A multiscale model for dislocations: from mesoscopic elasticity to macroscopic plasticity

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Abstract

A multiscale model for dislocations in single crystals is proposed. The aim of this paper is to provide homogenization of dislocation clusters from the meso- to the macro-scale. In particular we prove a new formula relating macroscopic strain incompatibility and the dislocation density. Moreover, it is shown that plasticity is recovered from homogenization of the purely elastic mesoscopic crystals with dislocations, where the appropriate functional space of Special functions of Bounded Deformation appear as a natural choice. Nonstandard defect and deformation internal variables and their evolution in time appear while novel differential relations are sketched in the non-Riemannian crystal with a thermodynamical model as based on those results.

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 motion of dislocations along the glide planes from the crystal wall to the solid-liquid interface can generate a too high stress concentration and be the cause of crystal loss of structure. The theory of dislocations is an old topic going back to the pioneer work of Volterra [39]. Crucial steps have later been provided by Burgers [4], Eshelby, Frank and Nabarro [11], among others (cf. survey results in, e.g., [29]). For the last half of past century we emphasize the contributions of Kröner [20] (see also [25]), in particular his works on the differential geometry of a crystal filled with dislocations and disclinations (the latter represent less frequent crystal line defects), which is interpreted as a non-Riemannian manifold.

In the theory of Kröner, the mesoscopic scale, i.e., the crystal viewed as a continuum adjacent to singular lines – the dislocations and/or the disclinations 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-line and the specific tools required to establish a rigorous link between the mesoscopic and macroscopic scales have been proposed in [36, 37], the goal being to homogenize the mesoscopic fields in order to well-define their macroscopic counterparts.

Homogenization from the meso- to the macroscale is investigated in this paper. The macroscale is defined as the scale where dislocations (disclinations are not considered in this work) are modelled by a set of PDEs where the macroscopic model variables are defined by homogenization of their mesoscopic counterparts. To define homogenized quantities, local averages of mesoscopic defect structures are provided, and thereby the singularities are regularized. Nonetheless these averages are obtained while keeping some important field concentration properties, such as the glide plane effects. By doing this, it is remarkable that these particular surfaces keep their specific meaning *across scales*, in terms of preferred directions for possible dislocation motion (though movement is not investigated in this paper). Moreover, in order to let diffuse and concentrated fields coexist, homogenization is perfomed in functional classes of defects such as Radon measures, functions of bounded – and of special bounded deformation [10, 33].

We recognize that the chosen local volume averaging is a rough kind of homogenisation. In fact, few fine properties of the homogenized fields are provided by this operation, but nevertheless key relations between variables are identified, from which a thermodynamic framework appears as a natural consequence. Let us emphasize that the advantage of our approach is that rather complex mesostructure can be considered, such as accumulation sets of dislocations, which are here called transfinite clusters (i.e., in the sense of Cantor notion of ordinal numbers [5]). As a matter of fact, mesoscopic dislocations may be any rectifiable loop (i.e., of finite length with a negligible set of non-regular points) and the mesoscopic clusters any transfinite union of conservative dislocations. Let us precise that the guideline of our approach is to introduce as few as possible assumptions, while making clear what is considered a definition, an assumption and a provable result. Moreover, we in general let the regularity properties of the fields appear from the analysis of the resulting PDEs.

The geometric framework as introduced by Kröner has in particular attracted attention of the author [34] since the geometry of the defects (dislocations, disclinations and point defects) can be envisaged as a way to recover and/or discover relations between model variables which do not necesserily appear clear if one restricts to a purely mechanical analysis. Another way to clarify the role of the model variables is to prove formulas (some of which might be well-known and widely used), which were otherwise heuristically inferred, formally justified, let alone only conjectured. This has been done in the series of papers [35–37] the last two of which introduce a new approach called "distributional". In fact, by working in the space of distributions and Radon measures [1, 31], we prove the relation between strain incompatibility and density of defects under precise field assumptions, and hence we stress the interrelations between the model variables.

The present paper is a key step in the construction of a multiscale distributional theory we focus on one particular formula appearing in Kröner's work [20]. 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 modeling of the behaviour of line defects in single crystals. In the present paper we provide a complete proof of such a formula at the macroscale as based on the mesoscopic results as proved in [35–37]. A new term appears in our result and this correction with respect to the celebrated Kröner's formula ($\mathrm{inc}\,\mathcal{E} = \kappa \times \nabla$ where $\mathrm{inc}\mathcal{E}$ is the strain incompatibility and κ the contortion tensors) has consequences in terms of modeling which are also investigated.

Section 2 recalls results from previous works, emphasizing the model variables and their relations at the meso-scale. Section 3 describes how the passage from the meso- to the macroscopic scale is performed. In Section 4, the (differential) relation between macroscopic strain incompatibility and the contortion curl is proved under precise field assumptions. In particular, the main result of this paper (i.e., Theorem 4) is found in §4.1. Let us emphasize that this result shows a newly introduced term with respect to

Kröner's formula, the interpretations of which are given in geometrical and physical terms in §4.6. In Section 4, we also address the elasto-plastic decompostion issue and we show how a "reference configuration" might be chosen in such a way that the resulting macroscopic displacement is, in mathematical terminology, a *special function of bounded variation*. Moreover, the convergence across scales is defined in Section §4.5, therefore bringing to light the precise mathematical relations between the meso- and macroscopic fields.

Applying the results from previous sections, we propose in Section 5 a conjecture on the time evolution of internal variables, and set the basis of a thermodynamical framework at the macroscale. Conclusions and current plans for future works are drawn in Section 6.

2 Preliminary results at the mesoscale: the basis of the distributional approach

The basis of the distributional approach can be found with more detail in the two references [36, 37], where the defect lines were assumed parallel to the z-axis, with a resulting elastic strain independent of z (in fact, those lines are the edge and screw dislocations and the wedge disclination). Hence they could be treated as a countable set of points in the plane (see Fig. 1(a) for an example of $2D$ isolated defects). In other words we considered 0-rectifiable sets in the sense of Mattila [24]. These two introductory works paved the way for the first extension of the theory to $3D$ dislocation in an elastic medium [35], where in addition to the three above-mentioned families of defects, we included the twist disclinations. The main results of these three papers are first recalled. Then, we will extend our results to 1-rectifiable dislocations.

2.1 Basic assumptions on the key mesoscopic deformation and defect variables

At the mesoscale, the assumed open, connected and simply-connected domain is denoted by $\Omega_\star \subset \mathbb{R}^3$, with the defect line(s) indicated by $\mathcal{L} \subset \Omega_\star$. Here and in the sequel, the $\star$ is chosen as a subscript to specify mesoscopic quantities. It will be dropped to denote their homogenized counterparts, as convergence to the macroscale is performed.

Definition 1 (Defect set) *A dislocation is a rectifiable curve in $3D$ in the sense of Mattila [24]. A rectifiable dislocation cluster $\mathcal{C}$ is the union of a countable family of dislocations containing at least one non-isolated line $\mathcal{L}$, and such that $\mathcal{H}^1(\mathcal{C})$ is finite. The entire defect set $\Upsilon \subset \Omega_\star$ is a countable union of rectifiable clusters $\mathcal{C}$ with finite $\mathcal{H}^1(\Upsilon)$.*

Let us remark that by Definition 1 (and by Theorem 15.11 of [24]) the set Υ can be approximated by a finite tending-to-infinity number of rectilinear segments $L^{(i)}$. Moreover, according to Cantor's [5] theory of transfinite sets, these families of clusters may consist of rather wild and complex geometries of sets (cf. Fig. 1(c)). In the present approach we assume that Υ possesses a sufficiently rich mathematical structure (i.e., that of transfinite sets) to reasonably represent a wide range of dislocation clusters, as real experiments and Nature might show (see, e.g., Fig. 1(b)).

Notations 1 *In this paper, a scalar, vector or tensor of any order are not typographically distinct symbols in the text. The tensor order is specified when equations* *are written, since in this case only, the vector v is written as v_i (with one index), and the tensor U as $U_{ij\dots}$ with a number of indices corresponding to its order.*

Moreover for a second-order tensor T, we denote by $\nabla \cdot T$ (resp. $T \cdot \nabla$) the first-order tensor given componentwise by $\partial_i T_{ij}$ (resp. $\partial_j T_{ij}$). The same convention holds for the left (resp. right) curl operator $\nabla\times$ (resp. $\times\nabla$), i.e., for a second-order tensor E, $(\nabla \times E)_{ij} = \epsilon_{ikl}\partial_k E_{lj}$ and $(E \times \nabla)_{ij} = \epsilon_{jkl}\partial_k E_{il}$ (otherwise written, $(E \times \nabla)^T = \nabla \times E^T$).

Notations 2 (Incompatibility) *The incompatibility operator* inc *is defined componentwise as*

$$\mathrm{inc}_{kl} := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q, \tag{2.1}$$

where ϵ_{ijk} is the Levi-Civita permutation symbol, i.e., its value is 1 if (i, j, k) is an even permutation of $(1, 2, 3)$, -1 if it is an odd permutation, and 0 if any 2 indices are repeated.

In the sequel, we say that a symmetric tensor E is compatible on $U \subset \Omega_\star$ if $\mathrm{inc}\, E$ vanishes on U.

Assumption 1 ($3D$ elastic strain) *The linear strain $\mathcal{E}^\star$ is a given symmetric L^1_{loc} $(\Omega_\star, \mathbb{R}^{3\times3})$-tensor compatible on $\Omega_\star \setminus \Upsilon$. In other words, the incompatibility tensor, as defined by the distribution $\eta^\star := \mathrm{inc}\, \mathcal{E}^\star = \nabla \times \mathcal{E}^\star \times \nabla$, vanishes everywhere on $\Omega_\star \setminus \Upsilon$. Moreover, the mesoscopic strain is linearly related to the mesoscopic stress $S^\star$, i.e.*

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

where $S^\star$ denotes the stress field, $C^\star$ and $\beta^\star$ stand for the 4th- and 2nd-order compliance and thermal dilation tensors, and T_0 is the reference temperature.

The invariant Burgers vector $B^{\star\mathcal{L}}$ is classically attached to every dislocation $\mathcal{L}$ [18]. In this work, the dislocation density is a second-order tensor. However, the chosen model defect variable will be the so-called *contortion tensor* (see, e.g., [34] for a discussion on its geometrical meaning) defined as follows.

Definition 2 (Dislocation densities)

PURE DISLOCATION DENSITY:
$$\Lambda^\star_{ij} := \sum_{\mathcal{L}\subset\Upsilon} \Lambda^{\star\mathcal{L}}_{ij} \quad \textit{with} \quad \Lambda^{\star\mathcal{L}}_{ij} := B^{\star\mathcal{L}}_j \tau_i \delta_{\mathcal{L}} \tag{2.2}$$

CONTORTION:
$$\kappa^\star_{ij} := \sum_{\mathcal{L}\subset\Upsilon} \kappa^{\star\mathcal{L}}_{ij} \quad \textit{with} \quad \kappa^{\star\mathcal{L}}_{ij} := \Lambda^{\star\mathcal{L}}_{ij} - \frac{1}{2}\Lambda^{\star\mathcal{L}}_{mm}\delta_{ij} \tag{2.3}$$

where $\delta_{\mathcal{L}}$ denotes the 1-dimensional Hausdorff measure concentrated on $\mathcal{L}$.

From the following classical theorem is proved in, e.g., [18], dislocations are either closed or end at the crystal boundary.

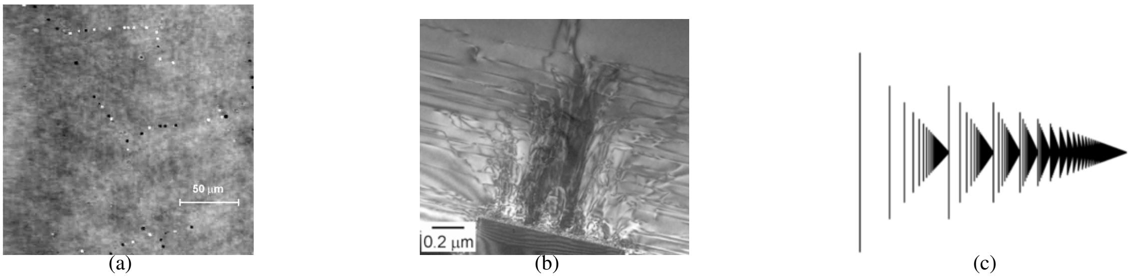
Theorem 1 (Conservation laws) *Dislocations are always closed or end at the boundary of $\Omega_\star$. Moreover, $\partial_i \Lambda^{\star\mathcal{L}}_{ij} = 0$.*

In general any smooth vector field can be decomposed into a solenoidal and an irrotational part, and this property can be easily extended to distribution fields. Similar decomposition of any symmetric tensor field into a compatible and a solenoidal part will here be recalled (see [37] for a proof, see also [13]).

Lemma 1 (Standard decomposition of a symmetric tensor) *Any symmetric 2^{nd}-order distribution tensor E can be decomposed into a compatible and a solenoidal symmetric part:*

$$E = E^c + E^s, \tag{2.4}$$

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



(a) (b) (c)

Figure 1: 1(a) As precipitates decorating dislocations in a GaAs sample is a typical $2D$ mesoscopic picture of dislocations; ©SEMILAB; 1(b) Dislocations in aluminum form complex mesoscopic structures, including accumulation sets, here called dislocation clusters; 1(c) Representation of a dislocation cluster as a ω^2-structure with ω the first ordinal transfinite number [5]. The lines can represent an isolated dislocation, a cluster of dislocations, or any countable accumulation set of defects with a given transfinite structure. The figure shows how these sets can be geometrically combined to form sets of higher density (i.e., clusters of rectifiable dislocations, clusters of clusters, etc).

2.2 The difficulty dealing with countable families of defects

In Nature, we observe sets of dislocations which are patently not a collection of isolated lines, as shown for instance in Fig. 1(b). So, any complete mathematical theory which aims at describing dislocation physics must allow for accumulation sets of defects. In our approach we consider countable families of defects, and following Cantor theory of transfinite number, we are able to describe a large variety of defect sets (such as accumulation of accumulation sets,. etc, cf. Fig 1(c)).

However, the extension of our theory (as introduced in [35–37]) to a countable – instead of finite number of defect lines poses several technical problems which we here briefly discuss.

Consider a countable family Υ of lines parallel to the z-axis and the planar countable set of points $l_0 := \Upsilon \cap \{z = z_0\}$. Consider also a series of weighted Dirac masses on l_0 indexed by $i \in \mathcal{I}$ where $\mathcal{I}$ is a countable subset of $\mathbb{N}$. Then its convergence as a measure implies that the sum of the weights must converge absolutely (i.e., the sum of the absolute value of the weights converges), as stated and proved in the following lemma.

