, \quad (5.28)$$

or equivalently as $\eta_k^* = \Theta_k^* + \epsilon_{k\alpha l} \partial_\alpha \kappa_{zl}^*$. \square

⁶Various notations are used in the literature to represent the defect densities. In particular, Nye (1953), Kröner (1980) and Kleinert (1989) give different definitions of the dislocation density and contortion tensors (without considering disclinations in the first two cases). We here follow Kröner's and Kleinert's notations for α_{ij}^* and Nye's original definition of κ_{ij}^* , with Nye's α_{ij}^* here denoted by α_{ji}^* . It should be recalled that the term "contortion" was introduced by Kondo (1952).

Proof. Consider any straight dislocation $L \in \mathcal{L}$ located at a given $x^L \in \Omega$. From Theorem 5.1, incompatibility writes as

$$\begin{aligned}\eta_k^* &= \delta_{kz} (\Omega_z^* \delta_L + \epsilon_{\alpha\gamma} (B_\gamma^* + \epsilon_{\beta\gamma} (\hat{x}_\beta - x_{0\beta}) \Omega_z^*) \partial_\alpha \delta_L) \\ &+ \delta_{k\kappa} \frac{1}{2} \epsilon_{\kappa\alpha} B_z^* \partial_\alpha \delta_L.\end{aligned}\quad (5.29)$$

Taking into account Eqs. (5.24), (5.25), (5.26), and (5.27), and the relation

$$\partial_\alpha ((x_\beta - x_{0\beta}) \delta_L) = \partial_\alpha \left((x_\beta^L - x_{0\beta}) \delta_L \right) = (x_\beta^L - x_{0\beta}) \partial_\alpha \delta_L,$$

it results from Theorem 5.1 that incompatibility can be written in the alternative formulation

$$\eta_k^*(x^L) = \Theta_k^*(x^L) + \epsilon_{\alpha\beta} \partial_\alpha \kappa_{k\beta}^*(x^L), \quad (5.30)$$

or equivalently as $\eta_k^*(x^L) = \Theta_k^*(x^L) + \epsilon_{k\alpha l} \partial_\alpha \kappa_{zl}^*(x^L)$. The result follows after summation on $L \in \mathcal{L}$ and using Eqs. (5.24), (5.25), (5.26), and (5.27). \square

First of all, the tensor $\bar{\partial}_j \bar{\partial}_l u_k^*$ is defined on the entire Ω in a similar way as $\bar{\partial}_j \omega_k^*$:

Definition 5.2

$$\bar{\partial}_j \bar{\partial}_l u_k^* := \partial_j \mathcal{E}_{kl}^* + \epsilon_{kpl} \bar{\partial}_j \omega_p^*. \quad (5.31)$$

By Proposition 3.1, the displacement field u_k^* is a multivalued function of index 2, which is obtained on Ω_L by recursive line integration of $\partial_j^{(s)} \partial_l^{(s)} u_k^* = \partial_j^{(s)} (\mathcal{E}_{kl}^* + \omega_{kl}^*)$ and hence by recursive integration of $\bar{\partial}_j \bar{\partial}_l u_k^*$.

Remark 5.3 *In the situation where, for a particular selection of the reference point, the dislocations have vanishing Burgers vectors, the disclination density equals the incompatibility*

$$\epsilon_{\alpha\beta} \partial_\alpha \bar{\partial}_\beta \omega_k^* = \Theta_k^* = \eta_k^*. \quad (5.32)$$

Using an arbitrary reference point, this expression is certainly false in the general case where disclinations coexist with dislocations. Moreover, the tensor $\bar{\partial}_j \bar{\partial}_l u_k^$ does not provide relevant information in terms of defect densities since $\epsilon_{iji} \bar{\partial}_j \bar{\partial}_l u_k^* = 0$ on Ω .*

The mesoscopic vectors and tensors Θ_k^* , Λ_k^* , α_k^* , κ_k^* and η_k^* are concentrated distributions on the defect lines which provide all the information on dislocation and disclination densities. However, homogenisation to the macro-scale still requires to clarify their link with the multiple-valued rotation and displacement fields. In order to resolve this problem, the tensors $\bar{\partial}_j \omega_k^*$ and $\bar{\partial}_j \bar{\partial}_l u_k^*$ are completed by appropriate concentrated effects in the defect lines, without however modifying their relationship with the multiple-valued displacement and rotation fields defined in Ω_L .

Definition 5.3

$$\bar{\partial}_\beta \omega_k^* := \bar{\partial}_\beta \omega_k^* - \kappa_{k\beta}^*, \quad (5.33)$$

$$\bar{\partial}_\alpha \bar{\partial}_\beta u_k^* := \bar{\partial}_\alpha \bar{\partial}_\beta u_k^* - \epsilon_{kp\beta} \kappa_{p\alpha}^* = \partial_\alpha \mathcal{E}_{k\beta}^* + \epsilon_{kp\beta} \bar{\partial}_\alpha \omega_p^*. \quad (5.34)$$

Theorem 5.3 *The vector and tensor distributions $\bar{\partial}_\beta \omega_k^*$ and $\bar{\partial}_\alpha \bar{\partial}_\beta u_k^*$ verify:*

$$\text{MESOSCOPIC DISCLINATION DENSITY} \quad \Theta_k^* = \epsilon_{\alpha\beta} \partial_\alpha \bar{\partial}_\beta \omega_k^*, \quad (5.35)$$

$$\text{MESOSCOPIC DISLOCATION DENSITY} \quad \alpha_k^* = \epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta u_k^*. \quad (5.36)$$

