doi:10.1017/S0956792512000010

A distributional approach to 2D Volterra dislocations at the continuum scale

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(*Received 29 October 2009; revised 4 January 2012; accepted 9 January 2012*)

We develop a theory to represent dislocations and disclinations in single crystals at the continuum (or mesoscopic) scale by directly modelling the defect densities as concentrated effects governed by the distribution theory. The displacement and rotation multi-valuedness is resolved by introducing the intrinsic and single-valued Frank and Burgers tensors from the distributional gradients of the strain field. Our approach provides a new understanding of the theory of line defects as developed by Kröner [10] and other authors [6, 9]. The fundamental identity relating the incompatibility tensor to the Frank and Burgers vectors (and which is a cornerstone of the theory of dislocations in single crystals) is proved in the 2D case under appropriate assumptions on the strain and strain curl growth in the vicinity of the assumed isolated defect lines. In general, our theory provides a rigorous framework for the treatment of crystal line defects at the mesoscopic scale and a basis to strengthen the theory of homogenisation from mesoscopic to macroscopic scale.

Key words: Dislocations; disclinations; distribution theory; strain incompatibility; defect density tensors

1 Introduction

Dislocations can be considered as the most complex class of defects for several kinds of single crystals such as Gallium Arsenide, Germanium or Sapphire. Even in Silicon single crystal growth, the rapid slip of dislocations, along the glide planes from the crystal wall to the solid–liquid interface, can generate high stress concentration and be the cause of crystal loss of structure. Therefore, the development of a relevant and accurate physical model represents a key issue with a view to reducing the dislocation density in the growing crystal by appropriate action on the processing conditions [5]. Unfortunately, the classical models used for that purpose, such as the Alexander–Haasen–Sumino model [13], exhibit drawbacks including their inability to model the dislocation slip over long distances within preferential planes, and hence, there is a strong need for a more relevant and better founded mathematical approach.

The physics of dislocations in single crystals cannot be easily captured since 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 (its precise definition is given in

Section 3.2). These properties play a fundamental role in the modelling of line defects in single crystals at the continuum scale and induce key conservation laws at the macro-scale. Aware of these principles and of previous pioneer works [3, 6, 8, 14, 17], Kröner [10] considers 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. The dislocation density shows to be divergence-free, and hence, obeys a dislocation conservation law. Survey contributions may be found in [8, 12]. On the contrary, no such conservation law could exist for a polycrystal since the dislocations abruptly end at the grain boundaries. Therefore the usual plasticity models, which are devoted to predict the behaviour of polycristalline materials and do not take this conservation law into account, are not able to capture the basic physics of dislocations in single crystals.

In the theory of Kröner [10], the mesoscopic scale is mainly used to give a meaning to the diffuse macroscopic dislocation density. However, at the mesoscopic scale the dislocation density is concentrated within the defect lines, and hence, particular tools are required to establish a rigorous link between the mesoscopic and macroscopic scales, the goal being to homegenise the mesoscopic fields in order to well-define their macroscopic counterparts. Without entering the homogenisation theory (which is not the objective of this work), it is of the utmost importance to observe that only additive (or extensive) fields, such as stresses or internal energy, are allowed to be homegenised. Indeed, homogenisation will typically consist in adding an ensemble of random samples, or in integrating the required field over a representative volume, etc., in order to get the searched average.

Having this issue in mind, the present paper is devoted to develop a mesoscopic theory of the geometry of crystal dislocations and disclinations (the latter represent less frequent crystal line defects which are considered for the sake of generality). Since dislocations and disclinations are lines at the continuum scale, concentrated effects are introduced in our model by means of the distribution theory [15]. In addition, since integration around the defect lines generates multiple-valued displacement and rotation fields with the dislocations/disclinations as branching lines, particular care is given to multi-valued functions. This combination of distributional effects and multi-valuedness is a key feature of the theory of line defects at the continuum scale but unfortunately the resulting difficulties have not well been addressed so far in the literature, the principal problem resulting from the fact that multiple-valued fields are never additive and hence cannot be homogenised. Our solution will consist in introducing new single-valued and intrinsic tensors called the Burgers and Frank tensors (cf. Section 2.2) and using these tensors everywhere possible in place of the multiple-valued displacement and rotation fields.

The principal contribution of this paper is to provide a theoretical framework for a combined treatment of distributions and multi-valued functions and to apply this theory to a set of isolated, moving or not, parallel line defects under the hypothesis of a $2D$ elastic strain field. Although distributions were already applied to several subjects of solid mechanics, such as fracture [2, 4], their use to highlight special aspects of the dislocation/disclination theory was not investigated so far to the knowledge of the authors.

As a main application of our theory, we here revisit the theory of Kröner [10] at the mesoscopic scale. In brief, Kröner states from physical reasons that the incompatibility of the macroscopic elastic strain is the curl of the dislocation density (as represented by the so-called contortion tensor) plus the disclination density if any. This relationship appears as a cornerstone for any modelling of the behaviour of line defects in single crystals. In the present paper, we provide a complete proof of the mesoscopic counterpart of this relation for a family of isolated $2D$ defect lines and under specific growth assumptions on the elastic strain behaviour in the vicinity of the defect line(s). Starting from the mesoscopic scale is required to achieve the proof. Previously, this equality was only known as a formal result without taking into account the concentrated or multi-valued nature of the involved fields.

So our principal objective will be to show that, for a set of isolated parallel rectilinear defect lines, the mesoscopic strain incompatibility

$$\eta^\star = -\nabla \times \mathscr{E}^\star \times \nabla, \tag{1.1}$$

writes as

$$\eta^\star = \Theta^\star + \nabla \times (\kappa^\star)^T, \tag{1.2}$$

where $\mathscr{E}^\star$ stands for the strain field while $\Theta^\star$ and $\kappa^\star$ denote appropriate measures of the defect densities defined for each defect line L as follows:

DISCLINATION DENSITY: $$\Theta^\star := \tau\delta_L \otimes \Omega^\star, \tag{1.3}$$

DISLOCATION DENSITY: $$\Lambda^\star := \tau\delta_L \otimes B^\star, \tag{1.4}$$

CONTORTION: $$\kappa^\star := \alpha^\star - \frac{I}{2}\operatorname{tr}\alpha^\star, \tag{1.5}$$

with the auxiliary defect density

$$\alpha^\star := \Lambda^\star + \Theta^\star \times (x - x_0). \tag{1.6}$$

In formulas (1.3)–(1.6), $\Omega^\star$ and $B^\star$ denote the Frank and Burgers vectors attached to the line L (cf. Section 3.2), δ_L and τ stand for the concentrated line measure and tangent vector along L, symbol $\otimes$ is used to denote the tensor product, and x_0 is a prescribed reference point.

To give a meaning to the above theorem and definitions, let us first observe that incompatibility is defined from (1.1) as the double (left and right) curl of the mesoscopic strain, in such a way that $\eta^\star$ classically vanishes whenever $\mathscr{E}^\star$ derives from an infinitesimal displacement $u^\star$. Also, $\eta^\star$ is a concentrated distribution on the defect lines. Then, a non-vanishing incompatibility necessarily involves that no single-valued rotation and displacement fields can be integrated from the linear strain, this resulting from some rotational and/or translational integration mismatch around the defect lines. On the other hand, equations (1.3) and (1.4) define $\Theta^\star$ and $\Lambda^\star$ as concentrated defect densities along the defect lines. Indeed, the Frank and Burgers vectors $\Omega^\star$ and $B^\star$ are defined on the defect lines only and hence, their multiplication by the concentrated δ_L provides tractable line densities. Multiplying the result by the tangent vector τ defines the second-order defect density tensors $\Theta^\star$ and $\Lambda^\star$ [10], which contain all the information provided by the Frank and Burgers vectors and the defect line orientation. According to these explanations, equation (1.2) appears as a precise relationship between incompatibility and rotational or translational line defects.