Lemma 2 *Let $\delta^{(i)}$, $i \in \mathcal{I} \subset \mathbb{N}$, stand for the Dirac measure at $\hat{x}^{(i)} \in l_0$ and $\sum_{i \in \mathcal{I}} C^{(i)} \delta^{(i)}$ be a Radon measure on $\Omega_{z_0} = \Omega \cap \{z = z_0\}$. Then the sum of the weights $C^{(i)}$ is locally absolutely convergent, this meaning its absolute convergence on any bounded subset $\{\hat{x}^{(i)}, i \in \mathcal{I}' \subset \mathcal{I}\}$ of l_0.*

Proof. Since $\sum_{i \in \mathcal{I}} C^{(i)} \delta^{(i)}$ is a Radon measure, then the sub-sum $\sum_{i \in \mathcal{I}'} C^{(i)} \delta^{(i)}$ is a finite Radon measure and can be indifferently carried out on every permutation of $\mathcal{I}'$. Hence, taking a test-function wich equals 1 on l_0, the sum of the weights converges for every permutation of $\mathcal{I}'$ and is absolutely convergent. □

A first difficulty arises from the different kinds of convergence that could be required. For instance, Lemma 2 might fail to hold if a (coarser) distributional convergence is required, that is, if convergence is provided only on, e.g., $\mathcal{C}_c^1(\Omega_\star)$. A second example is provided by those distributions that are the gradient of a summable function. If these distributions are concentrated on isolated points, they must be the sum of Dirac masses by Lemma 2, whereas this property might fail on a countable set. More generally, it is known [31] that a concentrated first-order distribution on isolated points is a sum of weighted Dirac masses and Dirac mass derivatives, while a concentrated measure on a countable set is a sum of weighted Dirac masses. However, it is false to claim that a concentrated first-order distribution on a countable set is a sum of Dirac masses and Dirac mass derivatives, as $1D$ counter-examples can show: the series $F = \sum_{i \in \mathcal{I} = \mathbb{N}_*} C^{(i)}(H^0 - H^{(i)})$, with $H^{(i)} = H(x - \hat{x}^{(i)}),\ \hat{x}^{(i)} = 1/i,\ H^0 = H(x)$ and H the step function, may be L^1_{loc} converging even if the sum of the weights $C^{(i)}$ diverges. To show this, it suffices to select suitable $C^{(i)}$ such that the partial sums defining F are enclosed between the L^1_{loc} functions $G(x)$ and $-G(x)$, with $G(x) = \log\left((1+x)/x\right)$ for $x > 0$ and $G(x) = 0$ for $x \leq 0$. Then $F \in L^1_{loc}$, in such a way that the distributional derivative of F, which cannot be the diverging series $-\sum_{i \in \mathcal{I}} C^{(i)} \delta^{(i)}$, exhibits a special behaviour near the origin to recover convergence.

This property at accumulation points of l_0 prevents a straightforward extension of the results obtained for isolated lines to more general, realistic and applicable situations. Nonetheless, the extension to a countable family of rectifiable defects is crucial for the two following reasons: (i) to consider curvilinear defects which are obtained by convergence of countably many rectilinear segments, (ii) to consider homogenization of mesoscopic defects to the macroscopic scale, where the limit of mesoscopic families naturally requires to pass from finite to countable quantities.

2.3 Governing assumptions at the mesoscale

The aim of this paper is to provide homogenization of dislocation clusters from the meso- to the macro-scale. Therefore a countable tending-to-infinity set of dislocation segments $\{L^{(i)} \subset \Upsilon\}_i$ each of which with unit tangent vector $\tau^{L^{(i)}}$ must be considered. However, as we have seen, a more complex mathematics governs the accumulation points of Υ (i.e., the clusters). To address this issue, the following assumptions on the mesoscopic strain curl must be made.

Assumption 2 (Mesoscopic nature of the Frank tensor) *The so-called (second-order) Frank tensor $\mathcal{E}^\star \times \nabla$ is a first-order distribution assumed to be such that the projection $p^\star := \sum_{L^{(i)} \subset \Upsilon} (\mathcal{E}^\star \times \nabla)\, \tau^{L^{(i)}}$ is a vector-valued Radon measure in the sense of Ambrosio et al. [1] on $\Omega_\star$, with a vector singular part $c^\star$ and regular part $r^\star := p^\star - c^\star \in L^1(\Omega_\star)$ s.t. the following quantities are purely concentrated on Υ:*

$$c^\star \quad , \quad \sum_{L^{(i)} \subset \Upsilon} \tau^{L^{(i)}} \cdot \nabla \times r^\star \quad \textit{and} \quad \sum_{L^{(i)} \subset \Upsilon} \nabla \left(\tau^{L^{(i)}} \cdot r^\star \right). \tag{2.5}$$

Moreover, we make the following assumption.

Assumption 3 (Total Burgers vector) *The total Burgers vector, as defined by* $B := \sum_{\mathcal{L}\subset\Upsilon} B^{\star\mathcal{L}}$ *has a finite norm.*

Assumption 3 is presented here as a model postulate in order to not overload this introduction with results from previous works. However, let us emphasize that the statement of Assumption 3 is a consequence of the decomposition results as proved in [37], and of Assumption 2. In fact, as relying on the hypotheses that some components of the strain and Frank tensor are Radon measures, it can be shown directly from the computations as found in the above-mentionned proofs and from Lemma 2 that for a countable set Υ of dislocation loops $\mathcal{L}$, one has $\sum_{\mathcal{L}\subset\Upsilon} ||B^{\star\mathcal{L}}|| < \infty$.

In this paper we limit ourseleves to the following class of dislocations.

Definition 3 (Conservative dislocation loops) *The mesoscopic dislocations* $\mathcal{L}$ *are simple loops in the three-dimensional space which have a Lipschitz-continuous tangent vector almost everywhere, in such a way that curvature* χ *is defined almost everywhere and is bounded. We also assume that the dislocations are torsion-free with a vanishing out-of-plane Burgers vector component, i.e.,* $\Lambda^\star(S)\sigma = 0$ *for every plane* $S \subset \Omega_\star$ *with unit normal* σ*. A conservative cluster* $\mathcal{C}$ *is defined as the union of a countable family of conservative dislocations such that* $\mathcal{H}^1(\mathcal{C}) < \infty$*. The entire defect set* $\Upsilon \subset \Omega_\star$ *is defined as a countable union of conservative clusters* $\mathcal{C}$ *satisfiying* $\mathcal{H}^1(\Upsilon) < \infty$*.*

Another manner to read Definition 3 is to say that we restrict ourselves to a set of dislocation loops admitting at most countable accumulation sets – the clusters, which themselves are restricted to lie in planes (as usually called *glide* or *slip planes*). Moreover, we do not consider rectilinear dislocations for a simple reason: by Theorem 1 they must end at the boundary and hence the scale separation between the meso- and the macroscopic description of matter can not be performed.

It has been proved in [35] that for a finite set of (skew) rectilinear dislocations, strain incompatibility satisfies the following structure theorem (viz., a mesoscopic *corrected* Kröner's formula). By an argument of *transfinite* recursion, we here provide a natural extension of this results for countable families of dislocation clusters Υ. To this aim, we first recall that the dislocation densities are given by Definition 2, while symbol $A_{m\leftrightarrow n}$ means that sum of tensor A_{mn} and its transposed A_{nm} is taken. Moreover, subscript $\mathcal{L}$ indicates, as usual, that the tensor represents a concentrated quantitity on the line $\mathcal{L}$, of which a sum is performed on Υ.

Theorem 2 (Incompatibility of a family of dislocation clusters) *Under Assumptions 1, 2 and 3, and provided Definition 3, incompatibility is the following first-order symmetric tensor distribution:*

$$\eta^\star_{mn} = \mathrm{inc}_{mn}(\mathcal{E}^\star) := \epsilon_{mkp}\epsilon_{nlq}\partial_k\partial_l\mathcal{E}^\star_{pq} = \sum_{\mathcal{L}\subset\Upsilon}\left[\tau^{\mathcal{L}}_m\tau^{\mathcal{L}}_k\hat{\eta}^{\star\mathcal{L}}_{kn}\right]_{m\leftrightarrow n}, \qquad (2.6)$$

where $\hat{\eta}^{\star\mathcal{L}}_{kn} = \tilde{\eta}^{\star\mathcal{L}}_{kn} - \frac{\delta_{kn}}{2}\tilde{\eta}^{\star\mathcal{L}}_{pp}$ *is called the Einstein tensor with* $\tilde{\eta}^{\star\mathcal{L}}_{kn} = \epsilon_{kij}\partial_i\kappa^{\star\mathcal{L}}_{nj}$ *known as the Kröner's tensor.*

Proof. Provided Assumption 2, Eq. (2.6) has been proved in [35] for a set of isolated skew (i.e., parallel but not necessarily coplanar) edge and screw dislocation lines in $3D$.

In a first step, provided Definition 3 and Theorem 1, this result can be extended in a natural way to a set of isolated segments (by *isolated*, it is meant that for each of these segments there exists a tube of finite width which contains only this segment). As compared to [35], the new terms that might appear here are due either to the fact that we consider segments with extremities inside Ω (instead of rectilinear lines) and to the line curvature. Since the lines are loops the contributions of the end points mutually cancel, while by the assumption that the dislocation be conservative, it is readily seen (cf. p. 108-109 of [35]) that the term due to curvature also vanishes.

In a second step, the passage from finite to countable segments is made by Assumption 3 and Lemma 2. To handle the accumulation sets, we introduce the so-called derived subset $\bar{\Upsilon}_1$ of Υ (i.e., according to Cantor theory of transfinite numbers [5], $\bar{\Upsilon}_1$ is defined as the accumulation set of Υ): the set $\bar{\Upsilon}_1$ is obtained by removing all isolated segments of Υ, for which (2.6) holds from the first step. Now, $\bar{\Upsilon}_1$ itself contains isolated and accumulation subsets and (2.6) may be proved again for every isolated segment of $\bar{\Upsilon}_1$. By a recursive procedure these two steps can be repeated since the derived set $\bar{\Upsilon}_k$ defined at step $k-1$ has (by the assumption of countability) a strictly decreasing cardinality. The result is eventually proved for every segment of Υ, and the proof is achieved by density and Theorem 15.11 of [24].

□

3 Homogenization of a transfinite family of rectifiable dislocation clusters

The aim of this section is to provide a macroscopic counterpart of Eq. (2.6). This will be achieved by taking local average values, in the spirit of a multiscale approach as proposed by Germain et al. [14] and later developped in, e.g., [15,26]. The main result of this section is that incompatibility of the homogenized strain reads $\operatorname{inc}\mathcal{E} = \tilde{\eta} - \frac{I}{2}\operatorname{tr}\tilde{\eta}$ with $\tilde{\eta} = \kappa \times \nabla$, and κ the homogenized contortion of the macroscopic crystal whose mesostructure at x consists of countably many rectifiable dislocation clusters. It this sense, we correct the celebrated Kröner's formula [20], $\operatorname{inc}\mathcal{E} = \kappa \times \nabla$, which, as we prove in Theorem 4, is missing the term $-\frac{I}{2}\operatorname{tr}\,(\kappa \times \nabla)$.

A crucial notion required to define homogenization is given in the following definition (we refer to [1] for detail).

Notion 1 (Radon measure) *Let U be an open subset of $\mathbb{R}^3$. A (tensor-valued) Radon measure $\mu \in \mathcal{M}(U)$ is a linear and continuous functional on $\mathcal{C}_c(U)$, the set of continuous functions with compact support in U. Moreover for any Borel set $A \subset U$, $\mu(A)$ is a set function such that (i) $\mu(\emptyset) = 0$, (ii) $\mu(\bigsqcup_i A^i) = \sum_i \mu(A_i)$ for any collection of pairwise disjoint sets $\{A^i\}$, and (iii) $\mu(K)$ is scalar- or tensor-valued (i.e., finite) as soon as $K \subset U$ is compact.*

Moreover, the following notation will be used:

Notations 3 $(f\mu)(A) = \int_A f d\mu := \sup \left\{ \sum_{z \in im(u)} z\mu(u^{-1}(z)) : u \textit{ measurable and simple and s.t. } u \le f \right\},$ *where $d\mu$ denotes the density of measure μ and $im(u)$ the co-domain of u (a function is said simple if its co-domain is a finite set).*

3.1 Preliminary results at the mesoscale

Let us consider the mesoscopic defect set Υ and the conservative dislocation loop $\mathcal{L} \subset \Upsilon \subset \Omega_\star$ with tangent vector τ and curvature χ. Let us also introduce the surface $B_\mathcal{L}$

enclosed by $\mathcal{L}$ and $\mathcal{I}_{\mathcal{L}} := \chi_{\Omega_\star \setminus \overline{B}_{\mathcal{L}}}$, the characteristic function of the complement of $\overline{B}_{\mathcal{L}}$ in $\Omega_\star$.

Observe that by multiplication with ϵ_{jkl}, one has that $\tilde{\eta}^{\star\mathcal{L}}_{kj} = \epsilon_{kpq}\partial_p \kappa^{\star\mathcal{L}}_{jq}$ is symmetric, together with $\hat{\eta}^{\star\mathcal{L}}_{kj} := \tilde{\eta}^{\star\mathcal{L}}_{kj} - \delta_{kj}\frac{\tilde{\eta}^{\star\mathcal{L}}_{pp}}{2}$. Moreover, by Eq. (2.6) of Theorem 2, one has, componentwise,

$$\eta^\star_{ij} = \sum_{\mathcal{L}\subset\Upsilon} \eta^{\star\mathcal{L}}_{ij} = \sum_{\mathcal{L}\subset\Upsilon} [\tau^{\mathcal{L}}_i \tau^{\mathcal{L}}_k \eta^{\star\mathcal{L}}_{kj}]_{i\leftrightarrow j}, \tag{3.1}$$

while the following identity also holds true:

$$\eta^\star_{ij} = \sum_{\mathcal{L}\subset\Upsilon} [\tau^{\mathcal{L}}_i \tau^{\mathcal{L}}_k \hat{\eta}^{\star\mathcal{L}}_{kj}]_{i\leftrightarrow j}. \tag{3.2}$$

It results from (3.1) and (3.2) that there exists for every $\mathcal{L}\subset\Upsilon$ a symmetric (gauge) second-order tensor field $\phi^{\mathcal{L}}$ such that $\tau\phi^{\mathcal{L}} = \phi^{\mathcal{L}}\tau = 0$, and satisfying

$$\eta^{\star\mathcal{L}}_{kj} = \hat{\eta}^{\star\mathcal{L}}_{kj} + \phi^{\mathcal{L}}_{kj}. \tag{3.3}$$

The decomposition property of a symmetric tensor into compatible and symmetric solenoidal parts of Lemma 1 yields $\phi = \nabla^S\tilde{\psi} + \hat{\psi}$ (we now drop the subscript $\mathcal{L}$, while subscript S indicates the symmetric part) where $\hat{\psi} = \nabla\times\varphi\times\nabla$ with $\nabla\cdot\varphi = 0$. One may take $\phi = \hat{\psi}$ since from the vector relations $\tau\left(\nabla^S\tilde{\psi}\right) = \left(\nabla^S\tilde{\psi}\right)\tau = 0$ and projections on $\{\sigma,\nu,\tau\}$ one has $\tilde{\psi} = 0$. Moreover, in order for $\tau\hat{\psi} = \hat{\psi}\tau$ to vanish, we introduce the scalar and vector fields $\bar{\varphi}$ and ψ, respectively (see Appendix A for the detailed computations) such that $\varphi = \tau\otimes\tau\bar{\varphi}\mathcal{I}_{\mathcal{L}} + \nabla^S\psi$ is solenoidal, with $\bar{\varphi}\mathcal{I}_{\mathcal{L}}$ solution of $\Delta(\bar{\varphi}\mathcal{I}_{\mathcal{L}}) = \operatorname{tr}(\Lambda^\star\times\nabla)$ and (in order for $\nabla\cdot\varphi = 0$ to vanish) $(\Delta + \nabla\nabla\cdot)\psi = -2\nu\bar{\varphi}\chi\mathcal{I}_{\mathcal{L}}$, where τ and ν are continuously extended on $\Omega_\star\setminus B_{\mathcal{L}}$. Therefore, recalling (2.3), and for any constant tensor $\hat{\varphi}$ and distribution field F, Eq. (3.3) rewrites as

$$\eta^\star_{kj} = \epsilon_{kpq}\partial_p\left(\kappa^\star_{jq} + \epsilon_{jmn}\partial_m\varphi_{qn} + \hat{\varphi}_{qj} + \partial_q F_j\right) - \frac{\delta_{kj}}{2}\epsilon_{mpq}\partial_p\kappa^\star_{mq}. \tag{3.4}$$

The above calculations suggest that the effective field to homogenize be the *effective contortion* $\tilde{\kappa}^\star$ besides the contortion $\kappa^\star$. Below and in the sequel, we use the notation $\fint_A := \frac{1}{|A|}\int_A$, where $|A|$ is the volume of A.