Proof. The first statement is a mere consequence of Eq. (5.28) while the second one follows from Eq. (5.33) by simple calculations, noting that $\bar{\partial}_m \omega_m^* = 0$ on Ω and that

$$\alpha_k^* = \kappa_{zk}^* - \kappa_{pp}^* \delta_{zk}. \quad (5.37)$$

□

Remark 5.4 Eqs. (5.35) and (5.24) directly show that

$$\int_S \epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta \omega_k^* dS = \int_S \Theta_k^* dS = \sum_{L \in \mathcal{L}_C} \Omega_k^{*L}, \quad (5.38)$$

where the domain S is bounded by the counterclockwise-oriented Jordan curve C , which encloses once each defect line of the subset \mathcal{L}_C of \mathcal{L} . Similarly, Eqs. (5.36) and (5.26) show that

$$\begin{aligned} \int_S \epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta u_k^* dS &= \int_S (\Lambda_k^* - \delta_{k\alpha} \epsilon_{\alpha\beta} \Theta_z^*(x_\beta - x_{0\beta})) dS, \\ &= \sum_{L \in \mathcal{L}_C} \left(B_k^{*L} - \delta_{k\alpha} \epsilon_{\alpha\beta} \Omega_z^{*L}(x_\beta^L - x_{0\beta}) \right). \end{aligned} \quad (5.39)$$

Remark 5.5 The vector $\bar{\partial}_l \omega_z^*$ does not verify Stokes theorem, neither in the classical sense, since $\epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta \omega_z^*$ is singular at x^L , nor in a measure theoretical sense, since $\epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta \omega_z^*$ is not a measure but a first-order distribution given by Eq. (5.22). As often observed in the literature, even in an inappropriate context, a formal use of Stokes theorem may give a correct final result. We here prefer to avoid any confusion and hence to mention that, in view of a clarification of Stokes' theorem in the context of defective crystals, the following formula holds and can be proved as a consequence of the previous definitions:

$$\int_C \bar{\partial}_l \omega_z^* dx_l = \int_{S_C} \epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta \omega_z^* dS. \quad (5.40)$$

6 Macroscopic analysis

6.1 A first approach to homogenisation from meso- to macro-scale

The mesoscopic results given in the previous sections are now homogenised (in an appropriate manner, whose description (Kröner, 2001) is not the purpose of this paper). Indeed, in the context of linear elasticity, the macroscopic elastic strain \mathcal{E}_{ij} is obtained by averaging the mesoscopic stress σ_{ij}^* and hence the macroscopic elastic incompatibility η_{ik} is obtained by averaging the mesoscopic incompatibility η_{ik}^* . Moreover the defect densities are homogenised and the macroscopic counterparts of Θ_k^* , Λ_k^* , α_k^* and κ_{ij}^* write as Θ_k , Λ_k , α_k , and κ_{ij} , with

$$\alpha_k = \kappa_{zk} - \kappa_{pp} \delta_{zk} \quad \text{and} \quad \kappa_{ij} = \delta_{iz} \alpha_j - \frac{1}{2} \alpha_z \delta_{ij}. \quad (6.1)$$

Definition 6.1 (Macroscopic Frank and Burgers tensors) *The Frank and Burgers vectors crossing a macroscopic surface S are defined as*

$$\Omega_k(S) := \int_S \Theta_k dS, \quad (6.2)$$

$$B_k(S) := \int_S \Lambda_k dS. \quad (6.3)$$

By homogenisation of Eqs. (5.33) and (5.34), the macroscopic counterparts of Definition 5.3 write as follows:

Definition 6.2

$$\bar{\partial}_\beta \omega_k := \epsilon_{kpq} \partial_p \mathcal{E}_{q\beta} - \kappa_{k\beta}, \quad (6.4)$$

$$\bar{\partial}_\alpha \bar{\partial}_\beta u_k := \partial_\alpha \mathcal{E}_{k\beta} + \epsilon_{kp\beta} \bar{\partial}_\alpha \omega_p, \quad (6.5)$$

where $\mathcal{E}_{k\beta}$ and $\kappa_{k\beta}$ define the macroscopic elastic strain and contortion.

Moreover, the macroscopic counterpart of Theorem 5.2 (i.e. the fundamental equation "inc $\mathcal{E} = \Theta + \text{curl } \kappa$ " of the continuum theory of defects by Kröner (1980)⁷) and Theorem 5.3 now follow from homogenisation of the mesoscopic defect densities and from Definition 6.2:

Theorem 6.1

$$\text{KRÖNER'S IDENTITY} \quad \eta_k = \Theta_k + \epsilon_{\alpha\beta} \partial_\alpha \kappa_{k\beta}, \quad (6.6)$$

$$\text{MACROSCOPIC DISCLINATION DENSITY} \quad \Theta_k = \epsilon_{\alpha\beta} \partial_\alpha \bar{\partial}_\beta \omega_k, \quad (6.7)$$

$$\text{MACROSCOPIC DISLOCATION DENSITY} \quad \alpha_k = \epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta u_k. \quad (6.8)$$

Remark 6.1 *By Stokes' theorem, if S is a region enclosed by a curve C , which might have only fractal regularity (Harrison and Norton, 1992), then $\Omega_k(S) = \int_C \bar{\partial}_\beta \omega_k dx_\beta$.*

Moreover, in the absence of disclinations, $B_k(S) = \int_S \alpha_k dS$.

The macroscopic density tensors Λ_k and κ_{ij} , as obtained from the single-valued mesoscopic densities, have a geometrical interpretation (Kröner, 1980; Anthony, 1970) which will be discussed in the following section. Indeed, α_k is directly related to the torsion of a body submitted to an incompatible purely elastic deformation to which a non-Riemannian connexion is attached due to the contortion κ_{ij} .