The basic concepts to represent the dislocated continuous medium are introduced in Section 2, together with the Burgers and Frank tensors. These tensors are used in Section 3 to resolve the multi-valuedness issue and to define the dislocation and disclination densities by appropriate integrals. In Section 4, the $2D$ distributional theory of the dislocated medium is established in the case of isolated parallel dislocations/disclinations, while conclusions are drawn in Section 5.

2 The dislocated continuous medium

At the mesoscopic scale, dislocations and disclinations are lines whose characteristic length is some average distance between neighbour defects. There is no need for a precise definition of this length which is simply assumed to be much larger than a typical diameter of the defect cores, as is generally the case in single crystal growth. Then, outside of the defect lines, the remaining of the medium is an elastic continuum.

In general, all kinematic fields (strain, displacement, rotation ...) are geometrically defined with respect to a reference configuration, which should be viewed as a motionless virtual picture of the evolving medium. In other words, strain, displacement and rotation are defined from the reference to the actual configuration. Whereas in general, in Continuum Mechanics the reference configuration is arbitrary, it will be chosen at the mesoscopic scale as isothermal, stress-free and without dislocations/disclinations (it is associated with a perfect lattice), and hence, the reference configuration is completely specified up to an arbitrary rigid body motion and uniform thermal dilation. Let us emphasise that, with this peculiar definition, the topologies of the reference and actual configurations (in which the "internal" and "external" observers of Kröner [10] are located) differ in the presence of dislocations/disclinations. In particular, any closed loop followed by the external observer around a defect line will correspond to a non-closed path for the internal observer (i.e. a path whose extremities differ). Nevertheless, the principal advantage of taking a perfect lattice as reference configuration is to give a precise geometrical meaning to the strain field, which is both frame-indifferent and invariant with respect to the mesoscopic reference configuration (up to the selection of the reference temperature). It should also be noted that a second and equivalent definition of the mesocopic strain can be obtained from the constitutive equations governing the elastic medium, by expressing the strain in terms of the frame-indifferent stress and temperature fields.

Contrarily to the strain and as long as a perfect lattice is selected as reference configuration for a dislocated medium, displacement and rotation show to be multi-valued fields at the mesoscale, and hence, take their values on a domain called a Riemann foliation (which in general neither is the reference nor the actual configuration). Its precise definition is given in Section 3. The Riemann foliation can be univoquely associated to the actual configuration if cuts are introduced in order to select one particular branch of the displacement and rotation. However, this approach causes major theoretical difficulties and will not be used in the sequel.

In this paper, linear thermo-elasticity will be considered (this assumption being generally valid in single-crystal growth). Then, the stress–strain–temperature relationship takes the following form:

$$\mathscr{E}^\star = C^\star \sigma^\star + \beta^\star (T^\star - T_0),$$

where $\sigma^\star$ denotes the stress field, $C^\star$ and $\beta^\star$ stand for the fourth- and second-order compliance and thermal dilation tensors, and T_0 is the reference temperature.

In linear thermoelasticity, it is usually said that strain, displacement and rotation become "infinitesimal", and hence, that the reference and actual configurations coincide. In the absence of defect lines, the strain is everywhere compatible ($\eta^{\star} = 0$) in such a way that single-valued rotation and displacement fields can be integrated from the strain field provided the domain be simply connected. This procedure will be recalled in Section 3. However, when disclinations or dislocations are present, rotation and displacement become multiple-valued and this multi-valuedness, therefore, appears as a reminiscence of the difference between Kröner's internal and external observers.

According to the above discussion, the starting field of our analysis is the assumed linear elastic strain, which is a single-valued and extensive field. The Burgers and Frank tensors are directly defined from the strain gradient and share its invariance and extensiveness properties. Also, these tensors appear as second-grade variables which can readily be used to model the free energy density with possible application to the modelling of dislocation/disclination motion. The Burgers and Frank vectors are integrated around the defect lines from their tensorial counterparts and will appear as key invariant quantities associated with the defect-lines, and from which the dislocation and disclination densities are defined.

2.1 Basic notations and assumptions

Some mathematical conventions are required for the presentation of our theory. First, the bounded or unbounded domain consists of a regular and a defective part.

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

Starting from the sole elastic strain, the defects are the lines along which the strain is not compatible.

Assumption 2.2 (Mesoscopic elastic strain) *Henceforth, we will assume that the linear strain is a given symmetric $L^1_{loc}(\Omega)$ tensor, which is also smooth and compatible on $\Omega_{\mathscr{L}}$. In other words, the incompatibility tensor $\eta^{\star}$, as defined componentwise by*

STRAIN INCOMPATIBILITY:
$$\eta^{\star}_{kl} := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathscr{E}^{\star}_{mn}, \tag{2.1}$$

where differentiation is carried out in the distribution sense, is assumed to vanish everywhere on $\Omega_{\mathscr{L}}$.

From now on, the classical indicial notation will be used together with Einstein's summation convention on repeated (or dummy) indices.

Careful analysis of equation (2.1) shows that the incompatibility tensor $\eta^{\star}_{kl}$ is a purely concentrated distribution (which is more complicated than a mere Radon measure) inside the defect lines. There is no other way to rigorously define the mesoscopic incompatibility and this consideration justifies our approach.

Now, the present analysis is restricted to isolated defect lines.

Assumption 2.3 (Defect lines) *The set of defect lines $\mathscr{L}$ will consist of a set of isolated rectifiable arcs $L^{(k)}$, $k \in \mathscr{I}$, without multiple points except possibly their end-points and on which the linear elastic strain is singular.*

Here, a set of isolated arcs means a set of arcs: (i) whose extremities form a set of isolated points of Ω in the classical sense and (ii) such that each point $\hat{x}$ of these arcs except their extremities can be located in a smooth surface $S(\hat{x})$ bounded by a loop $C(\hat{x})$ and such that $S(\hat{x}) \setminus \hat{x} \in \Omega_{\mathscr{L}}$.

2.2 The Frank and Burgers tensors

In the following essential definitions, the strain is considered as a distribution on Ω. First, the Frank tensor generalises the concept of rotation gradient to dislocated media.

Definition 2.1 (Frank tensor) The Frank tensor $\overline{\partial}_m \omega_k^\star$ is defined as the following distribution on Ω:

FRANK TENSOR:
$$\overline{\partial}_m \omega_k^\star := \epsilon_{kpq} \partial_p \mathscr{E}_{qm}^\star, \tag{2.2}$$

in such a way that

$$< \overline{\partial}_m \omega_k^\star, \varphi > := - \int_\Omega \epsilon_{kpq} \mathscr{E}_{qm}^\star \partial_p \varphi \, dV, \tag{2.3}$$

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

Let us recall that distributions are mathematically defined as linear and continuous functionals on smooth test-functions of compact support [15]. From a physical viewpoint, distributions are generalised functions which can exhibit concentrated effects of any kind.

Definition 2.1 shows that the Frank tensor reduces to the rotation gradient $\partial_m \omega_k^\star$ outside of the defect lines (i.e. in $\Omega_{\mathscr{L}}$). In addition, equations (2.1) and (2.2) show that the incompatibility tensor $\eta_{kl}^\star$ is the distributional curl of the Frank tensor

$$\eta_{kl}^\star = \epsilon_{kpm} \partial_p (\overline{\partial}_m \omega_l^\star). \tag{2.4}$$

Therefore, the Frank tensor comprises all the information required to integrate the multiple-valued rotation field $\omega_k^\star$ outside of the defect lines and to derive the concentrated incompatibility field inside the defect lines.