Definition 4 (Effective contortion) *Consider a conservative dislocation loop $\mathcal{L}$. Then we define componentwise*

EFFECTIVE MESOSCOPIC CONTORTION:
$$\tilde{\kappa}^{\star\mathcal{L}}_{jq} := \kappa^{\star\mathcal{L}}_{jq} + \epsilon_{jmn}\partial_m\varphi^{\star\mathcal{L}}_{nq} + \hat{\varphi}^{\star\mathcal{L}}_{qj} + \partial_q F^{\star\mathcal{L}}_j, \tag{3.5}$$

with the symmetric and solenoidal $\varphi^{\star\mathcal{L}} \in L^1_{loc}(\Omega_\star,\mathbb{R}^{3\times3})$ and $F \in W^{1,2}(\Omega_\star,\mathbb{R}^3)$ such that $\mu^{\star\mathcal{L}} := \nabla\times\varphi^{\star\mathcal{L}} + \nabla F^{\star\mathcal{L}}$ is a Radon measure (this is proved in Appendix A), with the constant tensor $\hat{\varphi}^{\star\mathcal{L}} := -\fint_{V^\star_x} d\mu^{\star\mathcal{L}}$, where $V^\star_x$ is a smooth neigbourhood of x.

Remark 1 *It immediately results from Assumption 3 and Definition 4 that*

$$\fint_{V^\star_x} d\kappa^{\star\mathcal{L}} = \fint_{V^\star_x} d\tilde{\kappa}^{\star\mathcal{L}} \quad \textit{and} \quad \fint_{V^\star_x} d\kappa^\star = \fint_{V^\star_x} d\tilde{\kappa}^\star, \tag{3.6}$$

where

$$\kappa^\star = \sum_{\mathcal{L}\subset\Upsilon} \kappa^{\star\mathcal{L}} \quad \textit{and} \quad \tilde{\kappa}^\star = \sum_{\mathcal{L}\subset\Upsilon} \tilde{\kappa}^{\star\mathcal{L}}. \tag{3.7}$$

From Eqs. (3.4) and (3.7), we rewrite Theorem 2 as follows.

Theorem 3 (Incompatibility of a family of dislocation clusters) *Under Assumptions 1, 2 and 3, and provided Definitions 3 and 4, incompatibility is the following first-order symmetric tensor distribution:*

$$\eta^\star = \operatorname{inc}(\mathcal{E}^\star) = \sum_{\mathcal{L}\subset\Upsilon} \eta^{\star\mathcal{L}} = \sum_{\mathcal{L}\subset\Upsilon} \left(\tilde{\kappa}^{\star\mathcal{L}} \times \nabla - \frac{I}{2}\operatorname{tr}\left(\kappa^{\star\mathcal{L}} \times \nabla\right)\right) = \tilde{\kappa}^\star \times \nabla - \frac{I}{2}\operatorname{tr}\left(\kappa^\star \times \nabla\right). \tag{3.8}$$

3.2 Passage from meso- to macro-scale

Let us consider the macroscopic single crystal as identified with a bounded smooth open and connected set Ω. A point x represents a macroscopic RVE (i.e., "representative volume element"), that is, x represents a bounded amount of mesoscopic matter, denoted by $V_x^\star$. Moreover, the mesostructure at x is given by Υ_x, the transfinite family of dislocation clusters. By Assumption 3 one has $\sum_{\mathcal{L}\subset\Upsilon_x} ||B^{\star\mathcal{L}}|| < \infty$ in such a way that the norm $||\mathcal{E}^\star||_{L^1(\Omega_\star)}$ and total variation $|\Lambda^\star|(\Omega_\star)$ are bounded (with $\Omega_\star \subset \mathbb{R}^3$). Therefore (since $\mathcal{E}^\star$ and $\Lambda^\star$ are linear in the Burgers vector), we may introduce the following Borel measures on $\mathbb{R}^3$ whose restrictions to $\Omega_\star$ are a finite Radon measures.

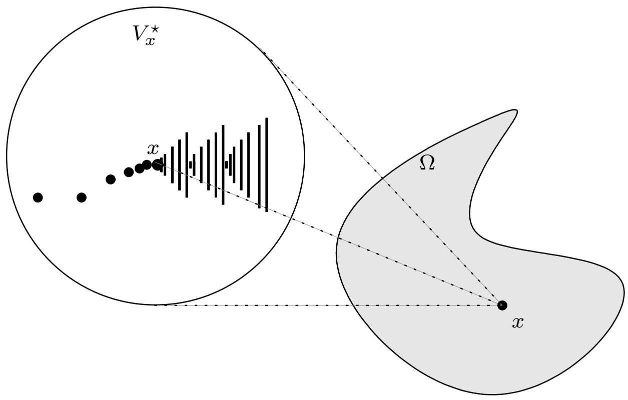


Figure 2: The representative volume $V_x^\star$ at $x \in \Omega$ and the mesoscopic defect structure Υ_x at x: black points mean isolated dislocations while the vertical segments represent accumulation sets of dislocations, i.e., a cluster. These clusters may in turn form accumulation sets.

Notations 4 *In the sequel, the concomitant uper subscript $\star$ and lower subscripts x are written to qualify all mesoscopic fields defined on a RVE at x. For instance $\mathcal{E}^\star$ will now read $\mathcal{E}_x^\star$ and $\kappa^\star$ or $\tilde{\kappa}^\star$ will now read $\kappa_x^\star$ or $\tilde{\kappa}_x^\star$ to emphasize that they are mesoscopic fields associated to the macroscopic point x.*

Let us recall that the mesoscopic strain $\mathcal{E}_x^\star \in L^1_{loc}(\Omega_\star)$, while the mesoscopic dislocation density $\Lambda_x^\star$ and contortion $\kappa_x^\star := \Lambda_x^\star - \frac{I}{2}\operatorname{tr}\Lambda_x^\star$ belong to $\mathcal{M}(\Omega_\star)$.

Definition 5 (Macroscopic measures) *The macroscopic strain $\mathcal{E}_x$ is a measure defined such that for every Borel set $A \subset \mathbb{R}^3$,*

$$x \in \Omega \mapsto \mathcal{E}_x(A) := \fint_A \mathcal{E}^\star_x(y)dy \tag{3.9}$$

where $\mathcal{E}^\star_x(y) = \mathcal{E}^\star(x+y)$. Moreover, the macroscopic dislocation density tensor Λ_x and contortion tensor κ are measures defined such that for every Borel set $A \subset \mathbb{R}^3$,

$$x \in \Omega \mapsto \Lambda_x(A) := \fint_A d\Lambda^\star_x(y) \qquad \text{and} \qquad x \in \Omega \mapsto \kappa_x(A) := \Lambda_x(A) - \frac{I}{2} \operatorname{tr} \Lambda_x(A), \tag{3.10}$$

where $\Lambda^\star_x(y) = \Lambda^\star(x+y)$.

Remark 2 *From Remark 1, Eqs. (2.3) and (3.10), it results that $\kappa_x = \sum_{\mathcal{L} \subset \Upsilon_x} \kappa^{\mathcal{L}}_x$ with $\kappa^{\mathcal{L}}_x(A) := \fint_A d\kappa^{\star\mathcal{L}}$ for every Borel set $A \subset \mathbb{R}^3$.*

Specializing the above measures to particular neigbourhoods, we introduce the associated homogenized fields as local average values at the macroscopic point x,

$$< \mathcal{E}_x > := \mathcal{E}_x(V^\star_x), \qquad < \Lambda_x > := \Lambda_x(V^\star_x), \qquad < \kappa_x > := \kappa_x(V^\star_x), \tag{3.11}$$

where the RVE at x is $V^\star_x$ is the ball centered at x and of radius R_x (see Fig. 2)[1].

By Assumption 3 and Definition 5 these three averages are finite at $x \in \Omega$. However, as functions of $x \in \Omega$, their regularity depends on the choice of the RVE $V^\star_x$. Therefore, we introduce the following mathematical postulate.

Postulate 1 (Measurability of the average values) *We postulate that appropriate RVE can be chosen to represent the dislocated macroscopic crystal with reasonable detail, by which we mean that $< \mathcal{E}_x >, < \Lambda_x >, < \kappa_x >$ are Radon measures on Ω.*

This postulate is not very strong, since we assume that the averaged values are as regular as their mesoscopic counterpart (and even less regular for the strain which we recall belongs to $L^r(\Omega), 1 \leq r < 2$ at the mesoscale). Let us emphasize that this postulate becomes a result as soon as a notion of convergence from the meso- to the macroscale is introduced in such a way that by sequential compactness the macroscopic fields appear as limits of bounded sequences at the mesoscopic scale within the class of Radon measures [1]. We do not want to enter into this kind of arguments at this stage and refer to §4.5 and Postulate 2 for a mechanical version of Postulate 1, and its subsequent consequences in mathematical terms. Let us recall that in mechanical terms, Postulate 1 means that the Bravais strain, the dislocation density and the contortion are bounded *extensive* macroscopic model variables.

Definition 6 (Bravais strain) *By Postulate 1, the Bravais strain[2] is defined as $\mathcal{E}^B := < \mathcal{E}_x > \in \mathcal{M}(\Omega)$.*

By Radon-Nykodým's decomposition [1], it is known that the Bravais strain is made of a diffuse (integrable) and a singular term. In the following assumption we make the classical hypothese that the singular part is concentrated on a two-dimensional set (interpreted as the glide planes).

[1] In practice, R_x is related to the mesoscopic dislocation density. Moreover R_x is chosen s.t. $l << R_x << L$ where l and L are characteristic lengths of the meso- and macro-scale.

[2] The term Bravais strain aims at not considering a-priori that it consists of a purely elastic quantity. In fact, the Bravais strain is the homogenized strain but is not the complete *macroscopic strain*. Auguste Bravais (1811-1863) is a French crystallographer, botanist, astronomer and physicist [3].

Assumption 4 (Bravais strain regularity) *We assume that there exist a rectifiable surface* Σ *such that* $\mathcal{E}^B = \bar{\mathcal{E}}^B dx + \hat{\mathcal{E}}^B \delta_\Sigma$*, where* δ_Σ *denotes the* 2*-dimensional Hausdorff measure concentrated on* Σ*. Here,* $\bar{\mathcal{E}}^B \in L^1(\Omega)$ *is the diffuse strain, while the singular part* $\hat{\mathcal{E}}^B \in L^\infty(\Sigma)$.

Definition 7 (Macroscopic contortion) *By Postulate 1, the macroscopic contortion*[3] *is defined as* $\kappa := <\kappa_x> \in \mathcal{M}(\Omega)$.

Since dislocation densities are concentrated on lines at the meso-scale, it is natural to let their homogenized counterparts still exhibit concentration properties on low-dimensional subsets of Ω. By Radon-Nykodým's decomposition, the contortion shows a part which is absolutely continuous with respect to the Lebesgue measure, with density $\bar{\kappa} dx$ and $\bar{\kappa} \in L^1(\Omega)$, and a part which is singular, denoted by k.

We propose two hypotheses for the contortion, and analyze their consequence on the strain regularity (cf. Remark 4).

Assumption 5 (Strong assumption on the contortion) *We assume that* $\bar{\kappa} \in L^2(\Omega)$*. Moreover, the singular part is concentrated on the (same as the above introduced) glide surface* Σ*. So, for every Borel set* $A \subset \Omega$ *we have* $\kappa(A) = \int_A d\kappa = \int_A \bar{\kappa} dx + k(A)$*, where* $k(A) = \hat{k}\delta_\Sigma(A)$ *with the restriction of* κ *to* Σ*,* $\hat{k} := \kappa_x\,(V_x^\star \cap \Sigma) \in L^\infty(\Sigma)$.

It is a well-known fact that every distribution vector can be decomposed into a pure gradient and a pure curl, both considered as distributions. Consider such a decomposition for the columns of $\bar{\kappa}$: $\bar{\kappa} = \bar{K}\nabla + K \times \nabla$ with $K \cdot \nabla = 0$. The following assumption is weaker than Assumption 5, since the regular contortion, and not its squared norm, is Lebesgue integrable. However the curl part of its above decomposition is assumed to be a Radon measure.

Assumption 6 (Weak assumption on the contortion) *Assume that the absolutely continuous part* $\bar{\kappa} \in L^1(\Omega; \mathbb{R}^{3\times 3})$ *is such that* $\bar{\kappa} \times \nabla$ *is a Radon measure*[4]*. In other terms we assume that* $K \in W^{1,1}(\Omega; \mathbb{R}^{3\times 3})$ *satisfies* $\Delta K \in \mathcal{M}(\Omega; \mathbb{R}^{3\times 3})$ *(in an ultra weak sense due to Stampacchia [32]), while* $\bar{K} \in W^{1,1}(\Omega)$*. Moreover we assume that the singular part is concentrated on* Σ*, i.e.,* $k = \hat{k}\delta_\Sigma$ *with* $\hat{k} = \kappa_x\,(V_x^\star \cap \Sigma) \in L^\infty(\Sigma; \mathbb{R}^{3\times 3})$.

4 The macroscopic elasto-plastic crystal

In this section we discuss several important properties of the macroscopic crystal, as a continuum with material, mechanical and mathematical properties depending on the underlying dislocation meso-structure. One theoretical difficulty when dealing with plasticity is to be able to have at hand a reference configuration with respect to which plasticity laws are postulated unambiguously. Here, the purely elastic mesoscopic crystal, as homogenized from the notions of Section 3, will allow us to precisely define elastic and plastic parts of a total compatible macroscopic strain. Moreover, we show how the natural functional space to describe the crystal is the space of functions of bounded deformations $SBV(\Omega)$, a class of functions introduced 30 years ago by Teman and Strang [33].

[3]This term comes from a notion of differential geometry which has a strong relation with our interpretation in terms of density of defects [34].