6.2 The non-Riemannian macroscopic body

The following geometric objects are introduced after homogenisation of the well-defined mesoscopic elastic strain and defect densities, in order to provide the model of a macroscopic body endowed with a law of parallel displacement together with internal torsion accounting for the defective crystal structure.

Definition 6.3

$$\text{METRIC TENSOR:} \quad g_{ij} := \delta_{ij} - 2\mathcal{E}_{ij}, \quad (6.9)$$

$$\text{TORSION:} \quad T_{k;ij} := -\frac{1}{2} \epsilon_{pij} (\alpha_{pk} - \epsilon_{kmn} \Theta_{pm} (x_n - x_{0n})), \quad (6.10)$$

SYMMETRIC CHRISTOFFEL SYMBOLS:

$$\tilde{\Gamma}_{k;ij} := \frac{1}{2} (\partial_i g_{kj} + \partial_j g_{ki} - \partial_k g_{ij}), \quad (6.11)$$

$$\text{CONTORTION:} \quad \Delta \Gamma_{k;ij} := T_{j;ik} + T_{i;jk} - T_{k;ji}, \quad (6.12)$$

NON SYMMETRIC CHRISTOFFEL SYMBOLS:

$$\Gamma_{k;ij} := \tilde{\Gamma}_{k;ij} - \Delta \Gamma_{k;ij}. \quad (6.13)$$

Remark 6.2 *The metric of the actual configuration $R(t)$ is δ_{ij} . Therefore, as required (cf Introduction and Remark 2.1) the reference configuration R_0 is nowhere used to introduce the above objects.*

⁷Note that different sign conventions for the rotation vector and incompatibility apply in Kröner's work.

Since small displacements are considered, no distinction is to be made between upper and lower indices.

Lemma 6.1 *The tensor g_{ij} defines a Riemannian metric. The symmetric Christoffel symbols $\tilde{\Gamma}_{k;ij}$ define a symmetric connexion compatible with this metric, while $T_{k;ij}$ and $\Delta\Gamma_{k;ij}$ are skew-symmetric tensors w.r.t. i and j and i and k , respectively. Moreover, the components of $T_{k;ij}$ for $i = z$ or $j = z$ vanish in the 2D case.*

Proof. The first statements follow from basic definitions (Dubrovin et al., 1992; Schouten, 1954) while the last one follows from the fact that, in the 2D case, $\alpha_{pk}(x^L)$ and $\Theta_{pm}(x^L)$ for $L \in \mathcal{L}$ are proportional to $\tau_p \delta_L(x^L)$ with τ_p standing for the tangent vector to the defect line. \square

Proposition 6.1 *The Cristoffel symbols $\Gamma_{k;ij}$ define a non-symmetric connexion compatible with the metric g_{ij} and whose torsion writes as $T_{k;ij}$.⁸*

Proof. It is easy to verify (Dubrovin et al., 1992) that $\Gamma_{k;ij}$ is a connexion since $\tilde{\Gamma}_{k;ij}$ is a connexion and $\Delta\Gamma_{k;ij}$ is a tensor. Denoting by ∇_k (resp. $\tilde{\nabla}_k$) the covariant gradient w.r.t. $\Gamma_{k;ij}$ (resp. $\tilde{\Gamma}_{k;ij}$), and recalling that a connexion is compatible with the metric g_{ij} if the covariant gradient of g_{ij} w.r.t. this connexion vanishes, we find by Eq. (6.13)

$$\begin{aligned}\nabla_k g_{ij} &= \partial_k g_{ij} - \Gamma_{l;ik} g_{lj} - \Gamma_{l;jk} g_{li} \\ &= \tilde{\nabla}_k g_{ij} + \Delta\Gamma_{l;ik} g_{lj} + \Delta\Gamma_{l;jk} g_{li},\end{aligned}\tag{6.14}$$

where in the right-hand side, the 1st term vanishes by Lemma 6.1 while the 2nd and 3rd terms cancel each other since $\Delta\Gamma_{l;jk} g_{li} = \Delta\Gamma_{i;jk} = -\Delta\Gamma_{j;ik}$. It results that the connexion torsion, i.e. the skew-symmetric part of $\Delta\Gamma_{j;ik}$ w.r.t. i and k , writes as

$$\begin{aligned}\frac{1}{2}(\Delta\Gamma_{j;ik} - \Delta\Gamma_{j;ki}) &= -\frac{1}{2}(\Delta\Gamma_{i;jk} - \Delta\Gamma_{k;ji}) = \frac{1}{2}((\Delta\Gamma_{k;ij} - \Delta\Gamma_{i;kj}) + \\ &(\Delta\Gamma_{k;ji} - \Delta\Gamma_{k;ij}) - (\Delta\Gamma_{i;jk} - \Delta\Gamma_{i;kj})).\end{aligned}\tag{6.15}$$

Observing that the 1st term in the right-hand side of Eq. (6.15) writes as $\Delta\Gamma_{k;ij}$ while, by Definition 6.3 (Eq. (6.12)), the left-hand side and the two remaining terms of the right-hand side of Eq. (6.15) are equal to $T_{j;ik}$, $T_{k;ji}$ and $-T_{i;jk}$, respectively, the proof is complete. \square

The following result shows $\Delta\Gamma_{k;ij}$ as directly linked to the contortion κ_{ij} .