The second key tensor used in our theory is the Burgers tensor, which plays in the construction of the displacement field a role analogous to the Frank tensor in the construction of the rotation field.

Definition 2.2 (Burgers tensor) For a selected reference point $x_0 \in \Omega_{\mathscr{L}}$, the Burgers tensor is defined on the entire domain Ω as the distribution

BURGERS TENSOR:
$$\overline{\partial}_l b_k^\star := \mathscr{E}_{kl}^\star + \epsilon_{kpq}(x_p - x_{0p})\overline{\partial}_l \omega_q^\star(x). \tag{2.5}$$

Both the Frank and Burgers tensors appear as single-valued extensive fields whose averages provide key information to model the behaviour of dislocations and disclinations at the macroscopic scale.

3 Multiple-valued fields and line invariants at the mesoscopic scale

In general, a multi-valued function from $\Omega_{\mathscr{L}}$ to $\mathbb{R}^N$ consists of a pair of single-valued mappings with appropriate properties

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

where F is the associated Riemann foliation [1]. In the present case of mesoscale elasticity, we will limit ourselves to multi-valued functions obtained by recursive line integration of single-valued mappings defined on $\Omega_{\mathscr{L}}$. Reducing these multiple line integrals to simple line integrals, the Riemann foliation shows to be the set of equivalence classes of paths inside $\Omega_{\mathscr{L}}$ from a given $x_0 \in \Omega_{\mathscr{L}}$ with homotopy as equivalence relationship. Accordingly, a multi-valued function will be called of index n on $\Omega_{\mathscr{L}}$ if its n-th differential is single-valued on $\Omega_{\mathscr{L}}$. No other kinds of multi-functions are considered in this work, whether $\mathscr{L}$ is a single line L or a more complex set of defect lines (with possible branchings, etc.).

3.1 Rotation and displacement vectors

The rotation and displacement vectors are defined from the linear strain together with the rotation and displacement $\omega_{0k}^\star$ and $u_{0k}^\star$ at a given point x_0.

Starting from the distributive Definition 2.1 of $\overline{\partial}_m \omega_k^\star$, the differential form $\overline{\partial}_m \omega_k^\star(\xi)\, d\xi_m$ is integrated along a regular parametric curve $\Gamma \subset \Omega_{\mathscr{L}}$ with endpoints $x_0, x \in \Omega_{\mathscr{L}}$. For selected x_0 and $\omega_{0k}^\star$, the multi-valued rotation vector is defined as

$$\omega_k^\star = \omega_{0k}^\star + \int_\Gamma \overline{\partial}_m \omega_k^\star(\xi)\, d\xi_m, \tag{3.1}$$

where $\omega_k^\star$ obviously depends on the path Γ and the rotation $\omega_{0k}^\star$ at x_0. Now, from the strain compatibility ($\eta_{kl}^\star = 0$) outside of the defect lines (i.e. in $\Omega_{\mathscr{L}}$), equation (2.4) also shows that $\omega_k^\star$ only depends on the path Γ through the equivalence class $\#\Gamma$ of all regular curves homotopic to Γ in $\Omega_{\mathscr{L}}$. Considering the set F of such equivalence classes for a selected x_0 and varying x, a discrete subset of classes is associated with each position x and these different classes (or path topologies) correspond to the different branches of the rotation $\omega_k^\star$ at x. Accordingly, F shows to be the Riemann foliation of the multiple-valued rotation field $\omega_k^\star$.

Following our approach, the Burgers tensor is then integrated in the same way as the Frank tensor along any parametric curve Γ, providing for selected $\omega^\star_{0k}$ and $u^\star_{0k}$ the index-2 multi-valued displacement vector $u^\star_k$

$$u^\star_k = u^\star_{0k} + \epsilon_{klm}\omega^\star_l(x_m - x_{0m}) + \int_\Gamma \overline{\partial}_l b^\star_k(\xi)\, d\xi_l, \tag{3.2}$$

which again depends on x and $\#\Gamma$ only (this following from (2.1) and (2.5)) and so is itself defined on the Riemann foliation F. It may be observed that $\overline{\partial}_l b^\star_k$ and the vector

$$b^\star_k = u^\star_k - \epsilon_{klm}\omega^\star_l(x_m - x_{0m}) \tag{3.3}$$

are related in the same way as $\overline{\partial}_m\omega^\star_k$ and $\omega^\star_k$, including the fact that $\overline{\partial}_l b^\star_k = \partial_l b^\star_k$ on $\Omega_{\mathscr{L}}$.

In general, every defect line will contribute to the rotation and displacement multi-valuedness, and hence, these latter fields are defined over $\Omega_{\mathscr{L}}$ and do not share the structure of a vector space. In other words, as it was already stated, the displacement and rotation fields cannot be added, and hence, are not extensive since their domains depend on the defect line locations. It will be seen in the next sections that the dislocation and disclination densities are defined from the displacement and rotation jumps around the defect lines. Nevertheless, it will also be seen that these jumps can be directly evaluated from the Burgers and Frank tensors and this will resolve the multi-valuedness issue.

3.2 Frank and Burgers vectors

Consider a regular parametric loop C (in case C is a planar loop, it is called a Jordan curve) and the equivalence class $\#C$ of all regular loops homotopic to C in $\Omega_{\mathscr{L}}$. Here, the extremity points play no role anymore and two loops are equivalent iff they can be continuously transformed into each other in $\Omega_{\mathscr{L}}$. For a selected reference point x_0, the jumps of the rotation and Burgers vectors $\omega^\star_k$ and $b^\star_k$ along $\#C$ depend on $\#C$ only and are calculated as

$$[\omega^\star_k] = \int_C \overline{\partial}_m\omega^\star_k(\xi)\, d\xi_m, \tag{3.4}$$

$$[b^\star_k] = [u^\star_k](x) - \epsilon_{klm}[\omega^\star_l](x_m - x_{0m}) = \int_C \overline{\partial}_l b^\star_k(\xi)\, d\xi_l. \tag{3.5}$$

Let us now focus on the case of a given isolated defect line $L^{(i)}$, $i \in \mathscr{I}$. The jump $[\omega^\star_k]$ of the rotation vector $\omega^\star_k$ around $L^{(i)}$ is defined as the jump of $\omega^\star_k$ along $\#C$ with C a loop enclosing once the defect line $L^{(i)}$ and no other defect line. It turns out that this jump is the same for any curve homotopic to C. Similarly, the jump $[b^\star_k]$ of the vector $b^\star_k$ around $L^{(i)}$ is defined as the jump of $b^\star_k$ along $\#C$ and is also the same for any curve homotopic to C, given x_0. These observations are summarised in the following well-known result [8].