[4]This is less demanding than requiring $\bar{\kappa} \in BV(\Omega; \mathbb{R}^{3\times 3})$.

4.1 Macrosopic strain incompatibility

Our key relation is the strain incompatibility as related to defects density, viz. Eq. (3.8). We here prove the macroscopic counterpart of Theorem 2 involving the homogenized fields.

Notations 5 *For any second-order tensors A, B, a, b we define $< A, B >= \sum_{i,j} < A_{ij}, B_{ij} >$ with $< \cdot >$ denoting the duality product, and $a \cdot b = \sum_{i,j} a_{ij} b_{ji}$ denoting the Euclidean scalar product.*

Theorem 4 (Macroscopic strain incompatibility) *Consider an open, bounded, connected set Ω, and a material point $x \in \Omega$ with its meso-structure $\Upsilon_x \subset V_x^\star$ defined as a countable family of conservative dislocation clusters. Assume that Theorem 3 holds on $\Omega_\star := V_x^\star$ for every $x \in \Omega$. From Definitions 6 and 7, Assumptions 4 and 5 or 6, the macroscopic strain incompatibility shows to be the following distribution:*

$$\mathrm{inc}\,(\mathcal{E}^B) := \nabla \times \mathcal{E}^B \times \nabla = \kappa \times \nabla - \frac{I}{2}\,\mathrm{tr}\,(\kappa \times \nabla)\,. \tag{4.1}$$

Proof. By definition of the Bravais strain, we have

$$< \mathcal{E}^B, \varphi >= \int_\Omega \varphi(x) dx \fint_{V_x^\star} \mathcal{E}_x^\star(y) dy. \tag{4.2}$$

By Definition 7, Eqs. (3.6) and (3.10), we introduce the Radon measure $\tilde{\kappa}$ as

$$\kappa = \fint_{V_x^\star} d\kappa_x^\star = \fint_{V_x^\star} d\tilde{\kappa}_x^\star =: \tilde{\kappa}. \tag{4.3}$$

in such a way that, for every test-function $\varphi \in \mathcal{C}_c(\Omega; \mathbb{R}^{3\times3})$, we have by Notion 1,

$$< \kappa, \varphi >:= \sup_{u \le \varphi} \left\{ \sum_{z \in im(u)} z\kappa(u^{-1}(z)) \right\} = \sup_{u \le \varphi} \left\{ \sum_{z \in im(u)} z\tilde{\kappa}(u^{-1}(z)) \right\} =:< \tilde{\kappa}, \varphi >, \tag{4.4}$$

where u is a simple function on the compact support of φ.

Let $V_x^\star$ be the ball at x and of radius R. Since $\kappa = \bar{\kappa} dx + k$ by Assumption 5 or 6, we prove the result in two parts.

Part A: $\kappa = \bar{\kappa} dx$ (with no concentrated part). Since $\bar{\kappa} = \kappa_x(V_x)$ and by Eqs. (4.3) and (4.4) we define $(\kappa \times \nabla)^{d^*} := \kappa \times \nabla - \frac{I}{2}\,\mathrm{tr}\,(\kappa \times \nabla)$ and write

$$\begin{aligned} < (\kappa \times \nabla)^{d^*}, \varphi > &= -\int_\Omega (\nabla \times \varphi) \cdot d\kappa + \frac{1}{2} \int_\Omega \epsilon_{mpn} \partial_p\,(\,\mathrm{tr}\,\varphi)\, d\kappa_{mn} \\ &= -\int_\Omega (\nabla \times \varphi) \cdot d\tilde{\kappa} + \frac{1}{2} \int_\Omega \epsilon_{mpn} \partial_p\,(\,\mathrm{tr}\,\varphi)\, d\tilde{\kappa}_{mn} \\ &= -\int_\Omega (\nabla \times \varphi)\, dx \cdot \fint_{V_x^\star} d\tilde{\kappa}_x^\star(y) + \frac{1}{2} \int_\Omega \epsilon_{mpn} \partial_p\,(\,\mathrm{tr}\,\varphi)\, dx \left(\fint_{V_x^\star} d\tilde{\kappa}_x^\star(y) \right)_{mn}. \end{aligned}$$

For $\epsilon > 0$, let us introduce $\xi = \frac{y-x}{\epsilon}$, $\varphi_x^\epsilon(\xi) = \varphi(x+\epsilon\xi)$ and[5] $\tilde{\kappa}_x^{\star\epsilon}(\xi) := \epsilon^{-1} \tilde{\kappa}_x^\star(x+\epsilon\xi)$.

[5]The scaling in ϵ for $\kappa_x^\star$ come from the scalings $\kappa_x^\star(x) \sim \delta_{\mathcal{L}}(x) dx \sim \epsilon^{-2} \delta_{\mathcal{L}}(\xi) \epsilon^3 d\xi \sim \epsilon \delta_{\mathcal{L}}(\xi) d\xi$.

By the relations $\partial_x = \epsilon^{-1}\partial_\xi, dy = \epsilon^3 d\xi$ and by the continuity of φ, we have (the blow-up of $V_x^\star$ being written $B(0,R/\epsilon)$)

$$
\begin{aligned}
< (\kappa\times\nabla)^{d^*}, \varphi > &= -\lim_{\epsilon\to 0}\frac{\epsilon}{|V_x^\star|}\int_\Omega dx \left(\int_{B(0,R/\epsilon)} (\nabla_x \times \varphi_x^\epsilon(\xi))\cdot d\tilde{\kappa}_x^{\star\epsilon}(\xi)\right. \\
&\quad \left. +\frac{1}{2}\int_{B(0,R/\epsilon)} \epsilon_{mpn}\frac{\partial}{\partial x_p}\,\mathrm{tr}\,\varphi_x^\epsilon(\xi)\,(d\tilde{\kappa}_x^{\star\epsilon}(\xi))_{mn}\right) \\
&= -\lim_{\epsilon\to 0}\frac{1}{|V_x^\star|}\int_\Omega dx \left(\int_{B(0,R/\epsilon)} \nabla_\xi \times \varphi_x^\epsilon(\xi)\cdot d\tilde{\kappa}_x^{\star\epsilon}(\xi)\right. \\
&\quad \left. +\frac{1}{2}\int_{B(0,R/\epsilon)} \epsilon_{mpn}\frac{\partial}{\partial \xi_p}\,\mathrm{tr}\,\varphi_x^\epsilon(\xi)\,(d\tilde{\kappa}_x^{\star\epsilon}(\xi))_{mn}\right),
\end{aligned}
$$

As $\epsilon \to 0$, the blown-up set $B(0,R/\epsilon)$ is identified with $\mathbb{R}^3$. By Theorem[6] 3 with $\Omega_\star = \mathbb{R}^3$, and since $\varphi_x^\epsilon \in \mathcal{C}_c(\mathbb{R}^3;\mathbb{R}^{3\times 3})$, we have

$$
\begin{aligned}
< (\kappa\times\nabla)^{d^*}, \varphi > &= \lim_{\epsilon\to 0}\frac{1}{|V_x^\star|}\int_\Omega dx < \left(\tilde{\kappa}_x^{\star\epsilon}\times\nabla_\xi - \frac{I}{2}\,\mathrm{tr}\,\left(\kappa_x^{\star\epsilon}\times\nabla_\xi\right)\right), \varphi_x^\epsilon > \\
&= \lim_{\epsilon\to 0}\frac{1}{|V_x^\star|}\int_\Omega dx < \nabla_\xi \times \mathcal{E}_x^{\star\epsilon}\times\nabla_\xi, \varphi_x^\epsilon >,
\end{aligned}
$$

which yields, since [7] $\mathcal{E}_x^{\star\epsilon}(\xi) := \epsilon\mathcal{E}_x^\star(x+\epsilon\xi)$,

$$
\begin{aligned}
< (\kappa\times\nabla)^{d^*}, \varphi > &= \lim_{\epsilon\to 0}\frac{\epsilon}{|V_x^\star|}\int_\Omega dx < \mathcal{E}_x^\star(x+\epsilon\xi), \nabla_\xi\times\varphi_x^\epsilon\times\nabla_\xi >, \\
&= \lim_{\epsilon\to 0}\frac{\epsilon}{|V_x^\star|}\int_\Omega dx \int_{B(0,R/\epsilon)} \mathcal{E}_x^\star(x+\epsilon\xi)\cdot(\nabla_\xi\times\varphi_x^\epsilon\times\nabla_\xi)\,d\xi,
\end{aligned}
$$

Since $y = x+\epsilon\xi, \partial_\xi = \epsilon\partial_y, \partial_x = \partial_y$, and $dy = \epsilon^3 d\xi$, the continuity of φ and Eq. (4.2) yield

$$
\begin{aligned}
< (\kappa\times\nabla)^{d^*}, \varphi > &= \lim_{\epsilon\to 0}\frac{1}{|V_x^\star|}\int_\Omega dx \int_{V_x^\star} \mathcal{E}_x^\star(y)\cdot(\nabla_y\times\varphi\times\nabla_y)\,dy \qquad (4.5)\\
&= \lim_{\epsilon\to 0}\int_\Omega dx \fint_{V_x^\star} \mathcal{E}_x^\star(y)\cdot(\nabla_x\times\varphi(x+\epsilon\xi)\times\nabla_x)\,dy \\
&= \int_\Omega (\nabla_x\times\varphi(x)\times\nabla_x)\,dx \fint_{V_x^\star}\mathcal{E}_x^\star(y)dy =< \nabla\times\mathcal{E}^B\times\nabla, \varphi >,
\end{aligned}
$$

which proves the claim by definition of the Bravais strain.

Part B: $\kappa = k = \hat{k}\delta_\Sigma$**.** The proof of this part mimicks part A, so we don't provide

[6] This is the reason why Theorem 3 had been valided for bounded as well as for unbounded domains.

[7] This scaling comes from the natural scaling if the strain were compatible, since $\nabla_\xi^S u(\xi) = \epsilon\nabla_x^S\tilde{u}(x)$.

any detail. Provided Assumptions 5 and 6, we have

$$
\begin{aligned}
&< (\kappa \times \nabla)^{d^*}, \varphi >= - \int_\Sigma \hat{k} \cdot \nabla \times \varphi dS(x) + \frac{1}{2} \int_\Sigma \epsilon_{mpn} \partial_p \left(\operatorname{tr} \varphi \right) \hat{k}_{mn} dS(x) \\
= &\; - \int_\Sigma dS(x) \left((\nabla \times \varphi) \cdot \fint_{V_x^\star} d\tilde{\kappa}_x^\star(y) + \frac{1}{2} \epsilon_{mpn} \partial_p \left(\operatorname{tr} \varphi \right) \left(\fint_{V_x^\star} d\tilde{\kappa}_x^\star(y) \right)_{mn} \right) \\
= &\; - \lim_{\epsilon \to 0} \frac{1}{|V_x^\star|} \int_\Sigma dS(x) \left(\int_{B(0,R/\epsilon)} \nabla_\xi \times \varphi_x^\epsilon(\xi) \cdot d\tilde{\kappa}_x^{\star\epsilon}(\xi) + \frac{1}{2} \int_{B(0,R/\epsilon)} \epsilon_{mpn} \frac{\partial}{\partial \xi_p} \operatorname{tr} \varphi_x^\epsilon(\xi) \left(d\tilde{\kappa}_x^{\star\epsilon}(\xi) \right)_{mn} \right) \\
= &\; \lim_{\epsilon \to 0} \frac{1}{|V_x^\star|} \int_\Sigma dS(x) < \nabla_\xi \times \mathcal{E}_x^{\star\epsilon} \times \nabla_\xi, \varphi_x^\epsilon > = < \nabla \times \left(\hat{\mathcal{E}}_x \delta_\Sigma \right) \times \nabla, \varphi >,
\end{aligned}
$$

proving the claim by definition of the Bravais strain and Assumption 4. □

4.2 Elasto-plastic decomposition

Notations 6 (Symmetric parts) *We use the notations $\nabla^S u := \frac{1}{2}(\nabla u + u \nabla)$ and $A^S := \frac{1}{2}\left(A + A^T\right)$ for any vector distribution u and second order tensor A.*

Any symmetric tensor field can be decomposed into compatible and solenoidal parts by Lemma 1. Moreover, according to Eq. (4.1), as soon as the contortion is known, the Bravais strain is determined up to a compatible field.

Remark 3 (Bravais strain decomposition) *The Bravais strain is decomposed as*

CANONICAL DECOMPOSITION OF THE BRAVAIS STRAIN: $$\mathcal{E}^B := \nabla^S \tilde{u} - \mathcal{E}^R \qquad (4.6)$$

where $(-\mathcal{E}^R)$ is symmetric, solenoidal and satisfies (4.1). To fix $\tilde{u}$ (up to piecewise constant displacements) one solves

$$\mathcal{L}_{0,1}(\tilde{u}) = 2 \nabla \cdot \mathcal{E}^B \qquad (4.7)$$

with the Lamé operator $\mathcal{L}_{\lambda,\mu} = \mu \Delta + (\mu + \lambda) \nabla \nabla \cdot$, whose distributional solution $\tilde{u}$ is given in terms of the Kelvin matrix [2]. Moreover, the symmetric and solenoidal $\mathcal{E}^R$ writes for some solenoidal distribution R as $\mathcal{E}^R = \nabla \times R \times \nabla$ where R is, by taking the double curl of (4.1), solution to

$$\nabla \times \mathcal{E}^R \times \nabla = \Delta \Delta R = -\nabla \times \mathcal{E}^B \times \nabla = -\left(\kappa \times \nabla - \frac{1}{2} \operatorname{tr}(\kappa \times \nabla) \right) \qquad (4.8)$$

which is unique provided appropriate boundary conditions are imposed at the crystal boundary.

It is observed by classical elliptic regularity results [8, 40] that $\kappa \in \mathcal{M}(\Omega) \subset H^{-2}_{loc}(\Omega)$, in such a way that in general $\mathcal{E}^R \in H^{-1}_{loc}(\Omega) = \left(H^1_{loc}(\Omega)\right)'$. However, according to Assumptions 5 and 6, the Bravais strain turns out to be more regular.

Remark 4 (Regularity of the residual strain) *Under the strong Assumption 5, it results from elliptic regularity results that $\mathcal{E}^R \in H^1_{loc}(\Omega; \mathbb{R}^{3\times3})$, since $\kappa \times \nabla \in H^{-1}_{loc}(\Omega)$. In fact, remark that for every test function $\Psi \in H^1_0(\Omega; \mathbb{R}^{3\times3})$, expression*

$$< \kappa \times \nabla, \Psi >= - \int_\Omega \bar{\kappa} \cdot \Psi \times \nabla dx - \int_\Sigma \hat{k} \cdot \Psi \times \nabla dS(x) \qquad (4.9)$$

defines a linear and continuous form on $H^1_0(\Omega; \mathbb{R}^{3\times3})$. Otherwise, under the weaker Assumption 6, we have $\kappa \times \nabla \in \mathcal{M}(\Omega) \subset H^{-2}_{loc}(\Omega; \mathbb{R}^{3\times3})$ and hence $\mathcal{E}^R \in L^2_{loc}(\Omega; \mathbb{R}^{3\times3})$.