Proposition 6.2 *In the 2D case, the contortion tensor $\Delta\Gamma_{k;ij}$ writes in terms of κ_{ij} as*

$$\begin{aligned}\Delta\Gamma_{k;ij} &= \delta_{k\kappa}(\delta_{i\alpha}\delta_{j\beta}\epsilon_{\kappa\alpha}\kappa_{z\beta}) + \delta_{i\alpha}\delta_{jz}\epsilon_{\alpha\tau}\kappa_{\tau\kappa} + \delta_{iz}\delta_{j\beta}\epsilon_{\beta\tau}\kappa_{\tau\kappa} \\ &\quad - \delta_{kz}\delta_{i\alpha}\delta_{j\beta}\epsilon_{\alpha\beta}\kappa_{zz}.\end{aligned}$$

Proof. For $k = z$, by Definition 6.3, the last statement of Lemma 6.1, and Eq. (6.1), it is found that $\Delta\Gamma_{z;ij} = \Delta\Gamma_{z;\alpha\beta}\delta_{i\alpha}\delta_{j\beta}$, with

$$\begin{aligned}\Delta\Gamma_{z;\alpha\beta} = T_{z;\alpha\beta} &= -\frac{1}{2}\epsilon_{\alpha\beta}\alpha_z = -\epsilon_{\alpha\beta}\kappa_{zz} \\ &= -\frac{1}{2}\epsilon_{\alpha\tau}\delta_{\tau\beta}\alpha_z = \epsilon_{\alpha\tau}\kappa_{\tau\beta}.\end{aligned}$$

⁸In the literature, a so-called Bravais' crystal is a macroscopic body endowed with a lattice where parallel displacement along the crystallographic lines is defined by the connexion $\Gamma_{k;ij}$ of Theorem 6.1 and where the metric is not defined by Eq. (6.9), but by the motion of an internal observer who would measure his own displacement by counting the atomic lattice steps, without feeling the body torsion (Kröner, 1980).

For $k = \kappa$, by Definition 6.3 and the last statement of Lemma 6.1, it is found that

$$\Delta\Gamma_{\kappa;ij} = \delta_{i\alpha}\delta_{j\beta}(T_{\kappa;\alpha\beta} + T_{\beta;\alpha\kappa} + T_{\alpha;\beta\kappa}) + \delta_{i\alpha}\delta_{jz}T_{z;\alpha\kappa} + \delta_{iz}\delta_{j\beta}T_{z;\beta\kappa},$$

with $T_{z;\xi\kappa} = \epsilon_{\xi\tau}\kappa_{\tau\kappa}$ and $T_{\xi;\tau\nu} = -\frac{1}{2}\epsilon_{\tau\nu}(\alpha_{\xi} + \epsilon_{\xi\gamma}\Theta_z(x_{\gamma} - x_{0\gamma}))$. Since the combination of the terms in Θ_z vanish in $\Delta\Gamma_{\kappa;ij}$, the proof is completed by observing that $\epsilon_{\alpha\beta}\alpha_{\kappa} + \epsilon_{\kappa\alpha}\alpha_{\beta} = (\epsilon_{\alpha\kappa}\epsilon_{\tau\nu})\epsilon_{\tau\beta}\alpha_{\nu} = \epsilon_{\alpha\kappa}\alpha_{\beta} = \epsilon_{\alpha\kappa}\kappa_{z\beta}$. \square

The following definition introduces two differential forms related, on the one hand (by Definitions 6.2 and 6.3, and Theorem 6.1 and Proposition 6.1) to the homogenisation of the well-defined mesoscopic defect measures and, on the other hand, as shown by the forthcoming theorem, to macroscopic incompatible rotation and distortion vectors.

Definition 6.4 *The following differential forms are introduced:*

$$d\omega_j := \bar{\partial}_{\beta}\omega_j dx_{\beta}, \quad (6.16)$$

$$d\beta_{kl} := -\Gamma_{l;k\beta} dx_{\beta}. \quad (6.17)$$

In the literature the existence of an elastic macroscopic distortion field is generally postulated (Mura, 1987; Head et al., 1993; Cermelli and Gurtin, 2001, 2002; Koslowski et al., 2002; Ariza and Ortiz, 2005) and the global distortion decomposition in elastic and plastic parts follows⁹. The point of view of the present paper is to avoid this kind of a-priori decomposition, which we believe cannot be rigorously justified. Nevertheless, the following theorem introduces rotation and distortion fields (which are not the global rotation and distortion related to the macroscopic strain) in the absence of disclinations. In contrast with the classical literature where it is basically postulated that dislocation density is the distortion curl, this relationship is here well-proved.

Theorem 6.2 *[Bravais rotation and distortion fields] If the macroscopic disclination density vanishes, there exists rotation and distortion fields defined as*

$$\text{BRAVAIS ROTATION} \quad \omega_j(x) := \omega_j^0 + \int_{x_0}^x d\omega_j, \quad (6.18)$$

$$\text{BRAVAIS DISTORTION} \quad \beta_{kl}(x) := \mathcal{E}_{kl}(x^0) - \epsilon_{klj}\omega_j^0 + \int_{x_0}^x d\beta_{kl}, \quad (6.19)$$

with $\beta_{kl} = \mathcal{E}_{kl} - \epsilon_{klj}\omega_j$, and where ω_j^0 is arbitrary and the integration is made on any line with endpoints x_0 and x . Moreover,

$$\partial_{\alpha}\beta_{k\beta} = \bar{\partial}_{\alpha}\bar{\partial}_{\beta}u_k \quad \text{and} \quad \epsilon_{\alpha\beta}\partial_{\alpha}\beta_{k\beta} = \alpha_k. \quad (6.20)$$

Proof. By Definition 6.3, the symmetric part of the connexion writes as

$$-\Gamma_{(l;k)\beta} dx_{\beta} = -\frac{1}{2}\partial_{\beta}g_{kl} dx_{\beta} = -\frac{1}{2}\partial_m g_{kl} dx_m = \partial_m \mathcal{E}_{kl} dx_m = d\mathcal{E}_{kl},$$

while, by Definition 6.3 and Proposition 6.2, the skew-symmetric part writes as

$$-\Gamma_{[l;k]\beta} = -\frac{1}{2}(\partial_k g_{l\beta} - \partial_l g_{k\beta}) + \Delta\Gamma_{l;k\beta} = \partial_k \mathcal{E}_{l\beta} - \partial_l \mathcal{E}_{k\beta} + \Delta\Gamma_{l;k\beta}.$$