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

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

Definition 3.2 (Frank and Burgers vectors) The Frank vector of an isolated defect line $L^{(i)},\ i \in \mathscr{I}$, is the invariant

$$\text{FRANK VECTOR:} \qquad \Omega_k^\star := [\omega_k^\star], \tag{3.6}$$

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

$$\text{BURGERS VECTOR:} \qquad B_k^\star := [b_k^\star] = [u_k^\star](x) - \epsilon_{klm}\Omega_l^\star(x_m - x_{0m}). \tag{3.7}$$

It should be emphasised from equations (3.4) and (3.5) that the Frank and Burgers vectors are accessible from the single-valued Frank and Burgers tensors $\bar{\partial}_m\omega_k^\star$ and $\bar{\partial}_l b_k$, without requiring use of the multiple-valued displacement and rotation fields. 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 can always be considered as a dislocation by appropriate choice of the common reference point x_0 while the reverse statement is false since $\Omega_k^\star$ might vanish and $[u_k^\star]$ not. In fact, two distinct reference points x_0 and x'_0 define two Burgers vectors obeying the relation $B_k^\star - B_k'^\star = \epsilon_{klm}(x_{0m} - x'_{0m})\Omega_l^\star$ (noting that $B_k^\star\Omega_k^\star$ is an invariant independent of the choice of x_0). Therefore, for a non-zero Frank vector, the vanishing of the Burgers vector depends on the choice of x_0.

This is why in the present paper, the word "dislocation" means in the general sense a dislocation and/or a disclination. A pure dislocation is a dislocation with vanishing Frank vector.

3.3 Defect densities

Having the Burgers and Frank tensors in hand and considering a set of isolated defect lines according to Assumption 2.3, let us now introduce the dislocation and disclination density tensors ($\Lambda_{ij}^\star$ and $\Theta_{ij}^\star$) as the basic physical tools to model defect density at the mesoscale [7, 9].

Definition 3.3 (Defect densities)

$$\text{DISCLINATION DENSITY:} \qquad \Theta_{ij}^\star := \sum_{k \in \mathscr{I} \subset \mathbb{N}} \Omega_j^{\star(k)} \tau_i^{(k)} \delta_{L^{(k)}} \ (i, j = 1 \cdots 3), \tag{3.8}$$

$$\text{DISLOCATION DENSITY:} \qquad \Lambda_{ij}^\star := \sum_{k \in \mathscr{I} \subset \mathbb{N}} B_j^{\star(k)} \tau_i^{(k)} \delta_{L^{(k)}} \ (i, j = 1 \cdots 3), \tag{3.9}$$

where $\delta_{L^{(k)}}$ is used to represent the $1D$ measure density (also called Hausdorff measure [11]) uniformly concentrated on the arc $L^{(k)}$ whose unit tangent vector is $\tau_i^{(k)}$, while $\Omega_j^{\star(k)}$ and $B_j^{\star(k)}$ denote the Frank and Burgers vectors of $L^{(k)}$, respectively.

From Definition 3.3 it appears that the dislocation and disclination densities are concentrated Radon measures inside the defect lines. These additive/extensive tensor fields contain the entire information provided by the Burgers and Frank vectors (viz. the invariant jumps of the displacement and rotation fields around the defect lines) together with the orientation of these defect lines.

Also, the above discussion shows that the dislocation and disclination densities can be fully integrated from the Burgers and Frank tensors. Therefore, besides the strain field which is the seminal ingredient of the present theory, the Burgers and Frank tensors appear as fundamental second-grade fields able to characterise the amount of defects on each single line or in the whole dislocated crystal. Together with the geometry of the defect set, these tensors provide the key defect measures called the dislocation and disclination density tensors, which now belong to a vector space and are easily shown to be divergence-free distributions and so are conservative fields [10]

$$\partial_i \Theta^\star_{ij} = 0, \tag{3.10}$$

$$\partial_i \Lambda^\star_{ij} = 0. \tag{3.11}$$

3.4 Additional remarks

Considering the possibly index-1 multi-valued rotation vector $\omega^\star_k$, it should be observed from Definition 2.1 that $\overline{\partial}_m \omega^\star_k = \partial_m \omega^\star_k$ on $\Omega_{\mathscr{L}}$ as a consequence of the classical relationship between infinitesimal rotation and deformation derivatives. However, $\overline{\partial}_m \omega^\star_k$ is defined by (2.2) as a distribution and, therefore, concentrated effects on $\mathscr{L}$ and its infinitesimal vicinity have to be added to $\partial_m \omega^\star_k$, justifying the use of the symbol $\overline{\partial}_m \omega^\star_k$ instead of $\partial_m \omega^\star_k$ without giving to $\overline{\partial}_m$ the meaning of an effective derivation operator.

In particular, in the vicinity of a defect line $\overline{\partial}_m \omega^\star_k$ is the finite part of an integral when acting against test-functions. Indeed, since $\partial_p \mathscr{E}^\star_{qm}$ might be non $L^1_{loc}(\Omega)$-integrable, from equation (2.3) the integral $< \epsilon_{kpq} \partial_p \mathscr{E}^\star_{qm}, \varphi >$ must be calculated on Ω as the limit

$$\lim_{\epsilon \to 0^+} \left(\int_{\Omega \setminus \odot_\epsilon} \epsilon_{kpq} \partial_p \mathscr{E}^\star_{qm} \varphi \, dV + \int_{\partial \odot_\epsilon \cap \Omega} \epsilon_{kpq} \mathscr{E}^\star_{qm} \varphi \, dS_p \right), \tag{3.12}$$

where symbol $\odot_\epsilon$ stands for a core of diameter 2ϵ enclosing the region $\mathscr{L}$ while $dS_p = n_p \, dS$ with n_p the outer unit normal from the core (so, $\odot_\epsilon$ is the intersection with Ω of the union of all closed spheres of radius ϵ centred on $\mathscr{L}$ and, if $\mathscr{L}$ consists of an single line L, $\odot_\epsilon$ is a tube of radius ϵ enclosing L).

The second term in (3.12) is precisely added to achieve convergence. One readily sees after integration by parts that (3.12) is equal to the right-hand side of (2.3) provided $\lim_{\epsilon \to 0} \Omega \setminus \odot_\epsilon = \Omega_{\mathscr{L}}$ (this hypothesis holds true for the lines satisfying Assumption 2.3).

Also, the vanishing of $\partial_m \omega^\star_k$ on $\Omega_{\mathscr{L}}$ does not imply that the distribution $\overline{\partial}_m \omega^\star_k$ vanishes as well. In fact from (3.12), it can be shown in that case that

$$< \overline{\partial}_m \omega^\star_k, \varphi >= \lim_{\epsilon \to 0} \int_{\partial \odot_\epsilon \cap \Omega} \epsilon_{kpq} \mathscr{E}^\star_{qm} \varphi \, dS_p = - \int_{\Omega} \epsilon_{kpq} \mathscr{E}^\star_{qm} \partial_p \varphi \, dV, \tag{3.13}$$

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

$$< \partial_l \overline{\partial}_m \omega_k^\star, \varphi >= - < \overline{\partial}_m \omega_k^\star, \partial_l \varphi >= \int_\Omega \epsilon_{kpn} \mathscr{E}^\star_{mn} \partial_p \partial_l \varphi \, dV. \tag{3.14}$$

4 Distributional analysis of incompatibility for isolated rectilinear dislocations

4.1 The 2D model for rectilinear dislocations

The present paper addresses the 2D problem only, this meaning that the strain $\mathscr{E}^\star_{ij}$ only depends on the coordinates x_α ($\alpha = 1, 2$) and 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. In general, in 2D elasticity, the strain is decomposed into three tensors:

$$\mathscr{E}^\star_{ij} = \underbrace{\delta_{\alpha i}\delta_{\beta j}\mathscr{E}^\star_{\alpha\beta}}_{\text{planar strain}} + \underbrace{\left(\delta_{iz}\delta_{j\gamma}\mathscr{E}^\star_{\gamma z} + \delta_{jz}\delta_{i\gamma}\mathscr{E}^\star_{\gamma z}\right)}_{\text{3D shear}} \qquad \underbrace{+\delta_{iz}\delta_{jz}\mathscr{E}^\star_{zz}.}_{\text{pure vertical compression/dilation}} \quad , \tag{4.1}$$

Then, at the mesoscale, a 2D set $\mathscr{L}$ of dislocations and/or disclinations consists of a set of isolated parallel lines $L^{(i)}$, $i \in \mathscr{I}$, on which the linear elastic strain is singular. These lines are assumed as parallel to the z-axis and the countable union of points located at the intersection between $\mathscr{L}$ and the $z = z_0$-plane is denoted by l_0, while Ω_{z_0} stands for the intersection of the domain Ω and the $z = z_0$-plane. In addition, the vectors $\eta_k^\star, \Theta_k^\star$ and $\Lambda_k^\star$ stand for the tensor components $\eta_{zk}^\star, \Theta_{zk}^\star$ and $\Lambda_{zk}^\star$. Greek indices are used to denote the values 1, 2 (instead of the Latin indices used in 3D to denote the values 1, 2 or 3). Moreover, $\epsilon_{\alpha\beta}$ denotes the permutation symbol $\epsilon_{z\alpha\beta}$.