Obviously, if κ is smooth in Ω, then the Bravais strain is also smooth and the problem is posed in classical, though far from trivial, terms at the macroscale (cf. Remark 7).

Definition 8 (Elastic and plastic strain decomposition) *Let us define the macroscopic stress density tensor as* $\sigma(x) =< \sigma_x >= \fint_{V(x)} \sigma_x^\star(y)dy$ *and assume that* $\sigma \in L^1(\Omega)$. *The elastic and plastic strains are defined as*

$$\text{MACROSCOPIC ELASTIC STRAIN:} \qquad \mathcal{E}^E := C\sigma + \beta(T - T_0) \tag{4.10}$$

$$\text{MACROSCOPIC PLASTIC STRAIN:} \qquad \mathcal{E}^P := \mathcal{E}^B - \mathcal{E}^E, \tag{4.11}$$

where C and β are the macroscopic thermo-elastic compliance and dilation tensors. Moreover, by Assumption 4, $\mathcal{E}^E \in L^1(\Omega)$ and $\mathcal{E}^P \in \mathcal{M}(\Omega)$.

The strain $\mathcal{E}^P$ should be understood as the part of the homogenized strain which is not elastic. Since we have homogenized by taking a volume average of the mesoscopic strain which was assumed elastic everywhere except on the dislocation lines, $\mathcal{E}^P$ represents the homogenization effect as generated by the mesoscopic *dislocation cores*.

4.3 Displacement of bounded deformation and glide surface

The following notion has been introduced by Temam and Strang [33] (see also [1,10]).

Notion 2 (Functions of bounded deformation) *A distribution u is of bounded deformation on Ω, i.e. $u \in BD(\Omega)$, if the symmetric part of its gradient is a Radon measure in the sense of Notion 1.*

Moreover, if a function is of bounded deformation it is locally Lebesgue integrable [33]. According to (4.6)-(4.8), (4.10)-(4.11), and Remark 4, we have established the existence of a displacement $\tilde{u} \in BD(\Omega)$ such that

$$\mathcal{E}^B + \mathcal{E}^R = \nabla^S \tilde{u} = \mathcal{E}^E + \mathcal{E}^P + \mathcal{E}^R \in \mathcal{M}(\Omega). \tag{4.12}$$

By Remark 4 and Definition 8, the sum $\mathcal{E}^E + \mathcal{E}^R \in L^1(\Omega)$. Hence by the decomposition property of BD fields [10] we know that $\mathcal{E}^P = \mathcal{E}^{P,r} + \mathcal{E}^{P,c}(\tilde{u}) + \mathcal{E}^{P,cantor}$, where $\mathcal{E}^{P,r} \in L^1(\Omega)$, $\mathcal{E}^{P,c}(\tilde{u}) := ([\tilde{u}] \otimes n\delta_\Sigma)^S$ with Σ the set of jump points of $\tilde{u}$ and n its unit normal, while $\mathcal{E}^{P,cantor}$ is the Cantor part of the plastic strain, that is, a diffuse measure s.t. $\mathcal{E}^{P,cantor}(S) = 0$ and $\mathcal{E}^{P,cantor}(A) = \infty$ for every surface $S \subset \Omega$ and volume $A \subset \Omega$. So, we may write

$$\nabla^S \tilde{u} = \mathcal{E} + \mathcal{E}^{P,c}(\tilde{u}) + \mathcal{E}^{P,cantor}, \tag{4.13}$$

where we have defined the total diffuse and regular Bravais strains as

$$\text{TOTAL DIFFUSE STRAIN} \qquad \mathcal{E} := \bar{\mathcal{E}}^B + \mathcal{E}^R \tag{4.14}$$

$$\text{REGULAR BRAVAIS STRAIN} \qquad \bar{\mathcal{E}}^B := \mathcal{E}^E + \mathcal{E}^{P,r} \tag{4.15}$$

while the remaining plastic strain is made of two terms: a purely concentrated part on a surface Σ with unit normal σ and a (fractal) Cantor part. By (4.13), we have $\operatorname{inc}\left(\mathcal{E} + \mathcal{E}^{P,c}(\tilde{u})\right) = -\operatorname{inc}\left(\mathcal{E}^{P,cantor}\right)$, whereby $\operatorname{inc}\left(\mathcal{E}^{P,cantor}\right) = 0$, since taking any smooth test-function Ψ with compact support and nonvanishing incompatibility it is observe that

$$< \mathcal{E} + \mathcal{E}^{P,c}(\tilde{u}), \operatorname{inc}\Psi >= - < \operatorname{inc}\mathcal{E}^{P,cantor}, \Psi >= - < \mathcal{E}^{P,cantor}, \operatorname{inc}\Psi >$$

necessarily implies that the distribution $\operatorname{inc} \mathcal{E}^{P,cantor}$ vanishes, since the LHS is finite. Hence

$$-\operatorname{inc}\left(\mathcal{E}^R + \mathcal{E}^{P,c}(\tilde{u})\right) = \operatorname{inc}\left(\mathcal{E}^B\right) = \kappa \times \nabla - \frac{I}{2} \operatorname{tr}\left(\kappa \times \nabla\right). \tag{4.16}$$

Let us emphasize that $\mathcal{E}$ is compatible in Ω only if $\mathcal{E}^{P,c}(\tilde{u}) = 0$ (i.e., in the absence of glide planes). It is otherwise compatible in $\Omega \setminus \Sigma$, and to this extend $\mathcal{E}$ is considered the countaerpart of the mesoscopic $\mathcal{E}^{\star}$.

The natural removal of the Cantor part is provided.

4.4 Displacement as a SBD function

Since $\mathcal{E}^{P,cantor} \in \mathcal{M}(\Omega) \subset H^{-2}_{loc}(\Omega)$is compatible we have the existence of the scalar gauge field $P^c \in L^2_{loc}(\Omega)$ such that $\mathcal{E}^{P,cantor} = \nabla P^c \nabla = \nabla^S(\nabla P^c)$ and $\Delta\Delta P^c = \nabla \cdot \mathcal{E}^{P,cantor} \cdot \nabla \in H^{-4}_{loc}(\Omega)$. By defining $u := \tilde{u} - \nabla P^c$ it follows that $\nabla^S u = \mathcal{E} + \left([\tilde{u}] \otimes n\delta_\Sigma\right)^S$, whose RHS is a Radon measure and hence [33] such that $\nabla P^c \in L^1_{loc}(\Omega)$. Hence $P^c \in W^{1,1}_{loc}(\Omega) \cap L^2_{loc}(\Omega)$ with by definition $\nabla P^c \in BD(\Omega)$. It therefore has a trace on both sides of Σ [10], satisfying the BD decomposition theorem [10]: $\mathcal{E}^{P,cantor} = \nabla^S\left(\nabla P^c\right) = \left([\nabla P^c] \otimes n\delta_{\Sigma^c}\right)^S + E^c\left(\nabla P^c\right)$ for some rectifiable surface Σ^c, which must be the empty set since all other terms are of Cantor-type (and in particular, are diffuse terms on Ω). In other terms, ∇P^c has no jump in Ω and therefore we have $u \in SBD(\Omega)$ satisfying the decomposition

STRAIN DECOMPOSITION $$\nabla^S u = \mathcal{E} + \mathcal{E}^{P,c}(u), \tag{4.17}$$

where $\mathcal{E}^{P,c}(u)$ is the plastic strain concentrated on the two-dimensional glide surfaces with normal n.

Remark 5 *Since the tensor distribution $\mathcal{E}^{P,c}(u)$ can be decomposed into a compatible and a solenoidal part as denoted by $\hat{\mathcal{E}}^{P,c}(u)$, the displacement field u might be defined such that*

STRAIN DECOMPOSITION $$\nabla^S u = \mathcal{E} + \hat{\mathcal{E}}^{P,c}(u). \tag{4.18}$$

4.5 Meso-macro convergence

Any mesostructure Υ_x at x is by definition the limit as $\epsilon \to 0$ of a countable mesostructures Υ_x^ϵ with less accumulation sets. The real ϵ defines the *mesoscopic scale at scale* ϵ.

Definition 9 (Transfinite cluster at scale ϵ) *Recall that the so-called $1st$ derived subset $\bar{\Upsilon}_x^{(1)}$ of Υ_x is the subset of Υ_x from which all isolated segments have been removed. The kth derived subset $\bar{\Upsilon}_x^{(k)}$ ($k \geq 1$) is defined as the subset of $\bar{\Upsilon}_x^{(k-1)}$ from which all isolated segments have been removed. The scale ϵ_k ($k \in \mathbb{N}_*$) is associated with the mesostructure $\Upsilon_x^k := \Upsilon_x^{k-1} \setminus \bar{\Upsilon}_x^{(k)}$ with the convention that $\Upsilon_x^0 = \Upsilon_x$. The mesostructure Υ_x^ϵ at scale $\epsilon \geq 0$ is identified with the mesostructure at scale $\epsilon_k = \lfloor \epsilon \rfloor$.*

Observe that the cardinality of Υ_x^ϵ converges to 0 as $\epsilon \to \infty$.

Definition 10 (Homogenization spectrum) *For $0 \leq \epsilon < \infty$, introduce $R_x^\epsilon := \frac{2}{\pi}\arctan(\frac{1}{\epsilon})R_x$, $V^\epsilon_{\Upsilon_x} := B(x, R_x^\epsilon) \setminus \Upsilon_x$ and define $V_x^\epsilon := \{x\} \cup \{V^\epsilon_{\Upsilon_x} \cup \Upsilon_x^\epsilon\}$, the RVE with ϵ-derived mesostructure (i.e., the complete mesostructure without all derived* *subsets of order* $> \epsilon$*, considered as invisible at scale* ϵ*). The* ϵ*-mesoscopic strain is defined as*

$$\mathcal{E}^\epsilon(x) := \mathcal{E}_x\left(V_x^\epsilon\right). \tag{4.19}$$

In particular its singular part is concentrated on Υ_x^ϵ*.*

By Definition 6 and Assumption 4 and since $V_x^\epsilon \to \{x\}$ as $\epsilon \to \infty$, we have for almost every $x \in \Omega$ the pointwise convergence [1], $\mathcal{E}_x^\star = \lim_{\epsilon\to\infty} \mathcal{E}^\epsilon(x)$, while from $V_x^\epsilon \to V_x^\star$ as $\epsilon \to 0$, convergence in the distribution sense follows as:

MESO-MACRO CONVERGENCE OF THE BRAVAIS STRAIN
$$\mathcal{E}^B = \lim_{\epsilon\to 0} \mathcal{E}^\epsilon. \tag{4.20}$$

where $\mathcal{E}^\epsilon \in L^s(\Omega)$ with $1 \leq s < 2$. As a consequence of (4.20) it immediately follows that, in the distribution sense,

$$\operatorname{inc}\left(\mathcal{E}^\epsilon\right) \to \operatorname{inc}\left(\mathcal{E}^B\right) \tag{4.21}$$

$$\mathcal{E}^\epsilon \times \nabla \to \mathcal{E}^B \times \nabla, \tag{4.22}$$

as $\epsilon \to 0$ and where $\mathcal{E}^B \times \nabla$ is the so-called macroscopic Frank tensor [36, 37].

The following result is proved in Appendix B. Let us recall the notation $\kappa^\epsilon := \sum_{\mathcal{L}\in\Upsilon_x^\epsilon} \kappa^{\mathcal{L}(\epsilon)}$ with $\kappa^{\mathcal{L}(\epsilon)} := \kappa_x^{\mathcal{L}}\left(V_x^\epsilon\right)$(cf. Definition 5 and Remark 2).

Corollary 1 (Meso-macro convergence of the contortion) *It results from Theorems 2 and 4 that*

$$\kappa = \lim_{\epsilon\to 0}\left(\kappa^\epsilon + G^{(\epsilon)} \times \nabla\right), \tag{4.23}$$

where $G^{(\epsilon)}$ *is a solenoidal tensor gauge field satisfying*

$$\Delta G^{(\epsilon)} = \kappa^\epsilon \times \nabla. \tag{4.24}$$

Moreover, in the distribution sense[8]*,*

$$\sum_{\mathcal{L}\in\Upsilon_x^\epsilon} (\sigma^{\mathcal{L}} \otimes \sigma^{\mathcal{L}} + \nu^{\mathcal{L}} \otimes \nu^{\mathcal{L}})\hat{\eta}^{\mathcal{L}(\epsilon)} \to 0 \tag{4.25}$$

where $\hat{\eta}^{\mathcal{L}(\epsilon)} := \tilde{\eta}^{\mathcal{L}(\epsilon)} - \frac{I}{2} \operatorname{tr} \tilde{\eta}^{\mathcal{L}(\epsilon)}$ *with* $\tilde{\eta}^{\mathcal{L}(\epsilon)} = \kappa^{\mathcal{L}(\epsilon)} \times \nabla$*.*

Let us now restate Postulate 1. By Assumption 2, the following definition can be made.

Definition 11 (Local macroscopic Burgers vector) *Let us define* B_x *at* $x \in \Omega$ *as*

$$B_x := \sum_{\mathcal{L}\in\Upsilon_x} ||B^{\star\mathcal{L}}||. \tag{4.26}$$

Postulate 2 (Continuity of the local macroscopic Burgers vector) *Let us assume that the RVEs can be chosen in such a way that* $x \mapsto B_x$ *is a continuous function from* Ω *to* $\mathbb{R}$*.*

A formulation of Postulate 2 in precise mathematical terms would require to rigorously define the meso- and macroscopic characteristic length l and L. It is however rather natural to validade Postulate 2 since one observes that two RVEs “close enough” have ”almost the same“ mesostructure, where the key argument is again Assumption 2. Let us emphasize that Postulate 2 is an alternative to Postulate 1.

[8]This limit can be interpreted in terms of a vanishing statistical mean. It explains why the key expression (3.1) only takes into account the projection of the strain incompatibility on the mesoscopic lines

Corollary 2 (The Bravais strain and the contortion are Radon measures) *From Definitons 10 and 11 and Postulate 2 it results that $\mathcal{E}^B$ and κ are a Radon measure from Ω to $\mathbb{R}^{3\times 3}$.*

Proof. The strain at scale ϵ, $\mathcal{E}^\epsilon : x \in \Omega \to \mathbb{R}^{3\times 3}$, is rewritten from Definition 11 and Eq. (4.19) as

$$\mathcal{E}^\epsilon = \int_{\mathbb{R}^3} \mathcal{E}_x^{\star(\epsilon)}(y)dy \quad \text{with} \quad \mathcal{E}_x^{\star(\epsilon)} := \mathcal{E}^\star \chi_{V_x^\epsilon} \quad \text{and} \quad x \in \Omega. \tag{4.27}$$

As direct consequence of Postulate 2 and from the boundedness of Ω, the finiteness of $\sup_{x\in\overline{\Omega}}\{\sum_{\mathcal{L}\in\Upsilon_x} ||B^{\star\mathcal{L}}||\}$ follows. Hence the equiboundedness of $\{\mathcal{E}^\epsilon\}_\epsilon$ also follows, since the strain is known to linearly depend on the mesoscopic Burgers vector [35]. This implies boundedness in the space of Radon measures $\mathcal{M}(\Omega;\mathbb{R}^{3\times 3})$ and hence by compactness of this class [1], convergence of (a subsequence) of $\mathcal{E}^\epsilon$ to a Radon measure identified, by Eq. (4.20), with $\mathcal{E}^B$. By compactness again, the statement for the contortion is immediate. □

4.6 Geometrical and physical interpretation of the correction term

Three types of arguments are given to understand the specific role of the newly introduced term $-\frac{I}{2}\,\mathrm{tr}\,(\kappa \times \nabla)$ in the corrected Kröner's formula (4.1). They are given in an increasing order of importance.