Observing, by Definitions 6.2 and 6.4 and Proposition 6.2, that $d\omega_j = \bar{\partial}_{\beta}\omega_j dx_{\beta} = -\frac{1}{2}\epsilon_{lkj}\Gamma_{[l;k]\beta} dx_{\beta}$, it results that $d\beta_{kl} = d\mathcal{E}_{kl} - \epsilon_{klj}d\omega_j$. Under the assumption of a vanishing macroscopic disclination density, the existence of well-defined Bravais rotation and distortion fields follows from Eqs. (6.16) and (6.20), Theorem 6.1, and Remark 6.1. Moreover, since $\partial_{\alpha}\beta_{k\beta} = \partial_{\alpha}\mathcal{E}_{k\beta} - \epsilon_{k\beta j}\bar{\partial}_{\alpha}\omega_j$, by Eq. (6.5), it equals $\bar{\partial}_{\alpha}\bar{\partial}_{\beta}u_k$, completing the proof by Eq. (6.8). \square

⁹In fact, the distortion is often considered as a constitutive variable in dislocation models (Davini, 1986; Gurtin, 2002; Ariza and Ortiz, 2005).

Remark 6.3 Referring to "Bravais" instead of "elastic" rotation and distortion fields is devoted to highlight that these quantities do not have a purely elastic meaning

Remark 6.4 The Bravais distortion does not derive from a Bravais displacement in the presence of dislocations. In fact, around a closed loop C , even if the macroscopic disclination density vanishes, the displacement differential as defined by $du_k := \beta_{k\alpha} dx_\alpha$ verifies by Theorem 6.2 the relationship:

$$\int_C du_k = \int_S \epsilon_{\beta\alpha} \partial_\beta \beta_{k\alpha} dS = \alpha_k(S). \quad (6.21)$$

Remark 6.5 Eq. (6.18) indicates that symbol $\bar{\partial}$ in Eq. (6.16) becomes a true derivation operator in the absence of disclinations.

Remark 6.6 Theorem 6.1 defines an operation of parallel displacement according to the Bravais lattice geometry. The parallel displacement of any vector v_i along a curve of tangent vector $dx_\alpha^{(1)}$ is such that $dx_\alpha^{(1)} \nabla_\alpha v_i = 0$ and hence that the components of v_i vary according to the law $d^{(1)}v_i = -\Gamma_{i;j\beta} v_j dx_\beta^{(1)}$ (Dubrovin et al., 1992). This shows the macroscopic Burgers vector and dislocation density together with the Bravais rotation and distortion fields as reminiscences of the defective crystal properties at the nanoscale. In fact, if $dx_\nu^{(1)}, dx_\xi^{(2)}$ are two infinitesimal vectors with the associated area $dS := \epsilon_{\nu\xi} dx_\nu^{(1)} dx_\xi^{(2)}$, it results from Eq. (6.10), Remark 6.1, and the skew symmetry of $T_{k;\alpha\beta}$ that, in the absence of disclinations,

$$dB_k = \alpha_k dS = -\epsilon_{\alpha\beta} \Gamma_{k;\alpha\beta} dS = -\Gamma_{k;\alpha\beta} (dx_\alpha^{(1)} dx_\beta^{(2)} - dx_\beta^{(1)} dx_\alpha^{(2)}),$$

whose right-hand side appears as a commutator verifying the relation

$$dB_k = \epsilon_{\alpha\beta} \bar{\partial}_\alpha \bar{\partial}_\beta u_k dS = -\epsilon_{\alpha\beta} d^{(\alpha)}(dx^{(\beta)}).$$

7 Concluding remarks

In this paper we have developed a 2D theory to analyse dislocated single crystals at the meso-scale by combining distributions with multiple-valued kinematic fields. The distributions are basically concentrated along the defect lines, which in turn form the branching lines of the multivalued fields. As a consequence of this analysis, a basic theorem relating the incompatibility tensor (as derived from the deformation field) to the Frank and Burgers vectors of the defect line has been established. This theory provides a framework for the homogenisation of the medium properties from meso- to macro-scale. In particular the macroscopic dislocation density is defined without stipulating an a-priori distortion decomposition into elastic and plastic parts (which does not exist, actually). The classical relationship between Bravais distortion and dislocation densities, instead of being a definition, now appears as a result taking its origin from the meso-scale analysis. Moreover, the torsion and contortion tensors, which both describe the defective macroscopic crystal, are now properly understood as averages of concentrated mesoscopic tensors. Since the latter are the differentials (in an appropriate sense) of multivalued mesoscopic fields, we have shown how mesoscopic multivaluedness is recovered in the geometric properties of the non-Riemannian macroscopic crystal. In particular, in contrast with the mesoscale (where defects are due to the multivaluedness of the rotation and displacement fields) the macroscopic Burgers vector now appears as the commutator of a non-closed differential operator related to the body torsion.

Extension to the 3D case is under investigation. Here, the handling of non-rectilinear curves will be required in the framework of the geometric-measure theory. This should eventually make it possible to consider a set of defect curves, freely occupying the crystal with possible intersections and accumulation regions-forming so-called dislocation clusters.