For 2D problems the incompatibility vector contains all the information provided by the general incompatibility tensor. Equation (2.4) becomes

$$\eta_k^\star := \epsilon_{\alpha\beta} \partial_\alpha \overline{\partial}_\beta \omega_k^\star. \tag{4.2}$$

In general, from equation (4.2) the incompatibility vector $\eta_k^\star$ expresses on the one hand the non-commutative action of the defect lines 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 lines.

In 2D elasticity, it is easy to show that the strain is compatible in a connected domain iff there are real numbers K, a_α and b such that

$$\begin{cases} \epsilon_{\alpha\gamma}\epsilon_{\beta\delta}\partial_\alpha\partial_\beta\mathscr{E}^\star_{\gamma\delta} = 0, \\ \epsilon_{\alpha\beta}\partial_\alpha\mathscr{E}^\star_{\beta z} = K, \\ \mathscr{E}^\star_{zz} = a_\alpha x_\alpha + b. \end{cases} \tag{4.3}$$

Also, in the 2D case the planar Frank vector $\Omega_\alpha^\star$ vanishes. Indeed, since

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

the planar Burgers vector simply writes as

$$B^\star_\tau = \int_C (\mathscr{E}^\star_{\beta\tau} + \epsilon_{\tau\gamma}(x_\gamma - x_{0\gamma})\overline{\partial}_\beta \omega^\star_z)\, dx_\beta - \epsilon_{\tau\gamma}(z - z_0)\Omega^\star_\gamma,$$

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

4.2 Classical examples of rectilinear line defects

This section is devoted to present the three classical examples of $2D$ line-defects for which the medium is assumed to be steady, isothermal and body force free outside the defect line L, which is assumed to be located along the z-axis (cf. [7, 16, 17]). The planar and polar coordinates are denoted by (x, y) or x_α and (r, θ), respectively. Symbols (e_x, e_y, e_z) or (e_α, e_z) stand for the Cartesian base vectors, while (e_r, e_θ, e_z) denote the local cylindrical base vectors. Detail of the distributional calculation of the Frank tensors is given in Appendix A.

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

$$u^\star_i e_i = \frac{B^\star_z \theta}{2\pi} e_z \quad \text{and} \quad \omega^\star_i e_i = \frac{1}{2}\nabla \times (u^\star_i e_i) = \frac{B^\star_z}{4\pi r} e_r, \tag{4.4}$$

in such a way that the jump $[\omega^\star_i]$ vanishes while the Cartesian components of the strain tensor are given by

$$[\mathscr{E}^\star_{ij}] = \frac{B^\star_z}{4\pi r}\begin{bmatrix} 0 & 0 & \sin\theta \\ 0 & 0 & -\cos\theta \\ \sin\theta & -\cos\theta & 0 \end{bmatrix}. \tag{4.5}$$

After some calculations, the Frank tensor writes as

$$[\overline{\partial}_m \omega^\star_k] = \frac{-B^\star_z}{4\pi r^2}\begin{bmatrix} \cos 2\theta & \sin 2\theta & 0 \\ \sin 2\theta & -\cos 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix} + \frac{B^\star_z}{4}\begin{bmatrix} -\delta_L & 0 & 0 \\ 0 & -\delta_L & 0 \\ 0 & 0 & 2\delta_L \end{bmatrix}, \tag{4.6}$$

where the first term does not belong to $L^1_{loc}(\Omega)$. The Burgers tensor can be calculated from the Frank tensor by means of equation (2.5). The Frank and Burgers vectors are integrated from the Frank and Burgers tensors by use of equations (3.4)–(3.7) showing that $\Omega^\star_k = 0$ and $B^\star_k = B^\star_z \delta_{kz}$ as expected.

It should be observed that the Frank tensor clearly consists of a diffuse part, which is exactly the rotation gradient outside of the dislocation, and a concentrated part directly related to the strain incompatibility as will be shown in the next sections.

- *Combined edge dislocation and concentrated force.* The displacement vector is

$$u^\star_i e_i = \frac{B^\star_y}{2\pi}\left(-\left(\log\frac{r}{R} + 1\right) e_x + \theta e_y \right), \tag{4.7}$$

with R a translation normalisation constant while the rotation $\omega_i^\star$ vanishes together with its jump. The Cartesian components of the strain write as

$$[\mathscr{E}_{ij}^\star] = \frac{-B_y^\star}{2\pi r}\begin{bmatrix}\cos\theta & \sin\theta & 0\\ \sin\theta & -\cos\theta & 0\\ 0 & 0 & 0\end{bmatrix}. \tag{4.8}$$

while the Frank tensor shows to be

$$[\overline{\partial}_m\omega_k^\star] = \frac{B_y^\star}{4}\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & \delta_L\\ 0 & 0 & 0\end{bmatrix}, \tag{4.9}$$

and so this tensor only consists of a concentrated part. Integrating the Frank and Burgers tensors around the defect line yields $\Omega_k^\star = 0$ and $B_k^\star = B_y^\star\delta_{ky}$.

It should be noticed that the above solution is the sum of the classical Volterra edge dislocation [7] and a concentrated force per unit line whose density reads

$$f_i^\star e_i = GB_y^\star\delta_L e_x, \tag{4.10}$$

with G, the shear modulus. This force is exerted on the dislocation perpendicularly to the Burgers vector as is easily shown by integrating the associated thermoelastic stress vector around the dislocation. To remove this concentrated force from the solution, it suffices to add the following single-valued contribution to the displacement field

$$\hat{u}_i^\star e_i = \frac{B_y^\star}{8\pi}\left[\left((3-\nu^*)\log\left(\frac{r}{R}\right)^2 - (1+\nu^*)\cos 2\theta\right)e_x + (1+\nu^*)\sin 2\theta e_y\right], \tag{4.11}$$

(with $\nu^* := \frac{\nu}{1-\nu}$ standing for the $2D$ Poisson coefficient) and the corresponding terms to the strain and rotation fields. This additional solution has vanishing Frank and Burgers vectors and the appropriate compensating force along the singular line L.

In general it should be mentioned that, corresponding to the three classical line defects (the screw and edge dislocations and the wedge disclination) there are exactly three dual stress concentrated line effects (the axial and planar forces per unit line and the axial moment per unit line) which may be exerted on the singular line L. All these effects can be separated from each other and from the line defect, and hence, the associated solutions have vanishing Frank and Burgers vectors. However, whereas these singular solutions have a compatible strain, and hence, single-valued displacement and rotation fields, their Airy function then becomes multiple-valued thence requiring the use of similar distributional techniques as developed in the present paper to treat the induced stress concentrated effects.