Argument of structure Recall that the contortion κ was defined from the dislocation density Λ in Definition 2 by

$$\kappa = \Lambda - \frac{I}{2}\,\mathrm{tr}\,\Lambda.$$

By Theorem 4, strain incompatibility η also shows this mathematical structure, since

$$\eta = \kappa \times \nabla - \frac{I}{2}\,\mathrm{tr}\,(\kappa \times \nabla).$$

This argument is not a mere aesthetic consideration. It has been shown in [34] that it also gives a hint that if the *first-grade defect variable* is chosen to be Λ, *the second-grade defect variable* should be $\kappa \times \nabla$. Moreover, this choice of defect model variables closes[9] the model in the sense that η can also be written as (cf. Eq. (4.22))

$$\eta = \nabla \times \overline{\partial}\omega,$$

with the Bravais strain $\mathcal{E}^B$ and Frank tensor $\overline{\partial}\omega := \mathcal{E}^B \times \nabla$ shosen as the *first- and second-grade deformation variables*.

Argument of geometry Considering for a while finite elasticity, it is known [6] that given a metric g, it writes as $g = \nabla\phi\nabla^T\phi$ for some diffeomeorphism ϕ such that $\Omega = \phi(\Omega_0)$ with Ω_0 and Ω the reference and current bodies, if and only if the 4th-order Riemann curvature tensor $\underline{\underline{\underline{\underline{R}}}}$ vanishes. In the small strain assumption in $3D$, let $g := I - 2\mathcal{E}^B$ be the *elastic metric*. Then, it is not hard to see [22,34]

[9] The model is closed in the sense that there is no need to further consider higher grade deformation and model variables since a common quantity, the incompatibility, renders those two families of variables non-independent from each other, as soon as grade 2 is considered.

that the above statement is equivalent to requiring that $\mathcal{E}^B$ be compatible in our sense: $\eta := \nabla \times \mathcal{E}^B \times \nabla = 0$ with $\eta = \underline{\underline{R}}^B - \frac{I}{2} \operatorname{tr} \underline{\underline{R}}^B$.

Therefore it immediately follows by identification with Eq. (4.1) that the Ricci tensor is the contortion curl, i.e.,

$$\underline{\underline{R}}^B = \kappa \times \nabla. \tag{4.28}$$

Let us also point out that tensor $G := R - \frac{g}{2} \operatorname{tr} R$ is precisely the so-called *Einstein tensor* (in the space-time manifold) appearing in the Einstein field equations. In our case, g is the linear elastic metric, R the contortion curl, while Einstein's energy-momentum G is identified in our theory with the strain incompatibility (under this small strain assumption).

Accepting now, in the spirit of Kröner's brillant intuition, that the dislocated crystal should be understood as a differential (non-Riemannian) manifold whose geometric properties (as metric, curvature, torsion, contortion, holonomic and anholonomic coordinates, connexion terms non-compatible with the metric, etc.) have a precise physical meaning [21], the newly-introduced trace term appearing in Eq. (4.1) allows us to make the crucial identification (4.28).

Argument of physics Let us determine the kind of line defect such that the correction term vanishes. It suffices to consider the mesoscopic term since its macroscopic counterpart follows from the homogenization process as described in Section 3. Definition 2 and direct calculations show that $\operatorname{tr}\ (\kappa \times \nabla) = \epsilon_{jpq}\partial_p \kappa^{\star\mathcal{L}}_{jq} = \epsilon_{jpq}\partial_p \left(B^{\star\mathcal{L}}_q \tau_j \delta_{\mathcal{L}}\right) = 0$ if at least one of the four following conditions is satisfied (with $\{\tau, \sigma, \nu\}$ the local Cartesian basis):

- $B^{\star\mathcal{L}}$ is parallel to τ
- $\chi \sigma_q B^{\star\mathcal{L}}_q = 0$
- $B^{\star\mathcal{L}}_q \sigma_q \partial_\nu \delta_{\mathcal{L}} = 0$
- $\partial_\sigma \delta_{\mathcal{L}} = 0$ with coplanar $B^{\star\mathcal{L}}$ and τ,

i.e., if one of the following situations is realized:

1. Straight dislocation lines of screw or edge type
2. Non-expanding pure edge dislocation loop
3. Conservative loop without cross-slip mechanism.

From the above four cases, the first three can be discarded (since in this paper we restrict ourselves to conservative loops, cf. Definition 3). However, the fourth situation is a very important mechanism in single-crystal plasticity, which can not be discarded a-priori. Therefore, cross-slip of conservative loops (see Figure 3 [17]) is interpreted as responsible for the correction term.

5 Applications of Theorem 4 for modeling purposes

The incompatibility-contortion relation has been analyzed so far in a statical, geometrical context. Given a dislocation mesostructure at $x \in \Omega$, we have proved that strain incompatibility and contortion are directly related through a static differential relation given by Theorem 4.

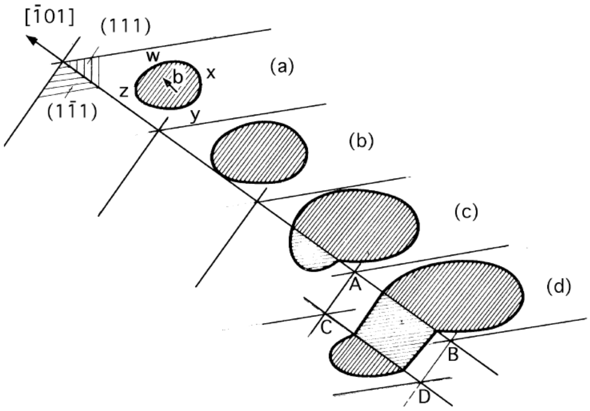


Figure 3: Cross-slip ((a)-(c)) or double cross-slip ((d)) mechanisms for conservative loops is responsible for the correction term in Kröner's formula [17]).

In the present section we show how this relation can be exploited to postulate evolution and/or optimization laws. Our starting point is the notion of Ricci flow [16] and the recent developments [27] as based on the landmark paper by Perelman [30]. In these references, from which we retain only introductory notions, the Ricci flow of a given connection (i.e., let us say, a scalar product on a differentiable manifold) is analyzed in detail to overcome a time singularity.

Here, we adapt the formalism of the authors, modify the flow, and show that it is solvable on each time interval. Surprisingly enough the flow proves these good properties directly from the incompatibility-contortion relation proved in Theorem 4. Another reference should here be [34] where it is shown that Riemann curvature, Cartan torsion and torsion contortion in the crystal differentiable manifold have a physical meaning in terms of defect quantities. Let us recall that the notion of crystal manifold is a 60-years-old and rich idea due to Kröner [20] and Kondo [19].

5.1 Flow of the Bravais strain

Assume for a while that the Bravais strain $\mathcal{E}^B$ is smooth. According to [34], $\kappa \times \nabla$ is identified with the so-called Ricci curvature R^B, writing componentwise as the trace $R^B_{jq} := R^B_{l;jlq}$ of the Riemann curvature tensor $R^B_{l;jmq}$ related to the following Bravais connection and curvature:

$$\text{BRAVAIS CONNECTION} \qquad \Gamma^B_{k;ij} := \frac{1}{2}\left(\partial_i g^B_{kj} + \partial_j g^B_{ki} - \partial_k g^B_{ij}\right), \tag{5.1}$$

$$\text{BRAVAIS CURVATURE} \qquad R^B_{l;kmq} := \left(\partial_q \Gamma^B_{l;km} + \tilde{g}^B_{np}\Gamma^B_{n;km}\Gamma^B_{p;lq}\right)_{[mq]} \tag{5.2}$$

with $\tilde{g}^B = I + 2\mathcal{E}^B$ the inverse of the

$$\text{BRAVAIS METRIC} \qquad g^B = I - 2\mathcal{E}^B \tag{5.3}$$

under the small strain assumption, and where $A_{[mn]}$ is a notation for $A_{mn} - A_{nm}$. Moreover let us introduce the scalar *Bravais curvature* as $R^B := R^B_{qq} = \mathrm{tr}\,(\kappa \times \nabla)$, and rewrite Theorem 4 as

$$\text{BRAVAIS FORMULA} \qquad \operatorname{inc} \mathcal{E}^B = \underline{\underline{R}}^B - \frac{I}{2} R^B. \tag{5.4}$$

The aim of this section is to analyze the consequences of (5.4). Introduce the so-called Einstein-Hilbert functional

$$\text{AVERAGE SCALAR CURVATURE} \qquad \psi(g^B) = \fint_\Omega R^B J^B dV, \tag{5.5}$$

where $J^B := \sqrt{|\det g^B|}$. Recalling that $\frac{d}{dt}\left(J^B\right) = \frac{1}{2} g^B \cdot \dot{g}^B$ and $\dot{R}^B = -\underline{\underline{R}}^B \cdot \dot{g}^B - \Delta \operatorname{tr} \dot{g}^B$ [27], while assuming that $\partial_N \operatorname{tr} \dot{\mathcal{E}}^B = \left(\nabla \cdot \dot{\mathcal{E}}^B\right) N = 0$ on $\partial\Omega$ with N the outward unit normal to Ω, the time derivative of (5.5) writes as:

$$\frac{d}{dt}\psi(g^B) = -\int_\Omega \left(\underline{\underline{R}}^B - \frac{g^B}{2} R^B\right) \cdot \dot{g}^B J^B dV. \tag{5.6}$$

Assuming small deformations (i.e., considering that the term $\mathcal{E}^B \cdot \dot{\mathcal{E}}^B$ is negligible as compared with the other terms of (5.6)) and according to Theorem 4, the flow of the Bravais strain is driven by strain incompatibility and reads from (4.28) (5.3) and (5.6),

$$\text{BRAVAIS FLOW} \qquad \frac{d}{dt}\mathcal{E}^B = -\frac{1}{2}\dot{g}^B = \frac{\alpha}{2}\left(\kappa \times \nabla - \frac{I}{2} \operatorname{tr}(\kappa \times \nabla)\right) = \frac{\alpha}{2} \operatorname{inc}\left(\mathcal{E}^B\right), \tag{5.7}$$

where α is a dimensional parameter[10] (scalar or tensorial) and where $\operatorname{inc}(\cdot)$ on the RHS is an elliptic operator of order two in the sense of Legendre and Hadamard[11]. Hence, provided appropriate boundary conditions, the incompatibility driven Bravais flow is parabolic and shows existence on every times interval, as opposed to ordinary Ricci flows [9, 16, 27, 30]. We postulate the following law.

Law 1 (Evolution by maximal[12] curvature) *The average scalar curvature $\psi(g^B)$ is increasing under the Bravais flow.*

Let us emphasize that the Bravais strain is a so-called *internal* variable, i.e., it is not a state – observable variable. Hence postulate such as Law 1 are not directly in contradiction with physical observations or measurements. Law 1 should be confronted to its physical consequences, in particular in terms of modeling. This issue will be initiated in the next section, but not developped in the present paper. So, for the moment, we admit that Law 1 is a pure conjecture.

Remark 6 *If the Bravais strain were non-smooth Radon measure, as it should be in principle, then Eq. (5.7) is nevertheless recovered in the distribution sense, since distributions are limits of smooth functions [31]. Moreover (5.7) shows by classical parabolic regularity results [12] that for smooth enough boundary and initial data, the Bravais strain is actually more regular than simply Radon measurable. For smooth data, the Bravais strain is smooth, and so is the contortion.*

[10] With the physical dimensions of a surface flow $[m^2/s]$.

[11] Since $f(u) = \frac{1}{2}|\nabla \times u|^2$ is rank-one convex [8].

[12] Among optimization principles in Mechanics, maximization has proven justified in thermodynamic analysis of many material processes, as for instance the celebrated Hill-Mandel principle of maximal dissipation in crack evolution [38].

As another consequence, we also have an evolution law for the incompatibility:

TIME EVOLUTION OF INCOMPATIBILITY

$$\frac{d}{dt}\operatorname{inc}\left(\mathcal{E}^B\right) = \frac{\alpha}{2}\operatorname{inc}\left(\operatorname{inc}\left(\mathcal{E}^B\right)\right) = \frac{\alpha}{2}\left(\Delta - \nabla\nabla\cdot\right)\mathcal{E}^B\left(\Delta - \cdot\nabla\nabla\right), \tag{5.8}$$

where $\operatorname{inc}(\operatorname{inc}(\cdot))$ on the RHS is an elliptic operator of order four in the sense of Legendre and Hadamard. Since $\operatorname{tr}\ \operatorname{inc} = \left(\Delta\operatorname{tr} - \nabla\cdot\nabla^T\cdot\right)$ with $\operatorname{tr}\ \left(\operatorname{inc}\mathcal{E}^B\right) = -\frac{1}{2}R^B$ and $\nabla\cdot\ \operatorname{inc} = \operatorname{inc}\cdot\nabla = 0$, by taking the trace of (5.8) we have the following evolution law for the scalar Bravais curvature.

Law 2 (Parabolic evolution of the curvature) *The scalar curvature satifies*

$$\dot{R}^B = \frac{\alpha}{2}\Delta R^B, \tag{5.9}$$

with appropriate initial and boundary conditions.

By classical parabolic regularity results [12], the minimal and maximal values of the scalar curvature depend on their bounds on $\partial\Omega$. So, if those are kept bounded in time, the process (5.9) stops in finite time. The resulting state is identified with the *thermodynamic equilibrium*.