A Appendix: Computation of 2D rectilinear dislocations

A.1 First group of solutions: planar displacement field

From the constitutive law $\sigma_{ij}^* = \lambda \mathcal{E}_{kk}^* \delta_{ij} + 2\mu \mathcal{E}_{ij}^*$ with λ, μ the Lamé coefficients and since $\mathcal{E}_{kk}^* = \mathcal{E}_{\gamma\gamma}^*$, the following planar law holds:

$$\sigma_{\alpha\beta}^* = \kappa^* \mathcal{E}_{\gamma\gamma}^* \delta_{\alpha\beta} + 2\mu \mathcal{E}_{\alpha\beta}^{*D}, \quad (\text{A.1})$$

with the planar compressibility modulus κ^* defined by $\kappa^* := \lambda + \mu$ and the planar deviatoric strain given by $\mathcal{E}_{\alpha\beta}^{*D} = \mathcal{E}_{\alpha\beta}^* - \frac{1}{2} \mathcal{E}_{\gamma\gamma}^* \delta_{\alpha\beta}$. From the equilibrium conditions $\partial_\beta \sigma_{\beta\gamma}^* = 0$ it follows that

$$\sigma_{\alpha\beta}^* = \epsilon_{\alpha\gamma} \epsilon_{\beta\delta} \partial_\gamma \partial_\delta F, \quad (\text{A.2})$$

for a smooth enough Airy function F , in such way that

$$\sigma_{\alpha\alpha}^* = \partial_\alpha^2 F = \Delta F. \quad (\text{A.3})$$

The relations between stress and strain are

$$\mathcal{E}_{\alpha\beta}^* = \frac{1 + \nu^*}{E^*} \sigma_{\alpha\beta}^* - \frac{\nu^*}{E^*} \sigma_{\gamma\gamma}^* \delta_{\alpha\beta}, \quad (\text{A.4})$$

with the 3D and planar elastic coefficients $E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}$, $\nu = \frac{\lambda}{2(\lambda + \mu)}$, $E^* := \frac{E}{1 - \nu^2}$, and $\nu^* := \frac{\nu}{1 - \nu}$.

The first compatibility condition Eq. (4.1) writes from Eqs. (A.3) and (A.4) as

$$\Delta \Delta F = 0.$$

In this and the following sections, functions of the complex variable $Z = x + iy$ and its conjugate \bar{Z} are now introduced. Remembering that, compared to holomorphic functions, analytical functions may be multivalued it is easily seen that given two analytic functions f and g , all real functions of the form

$$F = \Re\{\bar{Z}f + g\}$$

satisfy Eq. (A.2) and vice-versa. Eq. (A.3) then shows that

$$\sigma_{xx}^* + \sigma_{yy}^* = 4\Re\{f'(Z)\}.$$

From Eqs. (A.3) and (A.4) the deformation tensor is given by

$$\begin{cases} \mathcal{E}_{xx}^* + \mathcal{E}_{yy}^* = \frac{4(1-\nu^*)}{E^*} \Re\{f'(Z)\}, \\ \mathcal{E}_{yy}^* - \mathcal{E}_{xx}^* + 2i\mathcal{E}_{xy}^* = \frac{2(1+\nu^*)}{E^*} (\bar{Z}f''(Z) + g''(Z)), \end{cases} \quad (\text{A.5})$$

yielding after integration

$$\begin{aligned} E^*(u_x^* - iw_y^*) &= (3 - \nu^*)\bar{f}(Z) - (1 + \nu^*)(\bar{Z}f'(Z) + g'(Z)), \\ E^*\omega_z^* &= 4\Im\{f'(Z)\}. \end{aligned} \quad (\text{A.6})$$

It should be emphasised that $\mathcal{E}_{\alpha\beta}^*$ must be a single-valued field.

A.2 Second group of solutions: vertical displacement field

Another solution concerns the particular case where $u_\alpha^* = 0$, noting that each solution of 2D elasticity can be decomposed into a purely planar and a purely vertical solution. In fact, since stress equilibrium shows that

$$(\lambda + \mu)\partial_i\partial_j u_j^* + \mu\Delta u_i^* = 0,$$

it is easy to infer for $i = z$ that

$$u_z^* = \frac{(1 + \nu)}{E}\Re\{h(Z)\}, \quad (\text{A.7})$$

with $h(Z)$ an analytic function. Then

$$\mathcal{E}_{xz}^* - i\mathcal{E}_{yz}^* = \frac{(1 + \nu)}{2E}h'(Z). \quad (\text{A.8})$$

The function $h'(Z)$ must be uniform. The complex rotation is

$$\omega^* := \omega_x^* + i\omega_y^* = -\frac{i(1 + \nu)}{2E}\overline{h'(Z)}. \quad (\text{A.9})$$

In 2D isothermal linear elasticity without body forces, every displacement solution has planar components given by Eq. (A.6) and a vertical component given by Eq. (A.7) while the rotation vector has planar components given by Eq. (A.9) and a vertical component given by Eq. (A.7) (Sokolnikoff (1946) and Knopp (1996)).

A.3 The three 2D examples of rectilinear defects

In this section we consider two typical multivalued analytic functions $\log(Z)$ and $Z\log(Z)$. Starting from the general uniform strain expressions Eq. (A.5) or Eq. (A.8) it is easily observed that any of the holomorphic functions f'' (with $\Re\{f''\}$ single-valued), g'' and h' can provide a solution to the 2D problem. Since these functions can be expanded in Laurent series:

$$f''(Z) = \sum_{-\infty}^{+\infty} a_n Z^n, \quad g''(Z) = \sum_{-\infty}^{+\infty} b_n Z^n, \quad h'(Z) = \sum_{-\infty}^{+\infty} c_n Z^n,$$