- *Wedge disclination.* The multiple-valued planar displacement field is given by

$$u_i^\star e_i = \frac{\Omega_z^\star}{8\pi}\left[\left(2(1-\nu^*)x\log\frac{r}{R} - (1+\nu^*)x - 4y\theta\right)e_x\right.$$
$$\left. + \left(2(1-\nu^*)y\log\frac{r}{R} - (1+\nu^*)y + 4x\theta\right)e_y\right], \tag{4.12}$$

while the rotation vector is

$$\omega_i^\star e_i = \frac{\Omega_z^\star \theta}{2\pi} e_z, \tag{4.13}$$

and the Cartesian strain components write as

$$[\mathscr{E}_{ij}^\star] = \frac{\Omega_z^\star(1-\nu^*)}{4\pi}\begin{bmatrix} \log\frac{r}{R}+1 & 0 & 0 \\ 0 & \log\frac{r}{R}+1 & 0 \\ 0 & 0 & 0 \end{bmatrix} - \frac{\Omega_z^\star(1+\nu^*)}{8\pi}\begin{bmatrix} \cos 2\theta & \sin 2\theta & 0 \\ \sin 2\theta & -\cos 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{4.14}$$

Therefore, the $L^1(\Omega)$ Frank tensor is purely diffuse and writes as

$$[\overline{\partial}_m \omega_k^\star] = -\frac{\Omega_z^\star}{2\pi r}\begin{bmatrix} 0 & 0 & \sin\theta \\ 0 & 0 & -\cos\theta \\ 0 & 0 & 0 \end{bmatrix}. \tag{4.15}$$

Integrating the Frank and Burgers tensors around the defect line yields $\Omega_k^\star = \Omega_z^\star \delta_{kz}$ and $B_k^\star = 0$.

4.3 Mesoscopic incompatibility for a single defect line

In this and the following section, the theory of Kröner [10] is investigated at the mesoscopic scale. We begin by considering a single defect line L located along the z-axis as in Section 4.2. The radius r is the distance from a point x inside Ω to L, while the $1D$ measure density uniformly concentrated on L is denoted by δ_L.

Then, to establish the proof of our main theorem, an additional hypothesis is required. This 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 $O(r^{-1})$. For a straight defect line L, according to these examples, the hypotheses on the strain and Frank tensors read as follows.

Assumption 4.1 ($2D$ strain for line defects) *The strain tensor $\mathscr{E}_{ij}^\star$ is independent of the coordinate z, compatible on $\Omega_L = \Omega \setminus L$ in the sense that conditions (4.3) hold, smooth on Ω_L and L^1_{loc}-integrable on Ω.*

Assumption 4.2 (Local behaviour of the strain and Frank tensors) *The strain tensor $\mathscr{E}_{ij}^\star$ is $o(r^{-2})$ $(r \to 0^+)$ while the Frank tensor is $o(r^{-3})(r \to 0^+)$.*

The disclination and dislocation density tensors $\Theta_k^\star$ and $\Lambda_k^\star$ are then shown to be related by a fundamental distributional relation to the strain incompatibility.

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

$$\eta_k^\star = \delta_{kz}\eta_z^\star + \delta_{k\kappa}\eta_\kappa^\star, \tag{4.16}$$

with

$$\eta_z^\star = \Omega_z^\star \delta_L + \epsilon_{\alpha\gamma}\left(B_\gamma^\star - \epsilon_{\beta\gamma}x_{0\beta}\Omega_z^\star\right)\partial_\alpha \delta_L, \tag{4.17}$$

$$\eta_\kappa^\star = \frac{1}{2}\epsilon_{\kappa\alpha}B_z^\star \partial_\alpha \delta_L. \tag{4.18}$$

The detailed proof of this theorem is given in Appendix B.

4.4 Mesoscopic incompatibility for a set of isolated defect lines

To establish the theory of Kröner at the mesoscopic scale, the next step consists in rewriting Theorem 4.1 for a set of isolated defect lines.

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

$$\eta_k^\star = \delta_{kz}\eta_z^\star + \delta_{k\kappa}\eta_\kappa^\star, \tag{4.19}$$

with

$$\eta_z^\star = \sum_{i\in\mathscr{I}} \left(\Omega_z^{\star(i)}\delta_{L^{(i)}} + \epsilon_{\alpha\gamma}\left(B_\gamma^{\star(i)} + \epsilon_{\beta\gamma}(\hat{x}_\beta^{(i)} - x_{0\beta})\Omega_z^{\star(i)}\right)\partial_\alpha \delta_{L^{(i)}}\right), \tag{4.20}$$

$$\eta_\kappa^\star = \frac{1}{2}\epsilon_{\kappa\alpha}\sum_{i\in\mathscr{I}} B_z^{\star(i)}\partial_\alpha \delta_{L^{(i)}}. \tag{4.21}$$

The incompatibility decomposition is then rewritten in terms of the contortion tensor (a particular form of the dislocation density introduced by Nye, Kondo and Kröner [9, 10, 14]) and the disclination density, thereby providing a mesoscopic proof of Kröner's theory [10].

Theorem 4.3 (Incompatibility decomposition for 2D isolated defect lines) *The mesoscopic strain incompatibility for a set of isolated parallel rectilinear dislocations $\mathscr{L}$ writes as*

$$\eta_k^\star = \Theta_k^\star + \epsilon_{\alpha\beta}\partial_\alpha \kappa_{k\beta}^\star, \tag{4.22}$$

where $\kappa^\star_{k\beta}$ denotes the contortion tensor

$$\kappa^\star_{k\beta} = \delta_{kz}\alpha^\star_\beta - \frac{1}{2}\alpha^\star_z\delta_{k\beta}, \tag{4.23}$$

with $\alpha^\star_k$ standing for an auxiliary defect density vector

$$\alpha^\star_k := \Lambda^\star_k - \delta_{k\alpha}\epsilon_{\alpha\beta}\Theta^\star_z(x_\beta - x_{0\beta}), \tag{4.24}$$

and where x_0 is the selected reference point in Ω.

The latter fundamental result appears in Kröner's work [10] under assumptions which are not compatible with our approach. In fact, in his work this result follows in a straightforward manner from an "elastic-plastic" displacement gradient (or distortion) decomposition postulate, which itself requires the selection of a particular reference configuration and neither properly handle the intrinsic multi-valuedness of the mesoscopic problem nor the concentrated (and hence distributional) nature of the incompatibility field. Moreover, in our result the link between the defect densities and the Frank and Burgers vectors and tensors is clearly made, and precise assumptions on the strain field and the admissible defect structures are provided in order to validate the result.

4.5 Applications of the main result

In this section, the main result of Section 4.3 is applied to determine the Cartesian incompatibility components of the three rectilinear defect lines of Section 4.2. A distributional verification of these statements is provided in Appendix C.

- *Screw dislocation.* Since $B^\star_y = \Omega^\star_z = 0$, equations (4.17) and (4.18) yield

$$[\eta^\star_k] = \frac{B^\star_z}{2}\begin{bmatrix} \partial_y\delta_L \\ -\partial_x\delta_L \\ 0 \end{bmatrix}. \tag{4.25}$$

- *Edge dislocation.* Whereas $\overline{\partial}_m\omega^\star_k$ identically vanishes on Ω_L, it is easily seen that (4.17) and (4.18) with $B^\star_z = \Omega^\star_z = 0$ yield

$$[\eta^\star_k] = B^\star_y\begin{bmatrix} 0 \\ 0 \\ \partial_x\delta_L \end{bmatrix}. \tag{4.26}$$

- *Wedge disclination.* Incompatibility reads

$$[\eta^\star_k] = \Omega^\star_z\begin{bmatrix} 0 \\ 0 \\ \delta_L \end{bmatrix}. \tag{4.27}$$

The beautiful formulas (4.25)–(4.27) illustrate the completely concentrated nature of the incompatibility concept.