5.2 Physical interpretation of the Bravais flow

By Remark 3, recall that $\mathcal{E}^B := \nabla^S\tilde{u} - \mathcal{E}^R$ with $\tilde{u}$ a displacement field, $\mathcal{E}^R$ the residual strain satisfying $\nabla\cdot\mathcal{E}^R = 0$. By defining $u^B := \operatorname{tr}\mathcal{E}^B$, which physically is a variation of matter density, we first observe that in the small strain assumption ψ rewrites as

$$\psi(g^B) = \fint_\Omega R^B(1 - u^B)dV.$$

Since the physical meaning of $\mathcal{E}^B$ appears through its incompatibility and since $\mathcal{E}^B$ can be decomposed into a compatible and a divergence-free tensor by Lemma 1, we may for the sake of interpretation assume that $\nabla\cdot\mathcal{E}^B = 0$. It immediately follows from Eq. (5.4) that $-\frac{1}{2}R^B = \operatorname{tr}\ \left(\operatorname{inc}\mathcal{E}^B\right) = \Delta u^B$. As a consequence, integrating by parts (recall the assumption $\partial_N\dot{u}^B = 0$ on $\partial\Omega$), Law 1 rewrites as

$$0 \leq \frac{d}{dt}\psi(g^B) = -2\frac{d}{dt}\fint_\Omega |\nabla u^B|^2 dV, \tag{5.10}$$

meaning that $\fint_\Omega |\nabla u^B|^2 dV$ must be decreasing in time, whereby the following interpretation of the Bravais flow in mechanical terms is given:

Conjecture 1 (Thermodynamic uniformization process) *Under a Bravais flow, the lattice atom displacements tend to produce a dislocation meso-structure which has the macroscopic effect of increasing the (Bravais) curvature (up to its boundary values), while uniformizing the matter density. The thermodynamic equilibrium therefore consists of a state of the dislocated crystal where maximal uniformization has been reached, i.e., a state showing the maximal regions with uniform curvature and matter density.*

Remark 7 (Harmonic contortion at equilibrium) *Remark that uniform (Ricci) curvature means a smooth contortion, since the identification* $\underline{\underline{R}}^B = \kappa\times\nabla$ *immediately yields* $\underline{\underline{R}}^B\times\nabla = 0 = -\Delta\kappa + \nabla\nabla\cdot\kappa$, *whereby* $\Delta\kappa = \left(\kappa\cdot\nabla\right)\nabla$. *The contortion being an internal variable depending on the state variables* X_i *(in particular, temperature),* κ *shows to be harmonic at thermodynamic equilibrium (i.e., where in particular* $\nabla X_i = 0$*) since* $\Delta\kappa = \partial_{X_i}\left(\kappa\cdot\nabla\right)\cdot\nabla X_i = 0$.

5.3 Elements of thermodynamics in dislocated crystals

We consider a first-grade strain-based theory where the only state variable is the total diffuse strain $\mathcal{E}$ of Section 4.3. It is decomposed in three parts: the residual strain, the elastic strain and the regular plastic strain, each of which being considered as internal mechanical variables. The regular Bravais strain, being the sum of the latter two, is thereby also an internal mechanical variable. On the other hand, the only defect internal variable is assumed to be the contortion κ (see [34] for more detail). Classical thermodynamic relations are assumed for those fields (including the so-called complementary laws, whose brief exposition is taken from [23]). The fields can be summarized as follows.

Definition 12 (Thermodynamic system)

TOTAL DIFFUSE STRAIN	$\mathcal{E} = \bar{\mathcal{E}}^B + \mathcal{E}^R = \mathcal{E}^E + \mathcal{E}^*$	(5.11)
DECOMPOSITION OF THE REGULAR BRAVAIS STRAIN	$\bar{\mathcal{E}}^B := \mathcal{E}^E + \mathcal{E}^{P,r}$	(5.12)
DIFFUSE NONELASTIC STRAIN	$\mathcal{E}^* := \mathcal{E}^R + \mathcal{E}^{P,r}$	(5.13)
ATHERMAL SPECIFIC ENERGY POTENTIAL	$\Psi := \Psi\left(\mathcal{E};\mathcal{E}^E,\mathcal{E}^*;\kappa\right)$	(5.14)
DISSIPATION POTENTIAL	$\varphi := \varphi\left(\dot{\mathcal{E}}^*;\dot{\kappa}\right)$	(5.15)
STRESS	$\sigma := \rho\frac{\partial\Psi}{\partial\mathcal{E}^E} = \frac{\partial\varphi}{\partial\dot{\mathcal{E}}^*}$	(5.16)
DISLOCATION FORCE	$\gamma := \rho\frac{\partial\Psi}{\partial\kappa} = \frac{\partial\varphi}{\partial\dot{\kappa}}$	(5.17)
DISSIPATION	$\Phi := \sigma\cdot\dot{\mathcal{E}}^* + \gamma\cdot\dot{\kappa}$	(5.18)
LEGENDRE-FENCHEL TRANSFORM	$\varphi^* := \varphi^*(\sigma,\gamma) = \sup_{\dot{\mathcal{E}}^*,\dot{\kappa}}\{\Phi - \varphi\}$	(5.19)
EVOLUTION LAW FOR RATE OF NONELASTIC DEFORMATION	$\dot{\mathcal{E}}^* = \frac{\partial\varphi^*}{\partial\sigma}$	(5.20)
EVOLUTION LAW FOR RATE OF CONTORTION	$\dot{\kappa} = \frac{\partial\varphi^*}{\partial\gamma}$	(5.21)

Let us remark that $\mathcal{E}^*$ is sometimes called eigenstrain [28]. It appears as made of two parts. The first part is the residual strain, due to the presence of moving dislocations: it is non reversible unless one expels the dislocations through the crystal boundary. The second part is a strain which models all mechanical effects which depart from linear elasticity (i.e., nonlinear elasticity, higher-order strain terms, ductile damage, etc.)

Definition 13 (Nonelastic force) *Provided the stiffness tensor $S := C^{-1}$,*

NONELASTIC FORCE
$$f^* = -\nabla\cdot\left(S\left(\mathcal{E}^* + \hat{\mathcal{E}}^{P,c}(u)\right)\right).$$

Let us remark that if $S = 2\mu I_4 + \lambda I_2\otimes I_2$, the concentrated part of f^* reads $f^{*,c} = -\lambda\nabla\left([u]\cdot n\delta_\Sigma\right)^{S,s}$, where subscript S,s stands for the solenoidal symmetric part.

According to (4.10) and (4.17) we have $\nabla^S u = C\sigma + \mathcal{E}^* + \mathcal{E}^{P,c}(u)$, with the (a-priori known) glide surfaces Σ. Hence the momentum conservation on $\Omega\setminus\Sigma$ reads

MOMENTUM CONSERVATION
$$\rho\frac{\partial^2 u}{\partial t^2} - \nabla\cdot\left(A\left(\nabla^S u\right)\right) = f^{ext} + f^*, \quad (5.22)$$

with f^{ext} the externally applied load. The concentrated nonelastic strain is given on each Σ in terms of the jump of u by

$$\hat{\mathcal{E}}^{P,c}(u) = \left([u] \otimes n\delta_\Sigma\right)^{S,s}, \tag{5.23}$$

and vanishes as soon as the solution is regular enough, i.e., either if the nonelastic and external applied forces are smooth enough (which in general is not the case), or if $[u] \cdot n = 0$ which holds for conservative dislocations as soon as $[u]$ is identified with an effective Burgers vector. As soon as $\hat{\mathcal{E}}^{P,c}(u) = 0$, the total diffuse strain turns out to be compatible in Ω:

$$\operatorname{inc} \bar{\mathcal{E}}^B = - \operatorname{inc} \mathcal{E}^R \tag{5.24}$$

Besides the evolution of the Bravais strain, for which the Bravais flow (5.7) is postulated, the other internal mechanical variables show the following evolution in time.

Remark 8 (Evolution of the internal strains) *From (5.6), (5.12), (5.16) and (5.21) and from the incompatibility driven Bravais flow (5.7), one obtains (provided the assumption* $[u] \cdot n = 0$*)*

RATE OF PLASTIC DEFORMATION

$$\dot{\mathcal{E}}^{P,r} = \frac{\alpha}{2}\left[\left(\frac{d}{dt}\frac{\partial \varphi^*}{\partial \gamma}\right) \times \nabla - \frac{I}{2}\operatorname{tr}\left(\frac{d}{dt}\frac{\partial \varphi^*}{\partial \gamma}\right) \times \nabla\right] - C\frac{d}{dt}\frac{\partial \Psi}{\partial \mathcal{E}^E} \tag{5.25}$$

Moreover, according to (4.8) and (5.8), and since the residual strain is solenoidal, its rate is solution to

RATE OF RESIDUAL DEFORMATION

$$(\Delta - \nabla\nabla\cdot)\, \dot{\mathcal{E}}^R\, (\Delta - \cdot\nabla\nabla) = \Delta^2 \dot{\mathcal{E}}^R = - \operatorname{inc}\left(\dot{\underline{\underline{R}}}^B - \frac{I}{2}\dot{R}^B\right), \tag{5.26}$$

which is unique provided appropriate boundary conditions on $\dot{\mathcal{E}}^R$ *are prescribed. Eventually, considering the solution to (5.22) and (5.23), and assuming that the glide surfaces are motionless, one has*

RATE OF NONELASTIC DEFORMATION

$$\dot{\mathcal{E}}^* = \nabla^S \dot{u} - C\frac{d}{dt}\frac{\partial \Psi}{\partial \mathcal{E}^E} - \mathcal{E}^{P,c}(\dot{u}). \tag{5.27}$$

Remark 9 (Evolution of the total strain) *The total strain satisfies, by (5.7), (5.11) and (5.24),*

RATE OF TOTAL DIFFUSE STRAIN

$$\dot{\mathcal{E}} = \mathcal{L}^B(\mathcal{E}^R), \tag{5.28}$$

where the differential operator in space and time $\mathcal{L}^B$ *reads* $\mathcal{L}^B := -\frac{\alpha}{2}\operatorname{inc} + \frac{d}{dt}$.

6 Conclusive remarks

The first contribution of this paper is to provide a correction to Kröner's expression of macroscopic strain incompatibility as found in [20] as $\tilde{\eta} = \kappa \times \nabla$. In fact, the corrected version of the this formula as proved by the present approach reads

$$\operatorname{inc} \mathcal{E}^B = \kappa \times \nabla - \frac{I}{2}\operatorname{tr}\left(\kappa \times \nabla\right). \tag{6.1}$$

where the Bravais strain $\mathcal{E}^B$ is an internal deformation variable.

By the main theorem, expression (6.1) should be considered as a constraint to be verified by the Bravais strain field $\mathcal{E}^B$ – on the left hand-side as related to the behaviour of the defect densities (including their evolution in time) – on the right hand-side. Interpretations of this correction in terms of equation structure, subsequent consequences in differential geometry, and in physical terms have been given in Section 4.6.

The second contribution is towards the functional space used. In general, when (vector-) functions of bounded or of special bounded deformation are used in a context of Mechanics, the model vector fields are assumed to belong a priori to these function classes. In the present paper, this class appears a natural space, as following from distributional field assumptions at the meso- and macro-scale. Moreover, according to a classical decomposition theorem of gradients of BD- displacement, one part is Lebesgue integrable, the other is concentrated on the jump set of the displacement fields, while the third is a Cantor diffuse part. We prove that this latter part can be ommitted by just selecting another reference configuration (that is, by simply defining an appropriate displacement field). So, we prove that our distributional framework as based on mesoscopic Assumptions 1 and 2 and macroscopic Assumptions 5 and 4 immediately delivers a single-valued displacement field[13] which is of special bounded variation, i.e. whose Cantor part vanishes. Moreover, we provide an elastic-plastic decomposition of the Lebesgue part of the Bravais strain. In the literature [20], the relation between strain incompatibility and contortion is inferred following a postulated distortion decomposition into elastic and plastic parts. However, in contrast to our approach the latter approach cannot be rigorously justified, contrarily to the strain decomposition, since elastic and plastic rotations cannot be set apart without arbitrariness.

The last contribution is to confront Eq. (6.1), whose matematical structure is compared to the Einstein tensor, to other notions of differential geometry. In fact, (6.1) appears as a natural pseudo-Ricci flow if one conjectures that the crystal shows internal evolution of its dislocation density in order to maximize its average main curvature. This process is shown to be related to te uniformization of the mesostructure.

The process to regularize internal curvature and hence reduce incompatibility through this flow is only conjectured, but the author believes that it deserves attention with a view to future works in the direction of a thermomechanical closed model, whose basis was sketched in §5.3.

A Detail of subsection 3.1

Consider one single line $\mathcal{L}$ diffeomorphic to the circle with curvilinear abscissa s (with origin $s = 0$ at some $x_0 \in \mathcal{L}$) and tangent vector τ. For some $x \in \Omega_\star$ define $x_\mathcal{L} = s_\mathcal{L}\tau \in \mathcal{L}$ such that $x_\mathcal{L}$ minimizes its distance to x among all points of $\mathcal{L}$. Consider also the local Cartesian basis $\{\tau, \sigma, \nu\}$ at $x_\mathcal{L}$ and introduce the characteristic function $\mathcal{I}_\mathcal{L} := \chi_{\Omega_\star \setminus \bar{B}_\mathcal{L}}$ of the complement in $\Omega_\star$ of the closed surface $\bar{B}_\mathcal{L}$ enclosed by $\mathcal{L}$.

Recall that for a solenoidal φ, one has $\operatorname{tr}(\nabla \times \varphi \times \nabla) = \Delta \operatorname{tr} \varphi$ in such a way that (cf. Theorem 2) $\operatorname{tr} \eta^\star = 2\left(\tau_k\tau_j\tilde{\eta}^\star_{kj} - \frac{1}{2}\tilde{\eta}^\star_{kk}\right)$, while $\operatorname{tr} \hat{\eta}^\star = -\frac{1}{2}\operatorname{tr} \tilde{\eta}^\star$ and, by

[13] According to previous work [36,37] the single-valuedness of the displacement is not an natural assumption in the context of line-defects.

definition of ϕ and $\tilde{\eta}^\star$,

$$\begin{aligned}\Delta\left(\bar{\varphi}\mathcal{I}_{\mathcal{L}}\right) &= \Delta\,\mathrm{tr}\left(\tau\otimes\tau\bar{\varphi}\mathcal{I}_{\mathcal{L}}\right) = \mathrm{tr}\left(\nabla\times\varphi\times\nabla\right) = \mathrm{tr}\,\phi = \mathrm{tr}\left(\eta^\star-\hat{\eta}^\star\right)\\ &= 2\tau_k\tau_j\tilde{\eta}^\star_{kj}-\frac{1}{2}\,\mathrm{tr}\,\tilde{\eta}^\star = 2\tau_k\tau_j\left(\epsilon_{kpq}\partial_p\kappa^\star_{jq}\right)-\frac{1}{2}\epsilon_{kpq}\partial_p\kappa^\star_{kq},\end{aligned}$$

on $\Omega_\star\setminus\bar{B}_{\mathcal{L}}$ with $\tau(x):=\tau(x_{\mathcal{L}})$. Since $\epsilon_{ijk}\tau_i\tau_j=0=\epsilon_{ijk}\delta_{kj}$ one has

$$\begin{aligned}\tau_k\tau_j\left(\epsilon_{kpq}\partial_p\kappa^\star_{jq}\right)=\tau_k\tau_j\left(\epsilon_{kpq}\partial_p\Lambda^\star_{jq}\right) &= \tau_k\tau_j\epsilon_{kpq}\partial_p\left(B^\star_q\tau_j\delta_{\mathcal{L}}\right)=\epsilon_{kpq}\tau_kB^\star_q\partial_p\delta_{\mathcal{L}}\\ \epsilon_{kpq}\partial_p\kappa^\star_{kq} &= \epsilon_{kpq}\partial_p\left(B^\star_q\tau_k\delta_{\mathcal{L}}\right)=\epsilon_{kpq}\tau_kB^\star_q\partial_p\delta_{\mathcal{L}}+B^\star_q\epsilon_{kpq}\tau_p\chi\nu_k\delta_{\mathcal{L}},\end{aligned}$$

where the last term vanishes by Definition 3 (we have used the relations $\partial_i\tau_i=0$ and $\partial_i\tau_j=\chi\tau_i\nu_j$). Therefore

$$\Delta\left(\bar{\varphi}\mathcal{I}_{\mathcal{L}}\right)=\frac{3}{2}\epsilon_{kpq}\tau_kB^\star_q\partial_p\delta_{\mathcal{L}}.$$