inside their respective convergence annuli, primitivation shows that

$$\left\{ \begin{array}{l} f(Z) = \sum_{\substack{-\infty \\ n \neq -1, -2}}^{+\infty} \frac{a_n}{(n+1)(n+2)} Z^{n+2} - a_{-2} \ln(Z) + a_{-1} Z \ln(Z) + A_1 Z + A_0, \\ g(Z) = \sum_{\substack{-\infty \\ n \neq -1, -2}}^{+\infty} \frac{b_n}{(n+1)(n+2)} Z^{n+2} - b_{-2} \ln(Z) + b_{-1} Z \ln(Z) + B_1 Z + B_0, \\ h(Z) = \sum_{\substack{-\infty \\ n \neq -1}}^{+\infty} \frac{c_n}{n+1} Z^{n+1} + c_{-1} \ln(Z) + C_0, \end{array} \right.$$

with a_{-1} real in order that $\Re\{f'\}$ be uniform. The relevant cases are those which give rise to a dislocation or a disclination, i.e. such that the functions $\overline{f}, f', g', \Re\{h\}$ or $\Im\{f'\}$ are multivalued. Hence, in order to obtain non-vanishing rotation or displacement jumps, one needs to consider the following cases:

$$f(Z) = -a_{-2} \ln\left(\frac{Z}{R}\right) + a_{-1} Z \ln\left(\frac{Z}{R}\right), \quad a_{-1} \in \mathbb{R}, \quad (\text{A.10})$$

$$g(Z) = b_{-1} Z \ln\left(\frac{Z}{R}\right), \quad (\text{A.11})$$

$$h(Z) = c_{-1} \ln\left(\frac{Z}{R}\right), \quad c_{-1} \in i\mathbb{R}, \quad (\text{A.12})$$

where R is a constant length and to which any purely elastic term may always be added. In fact, from Eqs. (A.6), (A.7), (A.7) and (A.9), and from the definition $B^* := B_x^* + iB_y^*$ with B_k^* given by Eq. (3.11), it follows that:

$$\left\{ \begin{array}{l} \Omega_z^* = \frac{4}{E^*}[\Im\{f'\}], \\ \bar{B}^* : = B_x^* - iB_y^* = [u_x^*] - i[u_y] - \Omega_z^*(iz) \\ \quad = \frac{3-\nu^*}{E^*}[\bar{f}] - \frac{1+\nu^*}{E^*}\{\bar{Z}[f'] + [g']\} + \frac{4i\bar{Z}}{E^*}[\Im\{f'\}], \\ \Omega^* : = \Omega_x^* + i\Omega_y^* = -\frac{i(1+\nu)}{2E}[\bar{h}'], \\ B_z^* = [u_z^*] - \Re\{i\bar{Z}\Omega^*\} = \frac{1+\nu}{E}[\Re\{h\}] - \frac{1+\nu}{2E}\Re\{\bar{Z}[\bar{h}']\} = \frac{1+\nu}{E}[\Re\{h\}]. \end{array} \right.$$

It should immediately be noted that Ω^* vanishes identically since h' cannot be multivalued. From Eqs. (A.10)-(A.12) and some easy computations, the only possible solutions are given by the following proposition.

Proposition A.1 *For a straight defect line L in 2D elasticity, there are no more than three distinct defect classes. The two dislocation classes are the screw dislocation with a vertical Burgers vectors B_z^* , as generated by the analytical function h ($f = g = 0$), and the edge dislocation with a planar complex Burgers vector $B_x^* + iB_y^*$, as generated by the analytical function g ($f = h = 0$). There is a single class of disclinations, the wedge disclination, which has a vertical Frank vector Ω_z^* and is generated by the analytical function f ($g = h = 0$). These functions are:*

$$\begin{array}{ll} \text{WEDGE DISCLINATION} & f(Z) = \frac{E^*\Omega_z^*}{8\pi} z \ln\left(\frac{Z}{R}\right) \\ \text{EDGE DISLOCATION} & g(Z) = \frac{E^*(B_y^* + iB_x^*)}{2(1+\nu^*)\pi} Z \ln\left(\frac{Z}{R}\right) \\ \text{SCREW DISLOCATION} & h(Z) = \frac{iEB_z^*}{2\pi(1+\nu)} \ln\left(\frac{Z}{R}\right). \end{array}$$

For the edge dislocation, a detailed derivation is given by Eshelby (1966).

References

- Alexander, H., Haasen, P., 1968. Dislocations and plastic flow in the diamond structure. *Solid State Phys.* 22, 27-158.
- Alexander, H., 1986. *Dislocations in solids*. Ed. F. R. N. Nabarro, Vol. 7. North-Holland, Amsterdam.
- Almgren, F.J., 1986. Deformations and multiple-valued functions. *P. Symp. Pure Math.* 44, 29-130.
- Ambrosio, L., Fusco, N., Palara, D., 2000. *Functions of bounded variation and free discontinuity problems*. Oxford Mathematical Monographs, Oxford,
- Anthony, K.H., 1970. Die Theorie der Disklinationen. *Arch. Rational Mech. Anal.* 39, 1, 43-88.
- Anthony, K.H., 1970. Die Reduktion von nichteuklidischen geometrischen Objekten in eine euklidische Form und physikalische Deutung der Reduktion durch Eigenspannungszustände in Kristallen. *Arch. Rational Mech. Anal.* 37, 3, 161-180.
- Ariza, M.P., Ortiz, M., 2005. Discrete crystal elasticity and discrete dislocations in crystals. *Arch. Rational Mech. Anal.* 178, 2, 149-226.
- Brezis, H., 1983. *Analyse fonctionnelle*. Masson Editeur, Paris.
- Bilby, B.A., 1960. Continuous distribution of dislocations. *Solid Mechanics*, Eds.