5 Concluding remarks

In this paper a general theory revisiting the work of Kröner [10] has been developed to model line defects in single crystals at the mesoscopic scale. A rigorous definition of the dislocation and disclination density tensors as concentrated effects on the defect lines has been provided in the framework of the distribution theory. The main difficulty resulting from the multi-valuedness of the displacement and rotation vector fields in defective crystals has been addressed by defining the single-valued and second-grade Burgers and Frank tensors from the distributional strain gradient. Whereas, outside the defective lines both tensors are regular functions directly related to the displacement and rotation gradients, in addition they exhibit concentrated properties within the defect lines which may be linked to the displacement and rotation jumps around these lines.

Moreover, defining the incompatibility tensor as the distributional curl of the Frank tensor, the principal result of our work has been to express in the $2D$ case incompatibility as a function of the dislocation and disclination density tensors and their distributional gradients, and to prove this so-called Kröner's formula under precise strain growth assumptions in the vicinity of the assumed isolated defect line. Any violation of these conditions, nonetheless, appears as an exceptional effect in the framework of linear elasticity since, in that case, the infinitesimal strain is linearly related to the stress tensor, which itself obeys the momentum equations. Therefore, such violation would necessitate the abnormal presence of singular body forces or inertia terms in the vicinity of the defect line. Further work will deal with the general three-dimensional dynamic theory.

The ultimate objective of this work is to define extensive mesoscopic fields that can be homogenised from meso- to macro-scale in order to provide internal variables able to model the macroscopic behaviour of the dislocated medium. In the present paper this issue was addressed by introducing the Burgers and Frank tensors, the incompatibility tensor, and the dislocation and disclination densities. Since the same linear relationships connect these mesoscopic tensors and their homogenised counterparts, the Burgers and Frank tensors appear as fundamental quantities to model the elastic–plastic behaviour of the continuous medium. The macroscopic theory will be investigated in subsequent publications.

Appendix A Calculation of the Frank tensor for $2D$ rectilinear defect lines

In $2D$ the non-vanishing Cartesian components of the Frank tensor are from equation (2.2)

$$\bar{\partial}_\alpha \omega^\star_\beta = \epsilon_{\beta\gamma} \partial_\gamma \mathscr{E}^\star_{z\alpha}, \tag{A 1}$$

$$\bar{\partial}_\alpha \omega^\star_z = \epsilon_{\beta\gamma} \partial_\beta \mathscr{E}^\star_{\gamma\alpha}, \tag{A 2}$$

$$\bar{\partial}_z \omega^\star_z = \epsilon_{\alpha\beta} \partial_\alpha \mathscr{E}^\star_{\beta z} = -\bar{\partial}_\alpha \omega^\star_\alpha, \tag{A 3}$$

the third equation showing that only $\bar{\partial}_\alpha \omega^\star_\beta$ and $\bar{\partial}_\alpha \omega^\star_z$ have to be calculated. From equation (3.12) the effect of these distributions on a smooth $2D$ test-function φ with compact support in Ω_{z_0} writes as

$$< \bar{\partial}_\alpha \omega^\star_\beta, \varphi > = \lim_{\epsilon\to 0^+} \left(\int_{\Omega_{\epsilon,z_0}} \epsilon_{\beta\gamma} \partial_\gamma \mathscr{E}^\star_{z\alpha} \varphi \, dS + \int_{\partial\Omega_{\epsilon,z_0}\cap\Omega_{z_0}} \epsilon_{\beta\gamma} \mathscr{E}^\star_{z\alpha} \varphi n_\gamma \, ds \right), \tag{A 4}$$

$$< \bar{\partial}_\alpha \omega^\star_z, \varphi > = \lim_{\epsilon\to 0^+} \left(\int_{\Omega_{\epsilon,z_0}} \epsilon_{\beta\gamma} \partial_\beta \mathscr{E}^\star_{\gamma\alpha} \varphi \, dS + \int_{\partial\Omega_{\epsilon,z_0}\cap\Omega_{z_0}} \epsilon_{\beta\gamma} \mathscr{E}^\star_{\gamma\alpha} \varphi n_\beta \, ds \right), \tag{A 5}$$

with Ω_{ϵ,z_0} denoting the slice of $\Omega \setminus \odot_\epsilon$ at $z = z_0$ and n_γ standing for the unit outer normal vector from the core $\odot_\epsilon$.

The first right-hand side terms of (A 4) and (A 5) immediately show that the diffuse part of $\bar{\partial}_\alpha \omega^\star_\beta$ or $\bar{\partial}_\alpha \omega^\star_z$ is the simple derivative $\epsilon_{\beta\gamma}\partial_\gamma \mathscr{E}^\star_{z\alpha}$ or $\epsilon_{\beta\gamma}\partial_\beta \mathscr{E}^\star_{\gamma\alpha}$ outside of the defect line L. However, when acting against a test-function, the integrals have to be taken in Cauchy principal value. Then, some calculations easily provide the diffuse part of the Frank tensors as given by equations (4.6), (4.9) and (4.15).

In a second step, a particular φ is selected whose value is everywhere 1 in the core $\odot_\epsilon$. Then, the second right-hand side terms of (A 4) and (A 5) rewrite as follows:

$$\lim_{\epsilon\to 0^+} \left(\epsilon_{\beta\gamma} \int_0^{2\pi} \mathscr{E}^\star_{z\alpha} n_\gamma \epsilon \, d\theta \right), \tag{A 6}$$

$$\lim_{\epsilon\to 0^+} \left(\epsilon_{\beta\gamma} \int_0^{2\pi} \mathscr{E}^\star_{\gamma\alpha} n_\beta \epsilon \, d\theta \right), \tag{A 7}$$

with $(n_1, n_2) = (\cos\theta, \sin\theta)$. Passing to the limit directly provides from equations (4.5), (4.8) and (4.14) the concentrated part as of equations (4.6), (4.9) and (4.15).

Appendix B Proof of theorem 4.1

In this appendix, the notations of Section 4 are used. Moreover, the projection of the current point x on the defect line L is denoted by $\hat{x}$ and $(v_\alpha, 0)$ stands for the unit vector from $\hat{x}$ to x, and, for a planar curve C, the notation $dC_\alpha(x) = \epsilon_{\alpha\beta} dx_\beta$ is used for an infinitesimal vector normal to the curve.

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

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

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

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

Proof The second compatibility condition (4.3) is equivalent to

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

from which, in the 2D case

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

and

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

Since, under the assumptions of this lemma

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

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

Proof of Theorem 4.1 For some small enough $\epsilon > 0$, a tube $\odot_\epsilon$ can be constructed around L and inside Ω. Assuming that the smooth 3D test-function φ has its compact support containing a part of L, $\Omega_{\epsilon,z}$ denotes the slice of the open $\Omega \setminus \odot_\epsilon$ obtained for a given $\hat{x} \in L$, i.e.