A generic point of the line writes as $x'=s'\tau=x_{\mathcal{L}}(s')\in\mathcal{L}$ and a generic point outside the line writes in the local Cartesian basis as $x=x_{\mathcal{L}}+t\nu(s)+z\sigma(s)\in\Omega_\star$ where t and z are the coordinates along ν and σ, respectively. Moreover, the partial derivative operator is written as $\partial_p=\tau_p\partial_s+\sigma_p\partial_z+\nu_p\partial_t$, while $R^s_i=x_i-x'_i$ and $R^s=\sqrt{t^2+z^2}$ with $2\pi\delta_x(x')=\Delta\ln R^s$ where $\Delta=\partial^2_t+\partial^2_z$ Since there is no risk of confusion, subscript s is ommitted in the sequel, where we solve in $\Omega_\star\setminus\overline{B}_{\mathcal{L}}$,

$$\frac{2}{3}\Delta\left(\bar{\varphi}\mathcal{I}_{\mathcal{L}}\right)=\epsilon_{kpq}\tau_kB^\star_q\partial_p\int_{\mathcal{L}}\delta_x(x')dL(x')=\frac{\epsilon_{kpq}\tau_kB^\star_q}{2\pi}\partial_p\int_{\mathcal{L}}\Delta\ln R\,dL(x')=\frac{\epsilon_{kpq}\tau_kB^\star_q}{2\pi}\Delta\int_{\mathcal{L}}\partial_p\ln R\,dL(x')$$

(remark that the derivation term $\tau_p\partial_s$ identically vanishes because of the presence of $\epsilon_{kpq}\tau_k$ and hence Δ and ∂_p commute) of which a $L^1_{loc}(\Omega_\star)$-solution reads

$$\begin{aligned}\bar{\varphi}(x)=\bar{\varphi}\mathcal{I}_{\mathcal{L}}(x) &= \frac{3}{2}\frac{\epsilon_{kpq}\tau_kB^\star_q}{2\pi}\int_{\mathcal{L}}\partial_p\ln|x-x'|dL(x')=\frac{3}{2}\frac{\epsilon_{kpq}\tau_kB^\star_q}{2\pi}\int_{\mathcal{L}}\frac{x_p-x'_p}{R^2}dL(x')\\ &= \frac{3}{2}\frac{|B^\star|}{2\pi}\int_{\mathcal{L}}\frac{(x_l-x'_l)\sigma_l(x)}{R^2}dL(x'),\end{aligned}\qquad\text{(A.1)}$$

with $x\in\Omega_\star\setminus\overline{B}_{\mathcal{L}}$ (the last equality comes from the fact that the Burgers vector is restricted to lie in the plane of the dislocation loop– i.e., is torsion-free, by Definition 3), while $\bar{\varphi}\mathcal{I}_{\mathcal{L}}(x)=0$ if $x\in\overline{B}_{\mathcal{L}}$.

Recall that $\varphi=\tau\otimes\tau\bar{\varphi}\mathcal{I}_{\mathcal{L}}+\nabla^S\psi$ should be found solenoidal. In order for $\nabla\cdot\varphi$ to vanish, we solve for $x\in\Omega_\star\setminus\mathcal{L}$,

$$\mathcal{L}_{0,1}(\psi_j)(x)=\nabla\cdot\nabla^S\psi_j=f_j:=-2\partial_i\left(\tau_i\tau_j\bar{\varphi}\mathcal{I}_{\mathcal{L}}\right)=-2\partial_s\left(\tau_j\bar{\varphi}\mathcal{I}_{\mathcal{L}}\right),\qquad\text{(A.2)}$$

where symbol $\mathcal{L}_{\lambda,\mu}$ denotes the Lamé operator of elasticity [2]. The solution to (A.2) is given in terms of the Kelvin matrix [2],

$$\Gamma(x)=-\frac{3}{16\pi}\frac{I}{|x|}-\frac{1}{16\pi}\frac{x\otimes x}{|x|^3}$$

and reads (by part integration and since $\mathcal{L}$ is closed)

$$\psi_i(x)=\int_{\Omega_\star}\Gamma_{ik}(x-y)f_k(y)dy=2\int_{\Omega_\star\setminus\bar{B}_{\mathcal{L}}}\partial'_s\Gamma_{ik}(x-y)\left(\tau_k\bar{\varphi}\right)(y)dy,\qquad\text{(A.3)}$$

where $x \in \Omega_\star \setminus \mathcal{L}$, $\partial'_s := \partial_{s'}$ and $y = s'\tau + t'\nu + z'\sigma \in \Omega_\star \setminus \overline{B}_\mathcal{L}$, and which is recognized as a $W^{1,1}_{loc}(\Omega_\star)$-function. So, by (A.1) and (A.3) we have obtained the decomposition $\phi = \nabla \times \varphi \times \nabla$ with $\nabla \cdot \varphi = 0$ and $\varphi = \tau \otimes \tau \bar{\varphi} \mathcal{I}_\mathcal{L} + \nabla^S \psi \in L^1_{loc}(\Omega_\star)$.

With a view to Eq. (3.5), let us compute $(\tau \otimes \tau \bar{\varphi} \mathcal{I}_\mathcal{L}) \times \nabla$ in $\Omega_\star \setminus \overline{B}_\mathcal{L}$:

$$\begin{aligned} \epsilon_{qnj}\partial_n (\tau_i\tau_j\bar{\varphi}\mathcal{I}_\mathcal{L}) &= \epsilon_{qnj} (\tau_n\tau_j\chi\nu_i\bar{\varphi}\mathcal{I}_\mathcal{L} + \tau_i\tau_n\chi\nu_j\bar{\varphi}\mathcal{I}_\mathcal{L} + \mathcal{I}_\mathcal{L}\tau_i\tau_j\partial_n\bar{\varphi} + \tau_i\tau_j\bar{\varphi}(-\nu_n\delta_\mathcal{L})) \\ &= -\sigma_q\tau_i (\chi\bar{\varphi}\mathcal{I}_\mathcal{L} + \bar{\varphi}\delta_\mathcal{L}) + \mathcal{I}_\mathcal{L}\epsilon_{qnj}\tau_i\tau_j\partial_n\bar{\varphi}, \end{aligned}$$

where we observe that the first term of the RHS is the sum of a $L^1_{loc}(\Omega)$-term and of a concentrated measure, while the last one is not necessarily a measure. Moreover, also the following term is not necessarily a measure:

$$\left(\nabla^S\psi \times \nabla\right)_{iq} = -\int_{\Omega_\star\setminus\bar{B}_\mathcal{L}} \epsilon_{qnj}\partial_n\partial_i\partial_s\Gamma_{jk}(x-y)\tau_k\bar{\varphi}(y)dy, \tag{A.4}$$

where $x \in \Omega_\star \setminus \mathcal{L}$ and all three partial derivation intended w.r.t. x (we have used the fact that $\partial'_s\Gamma = -\partial_s\Gamma$).

In order to remove these two non-measure terms from $\epsilon_{qnj}\partial_n\varphi_{ij}$ in $\Omega_\star \setminus \overline{B}_\mathcal{L}$, let us seek a distribution vector F_q satisfying

$$\begin{aligned} \Delta F_q &= \partial_i^2 F_q = -\partial_i \left(\mathcal{I}_\mathcal{L}\epsilon_{qnj}\tau_i\tau_j\partial_n\bar{\varphi} + \left(\nabla^S\psi \times \nabla\right)_{iq}\right) \\ &= -\partial_s (\mathcal{I}_\mathcal{L}\epsilon_{qnj}\tau_j\partial_n\bar{\varphi}) + \int_{\Omega_\star\setminus\bar{B}_\mathcal{L}} \epsilon_{qnj}\partial_n\partial_s\Delta\Gamma_{jk}(x-y)\tau_k\bar{\varphi}(y)dy \\ &= -\partial_s \left(\mathcal{I}_\mathcal{L}\epsilon_{qnj}\tau_j\partial_n\bar{\varphi} - \int_{\Omega_\star\setminus\bar{B}_\mathcal{L}} \epsilon_{qnj}\partial_n (\delta_{jk}\delta_x(y) - \partial_j\partial_l\Gamma_{lk}(x-y))\tau_k\bar{\varphi}(y)dy\right) =: g_q, \\ &= -\mathcal{I}_\mathcal{L}\partial_s (\epsilon_{qnj}\tau_j\partial_n\bar{\varphi} - \epsilon_{qnk}\partial_n(\tau_k\bar{\varphi}))(x) = -\mathcal{I}_\mathcal{L}\partial_s(\sigma_q\chi\bar{\varphi})(x). \end{aligned} \tag{A.5}$$

To show existence of a solution to (A.5), we shall use a crucial result from [7] (see also [2]), stating that $\bar{\varphi}$ – and hence by Definition 3 the RHS of (A.5) is according to expression (A.1) a bounded linear operator on $L^2(\Sigma_\mathcal{L})$ where $\Sigma_\mathcal{L}$ is the plane of the loop, in such a way that a weak solution to (A.5) exists [32] in $W^{2,2}_{loc}(\Omega_\star)$ up to a constant vector. It follows from (A.5) that

$$\partial_i F_q = -\left(\mathcal{I}_\mathcal{L}\epsilon_{qnj}\tau_i\tau_j\partial_n\bar{\varphi} + \left(\nabla^S\psi \times \nabla\right)_{iq}\right) + \epsilon_{imn}\partial_m G_{nq}, \tag{A.6}$$

for a solenoidal gauge tensor field $G \in W^{1,2}_{loc}(\Omega_\star)$ weak solution, by (A.1), (A.5) and [32], of $\Delta G_{pq} = I_\mathcal{L}\epsilon_{qnj}\sigma_p\tau_j\chi\partial_n\bar{\varphi}$. As a result $\mu := \varphi \times \nabla + \nabla F$ is a Radon measure.

B Proof of Corollary 2

By Theorems 2 and 4 and from Eqs. (4.20) and (4.21), we have in the distribution sense that

$$\operatorname{inc}\mathcal{E}^B = \lim_{\epsilon\to 0} \operatorname{inc}\mathcal{E}^\epsilon = \lim_{\epsilon\to 0} \sum_{\mathcal{L}\subset\Upsilon_x^\epsilon} 2\left[\tau^\mathcal{L}\otimes\tau^\mathcal{L}\hat{\eta}^{\mathcal{L}(\epsilon)}\right]^S = \kappa\times\nabla - \frac{I}{2}\operatorname{tr}(\kappa\times\nabla), \tag{B.1}$$

where $\hat{\eta}^{\mathcal{L}(\epsilon)} = \left(\tilde{\eta}^{\mathcal{L}(\epsilon)}\right)^{d*} := \tilde{\eta}^{\mathcal{L}(\epsilon)} - \frac{I}{2}\operatorname{tr}\tilde{\eta}^{\mathcal{L}(\epsilon)}$ with $\tilde{\eta}^{\mathcal{L}(\epsilon)} = \kappa^{\mathcal{L}(\epsilon)} \times \nabla$ and where we recall that $\kappa^{\mathcal{L}(\epsilon)} = \kappa_x^\mathcal{L}(V_x^\epsilon)$.

Since the identity tensor in the local basis attached to $\mathcal{L}$ reads $(Id)^{\mathcal{L}} = \tau^{\mathcal{L}} \otimes \tau^{\mathcal{L}} + \sigma^{\mathcal{L}} \otimes \sigma^{\mathcal{L}} + \nu^{\mathcal{L}} \otimes \nu^{\mathcal{L}}$, we may infer from (B.1) that

$$\sum_{\mathcal{L}\subset\Upsilon_x^\epsilon} 2\left[\tau^{\mathcal{L}} \otimes \tau^{\mathcal{L}} \hat{\eta}^{\mathcal{L}(\epsilon)}\right]^S = \sum_{\mathcal{L}\subset\Upsilon_x^\epsilon} 2\hat{\eta}^{\mathcal{L}(\epsilon)} - \sum_{\mathcal{L}\subset\Upsilon_x^\epsilon} 2\left[(\sigma^{\mathcal{L}} \otimes \sigma^{\mathcal{L}} + \nu^{\mathcal{L}} \otimes \nu^{\mathcal{L}})\hat{\eta}^{\mathcal{L}(\epsilon)}\right]^S \quad (B.2)$$

By (B.1) and (B.2) it results that, as $\epsilon \to 0$ and in the distribution sense,

1. $\sum_{\mathcal{L}\in\Upsilon_x^\epsilon} (\sigma^{\mathcal{L}} \otimes \sigma^{\mathcal{L}} + \nu^{\mathcal{L}} \otimes \nu^{\mathcal{L}}) \left[\left(\kappa^{\mathcal{L}(\epsilon)} \times \nabla\right)^{d*}\right]^S = \sum_{\mathcal{L}\in\Upsilon_x^\epsilon} (\sigma^{\mathcal{L}} \otimes \sigma^{\mathcal{L}} + \nu^{\mathcal{L}} \otimes \nu^{\mathcal{L}})\hat{\eta}^{\mathcal{L}(\epsilon)} \to 0$
2. $\sum_{\mathcal{L}\in\Upsilon_x^\epsilon} 2\left[\kappa^{\mathcal{L}(\epsilon)} \times \nabla\right] \to \kappa \times \nabla.$

The second equation above can be rewritten as $\sum_{\mathcal{L}\in\Upsilon_x^\epsilon} 2\kappa^{\mathcal{L}(\epsilon)} \times \nabla \to \kappa \times \nabla$ from which it is inferred that

$$\kappa = \lim_{\epsilon\to 0} 2\kappa^\epsilon + \Phi\nabla,$$

as $\epsilon \to 0$, where Φ is a gauge vector distribution field and where $\kappa^\epsilon := \sum_{\mathcal{L}\in\Upsilon_x^\epsilon} \kappa^{\mathcal{L}(\epsilon)}$. Let Φ be chosen such that, by Eq. (2.3) and Theorem 1,

$$\Phi\nabla \cdot \nabla = \Delta\Phi = -\lim_{\epsilon\to 0} \kappa^\epsilon \cdot \nabla. \quad (B.3)$$

Eq. (B.3) implies that for some gauge (solenoidal) field $G^{(\epsilon)}$,

$$\Phi\nabla = -\lim_{\epsilon\to 0} \kappa^\epsilon + G \times \nabla, \quad (B.4)$$

in such a way that Eq. (4.23) follows as soon as $G^{(\epsilon)}$ is chosen to satisfying

$$\Delta G = \lim_{\epsilon\to 0} \kappa^\epsilon \times \nabla = \lim_{\epsilon\to 0} \tilde{\eta}^\epsilon = \tilde{\eta},$$

where $\tilde{\eta}^\epsilon := \sum_{\mathcal{L}\in\Upsilon_x^\epsilon} \tilde{\eta}^{\mathcal{L}(\epsilon)}$ and $\tilde{\eta}$ are Kröner's incompatibility at scale ϵ and at the macroscle, since $\Upsilon_x^{(0)} = \Upsilon_x$.

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