- N. Sneddon and R. Hillin Progress, Vol. 1. North-Holland, Amsterdam.
- Burgers, J.M., 1939. Some considerations on the field of stress connected with dislocations in a regular crystal lattice. Proc. K. Ned. Akad. 42, 293-324.
- Cermelli, P., Gurtin, M.E., 2001. On the characterization of geometrically necessary dislocations in finite plasticity. J. Mech. Phys. Solids 49, 1539-1568.
- Cosserat, E. and F., 1909. Théorie des corps déformables. Hermann, Paris.
- Davini, C., 1986. A proposal for a continuum theory of defective crystals. Arch. Rational Mech. Anal. 96, 4, 295-317.
- Dubrovin, B.A., Fomenko, A.T., Novikov, S.P., 1992. Modern geometry-methods and applications, Part 1 (2nd edn.). Springer-Verlag, New-York.
- Eshelby, J.D., Frank, F.C., Nabarro, F.R.N., 1951. The equilibrium linear arrays of dislocations. Phil. Mag. 42, 351-364.
- Eshelby, J.D., 1956. The continuum theory of lattice defect. Solid State Physics, Eds. F. Seitz and D. Turnbull, Vol. 3. Academic Press, New-York.
- Eshelby, J.D., 1966. A simple derivation of the elastic field of an edge dislocation. Brit. J. Appl. Phys. 17, 1131-1135.
- Estrada, R., Kanwal, R.P., 1989. Regularization, pseudofunction, and Hadamard finite part. J. Math. Anal. Appl. 141, 195-207.
- Evans, L.C., Gariépy, R., 1992. Measure theory and fine properties of functions. CRC Press, New York.
- Gurtin, M.E., 2002. A gradient theory of single-crystals viscoplasticity that accounts for geometrically necessary dislocations. J. Mech. Phys. Solids 50, 5-32.
- Harrison, J., Norton, A., 1992. The Gauss-Green theorem for fractal boundaries. Duke Math. J. 67, 3, 575-588.
- Head, A.K., Howison, S.D., Ockendon, J.R., Tighe, S.P., 1993. An equilibrium theory of dislocation continua. Siam Rev. 35, 4, 580-609.
- Jordan, A.S., Von Neida, A.R., Caruso, R., 2000. The theory and practise of dislocation reduction in *GaAs* and *InP*. J. of Cryst. Growth 218, 555-573.
- Kleinert, H., 1989. Gauge fields in condensed matter, Vol.1. World Scientific Publishing, Singapore.
- Knopp, K., 1996. Theory of functions, Part 1&2. Dover Publications, New York.
- Kondo, K., 1952. On the geometrical and physical foundations of the theory of yielding (in Proc. 2nd Japan Nat. Congr. Applied Mechanics). Tokyo.
- Kondo, K., 1962. Non-Riemannian geometry of imperfect crystals from a macroscopic viewpoint (in RAAG Memoirs of the unifying study of basic problems in engineering and physical science by means of geometry, ed. K. Kondo, Vol. 3). Tokyo.
- Koslowski, M., Cuitino, A.M., Ortiz, M., 2002. A phase field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystal. J. Mech. Phys. Solids 50, 2597-2635.
- Kratochvil, J., Dillon, O.W., 1969. Thermodynamics of elastic-plastic materials as a theory with internal variables. J. Appl. Phys. 40, 8, 3207-3218.
- Kröner, E., 1955. Die Spannungsfunktionen der dreidimensionalen anisotropen Elastizitätstheorie. Z. Physik 140.
- Kröner, E., 1980. Continuum theory of defects. Physiques des défauts, Les Houches session XXXV, Course 3, ed. R. Balian.
- Kröner, E., 1990. The differential geometry of elementary point and line defects in Bravais crystals. Int. J. Theor. Phys. 29, 11, 1219-1237.
- Kröner, E., 2001. Benefits and shortcomings of the continuous theory of dislocations. Int. J. Solids Struc. 38, 1115-1134.
- Maroudas, D., Brown, R.A., 1991. On the prediction of dislocation formation in semiconductor crystals grown from the melt: analysis of the Haasen model for plastic deformation dynamics. J. of Cryst. Growth 108.
- Mattila, P., 1995. Geometry of sets and measures in Euclidean spaces-Fractals

- and rectifiability. Cambridge studies in advanced mathematics, Cambridge, 1995.
- Mawhin, J., 1992. Analyse: fondements, techniques, evolutions. De Boek Université, Louvain-la-Neuve.
- Mura, T., 1987. Micromechanics of defects in solids (2nd edn.). Kluwer Academic Publishers, Boston.
- Nye, J.F., 1953. Some geometrical relations in dislocated crystals. *Acta Metall.* 1, 153-162.
- Remmert, R., 1996. From Riemann surfaces to Riemann spaces. Proceedings of the colloquium to the memory of Jean Dieudonné, Nice, France, January 1996, Société Mathématique de France, Sémin. Congr. 3.
- Schouten, J.A., 1954. Ricci-Calculus (2nd edn.). Springer Verlag, Berlin.
- Schwartz, L., 1957. Théorie des distributions. Hermann, Paris.
- Sokolnikoff, I.S., 1946. Mathematical theory of elasticity. Mc Graw-Hill, New-York.
- Thom, R., 1980. Concepts in the theory of ordered media. *Physiques des défauts, Les Houches session XXXV, Course 6*, ed. R. Balian.
- Van den Bogaert, N., Dupret, F., 1997. Dynamic global simulation of the Czochralski process: I. Principles of the method; II. Analysis of the growth of a Ge crystal. *J. Cryst. Growth* 171, 65-76; 77-93.
- Volterra, V., 1907. Sur l'équilibre des corps élastiques multiplement connexes. *Ann. Sci. École Norm. Sup.* 3, 24, 401-517.