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

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

▲ Let us firstly treat the left-hand side of equation (4.16). From Definition 2.1 and equations (2.2), (2.3) and (4.2), it follows that

$$< \eta^\star_k, \varphi > = \int_L dz \lim_{\epsilon\to 0^+} \Pi_k(z, \varphi, \epsilon), \tag{B 1}$$

where

$$\Pi_k(z, \varphi, \epsilon) := -\int_{\Omega_{\epsilon,z}} \epsilon_{\alpha\beta}\overline{\partial}_\beta \omega^\star_k \partial_\alpha \varphi \, dS - \int_{C_{\epsilon,z}} \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\mathscr{E}^\star_{\beta n}\partial_\alpha \varphi \, dC_\gamma, \tag{B 2}$$

and with $dC_\alpha(x) = \epsilon_{\alpha\beta}dx_\beta$ standing for an infinitesimal vector normal to the curve. Then, the boundedness of $|\partial_\tau\partial_\delta\varphi|$ on Ω_L provides the following Taylor expansions of φ and $\partial_\alpha\varphi$ around $\hat{x}$:

$$\varphi(x) = \varphi(\hat{x}) + r\nu_\alpha \partial_\alpha \varphi(\hat{x}) + \frac{r^2}{2}\nu_\tau \nu_\delta \partial_\tau \partial_\delta \varphi\,(\hat{x} + \gamma_1(x - \hat{x})), \tag{B 3}$$

$$\partial_\alpha \varphi(x) = \partial_\alpha \varphi(\hat{x}) + r\nu_\tau \partial_\tau \partial_\alpha \varphi\,(\hat{x} + \gamma_2(x - \hat{x})), \tag{B 4}$$

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

▲ Consider the first term of the right-hand side of (B 2), noted $\hat{\Pi}_k$. From the strain compatibility on Ω_L and Gauss-Green's theorem, this term writes as

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

Since $r\nu_\alpha := x_\alpha - \hat{x}_\alpha = x_\alpha$, equation (B 3) and Assumption 4.2 show that, for $\epsilon \to 0^+$,

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

▲ Consider the second term of the right-hand side of (B 2), noted $\Pi_k^\star$. On account of Assumption 4.2 and from expansion (B 4), this term may be rewritten as

$$\Pi_k^\star(z,\varphi,\epsilon) := -\int_{C_{\epsilon,z}} \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\mathscr{E}^\star_{\beta n}\partial_\alpha\varphi dC_\gamma$$
$$= -\partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\mathscr{E}^\star_{\beta n}dC_\gamma + o(1).$$

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

$$\Pi_k = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} \left(x_\alpha\overline{\partial}_\tau\omega_k^\star - \epsilon_{\alpha\beta}\epsilon_{k\gamma n}\epsilon_{\gamma\tau}\mathscr{E}^\star_{\beta n}\right)dx_\tau + \Omega_k^\star\varphi(\hat{x}) + o(1). \tag{B 5}$$

▲ Consider the first term of the right-hand side of (B 5), noted Π_k', and take $\xi = \gamma$ in the identity

$$\epsilon_{k\xi n}\epsilon_{\gamma\tau} = \delta_{kz}(\delta_{\gamma\xi}\delta_{n\tau} - \delta_{n\gamma}\delta_{\tau\xi}) - \delta_{nz}(\delta_{\gamma\xi}\delta_{k\tau} - \delta_{k\gamma}\delta_{\tau\xi}), \tag{B 6}$$

in such a way that

$$\Pi_k' = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} (x_\alpha\overline{\partial}_\tau\omega_k^\star - \delta_{kz}\epsilon_{\alpha\beta}\mathscr{E}^\star_{\beta\tau} + \delta_{k\tau}\epsilon_{\alpha\beta}\mathscr{E}^\star_{\beta z})\,dx_\tau. \tag{B 7}$$

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

• When $k = z$, Definition 2.2 shows that

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

which, after multiplication by $\epsilon_{\tau\alpha}$ and using (B 6) with τ, α and z substituted for k, ξ and n, is inserted into (B 7), thence yielding

$$\Pi_z' = \partial_\alpha\varphi(\hat{x})\int_{C_{\epsilon,z}} (\epsilon_{\tau\alpha}\overline{\partial}_\beta b_\tau^\star + x_{0\alpha}\overline{\partial}_\beta\omega_z^\star + (z - z_0)\overline{\partial}_\beta\omega_\alpha^\star)\,dx_\beta, \tag{B 8}$$

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

$$\lim_{\epsilon\to 0^+}\Pi_z' = \ll \{\epsilon_{\alpha\tau}B_\tau^\star - (z - z_0)\Omega_\alpha^\star - x_{0\alpha}\Omega_z^\star\}\partial_\alpha\delta_0, \varphi_z \gg, \tag{B 9}$$

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 2.2 shows that

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

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

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

Then, by the Lemma with a permutation of κ and α, (B 7) also writes as

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

On the other hand, from (B 7) and the Lemma (i.e. from strain compatibility) it follows that:

$$\begin{aligned}\Pi'_\kappa &= \partial_\alpha\varphi(\hat{x}) \int_{C_{\epsilon,z}} (-\epsilon_{\kappa\beta}\mathscr{E}^\star_{\beta z}dx_\alpha + \epsilon_{\alpha\beta}\mathscr{E}^\star_{\beta z}dx_\kappa) + o(1)\\ &= \partial_\alpha\varphi(\hat{x}) \int_{C_{\epsilon,z}} \epsilon_{\alpha\kappa}\mathscr{E}^\star_{\beta z}dx_\beta + o(1). \end{aligned} \tag{B 10}$$

By summing this latter expression of Π'_κ with (B 10), from the definitions of the Frank and Burgers vector it follows that:

$$\Pi'_\kappa = \frac{1}{2}\partial_\alpha\varphi(\hat{x})\epsilon_{\alpha\kappa}(B^\star_z - \epsilon_{\gamma\beta}\Omega^\star_\gamma x_{0\beta}) + o(1). \tag{B 11}$$

Hence, in the limit $\epsilon \to 0^+$ (B 11) writes as

$$\lim_{\epsilon\to 0^+} \Pi'_\kappa = \ll \left\{\frac{1}{2}\epsilon_{\kappa\alpha}B^\star_z - \frac{1}{2}\epsilon_{\kappa\alpha}\epsilon_{\gamma\beta}\Omega^\star_\gamma x_{0\beta}\right\}\partial_\alpha\delta_0, \varphi_z \gg . \tag{B 12}$$

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

$$\lim_{\epsilon\to 0^+} \Pi_k(z,\varphi,\epsilon) = \lim_{\epsilon\to 0^+} \Pi'_k(z,\varphi,\epsilon) + \ll \Omega^\star_k\delta_0, \varphi_z \gg . \tag{B 13}$$

As suggested by (B 1), to obtain the result for the entire domain Ω it suffices to integrate (B 8) and (B 11) and the expression $\Omega^\star_k\ \varphi(\hat{x})$ over L, in order to replace δ_0 by the line measure δ_L in (B 9), (B 12) and (B 13). By (B 1) the proof is then achieved. □

Appendix C Verification of the main result for 2D rectilinear defect lines

- S*crew dislocation*. The result is easily verified with use of equation (3.14). One needs to compute $< \eta^\star_k, \varphi >= \int_\Omega \epsilon_{kpn}\epsilon_{\alpha\beta}\mathscr{E}^\star_{\beta n}\partial_p\partial_\alpha\varphi\, dV$, that is to calculate the integral of

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

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

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

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

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

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

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

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

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

  achieving the third verification.

Acknowledgements

The first author has been supported by Fundação para a Ciência e a Tecnologia (Ciência 2007, PEst OE/MAT/UI0209/2011 & FCT Project: PTDC/EME-PME/108751/2008).

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