The non-Riemannian dislocated crystal: a tribute to Ekkehart Kröner (1919-2000)

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Abstract

This expository paper is a tribute to Ekkehart Kröner's results on the intrinsic non-Riemannian geometrical nature of a single crystal filled with point and/or line defects. A new perspective on this old theory is proposed, intended to contribute to the debate around the still open Kröner's question: "what are the dynamical variables of our theory?"

1 Introduction

In the field of solid state physics, in particular physics of defects, the legacy of Ekkehart Kröner who died ten years ago at the age of 81, is invaluable. He has been actively publishing for 50 years, mostly as a single author, on the physical understanding of defective solids, but also on their mathematical structure. One could make a distinction between a first series of paper [19]-[21] where he constructs an original approach to understand dislocations, and a later series [22]-[26] where he raises questions, while reporting new knowledge in the field.

Most of the theory can be found in the course [21] but since Kröner also distilled many comments, ideas, and computations along other publications, the idea of writing the present tribute grew up. It is especially intended to commemorate the 10th anniversary of his death, in order, not to recall (because the author has no privileged relationship with Kröner to do so), but to enlighten Kröner's ideas and show how they are found rich enough by the author to be diffused, revisited and emphasized today.

It should be pointed out that Anthony [2, 3] is one of Kröner's direct students who also greatly contributed to understand defect lines (in particular, disclinations). Since then, many contributions to the field (nonlinear dislocations, dislocation motion, thermodynamic of defective crystals, etc.) have appeared, but surprisingly enough, few only cite Kröner. This is probably due to the lack of real school following him, but also due to scientific reasons: indeed, Kröner's theory is formulated in physical terms, but appeals to complex mathematical concepts, the combination of which is only rarely seen in the literature.

It should be emphasized that de León, Epstein, Kleinert, Lazar, Maugin and co-authors [11, 14, 8, 15, 27] (cf. the well-documented survey [28] and the references therein) have produced significant results not only by following, but especially by completing the ideas of Kröner.

So, the present paper is intended to (i) collect and show Kröner's results in the light of a new presentation, (ii) describe the non-Riemannian crystal and show how it can help to select appropriate deformation and internal (thermodynamic) variables, (iii) participate to the debate around Kröner's question: "what are the dynamical variables of our theory?" [24]

It will be especially stressed that the crystal geometry and the physical laws governing defects are inseparable, as is the case in the Einstein's General Theory of Relativity. However, we entirely agree with Noll when he writes [29] that "the geometry [must be] the natural outcome, not the first assumption, of the theory" (i.e., as in the *Continuous Distribution of Dislocation* (CDD) theory of Bilby et al. [6]). Many geometrical tools and mathematical theory required for a rigorous description of the dislocated crystal geometry can be found in the landmark papers by Noll [29] and Wang [38], while also pointing out a recent book on Continuum Mechanics in that spirit [13].

The approach followed here and detailed in [35]-[37] is nonetheless distinct from the CDD theory. Single crystals growing from the melt are considered where high temperature gradients are unavoidable and hence where point defects are present [34]. Moreover, since there are no internal boundaries, the defect lines can take in principle any orientation while forming either loops or lines ending at the crystal boundary. Note also that for a complete theory, and in particular to obtain a multiscale model, line-defect clusters must be considered [37]. However, for the purpose of simplicity in the exposition of the theory, we will consider a tridimensional crystal filled with a network of rectilinear parallel disclinations and/or dislocations.

Particular to the chosen approach is the distinction between scales, where the macroscale is recovered from the mesoscale by a homogenization process: the singularities (i.e., the defect lines) have been erased and hence the density of defects (dislocations and/or disclinations) are recovered by means of smooth fields which we will show responsible for curvature and torsion of the crystal intrisic geometry. Also, the density of point defects will show responsible for the appearance of non-metric terms. In the present approach, only objective fields are considered to describe defective matter: they are defined across scales although their physical meaning might differ. Moreover, no elasto-plastic decomposition and no prescription of any reference configuration are required, and there is no assumption of static equilibrium (vanishing stress divergence).

2 Preliminar results at the continuum scale

Notation 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 $U_{ij...}$ with a number of indices corresponding to its order.*

The present section focuses on the mesoscopic scale, where dislocations and disclinations are lines and whose characteristic length is some average distance between neighboring defects. The remaining of the medium is a continuum governed by linear elasticity. At time t, the body is referred to as $\mathcal{R}^\star(t)$ to represent any random sample corresponding to a given crystal growth experiment. In the crystal domain Ω, the meso-scale physics will then be represented by a nowhere dense set of defect lines which in $2D$ are parallel to each other.

Definition 2.1 ($2D$ mesoscopic defect lines) *At the meso-scale, a 2D set of dislocations and/or disclinations $\mathcal{L} \subset \Omega$ is a closed set of Ω (this meaning the intersection with Ω*

of a closed set of $\mathbb{R}^3$) formed by a countable union of parallel lines $L^{(i)}, i \in \mathcal{I} \subset \mathbb{N}$, whose adherence is itself a countable union of lines and where the linear elastic strain is singular. In the sequel, these lines will be assumed as parallel to the z-axis.

Since accumulation points (to be understood as clusters of parallel lines) might appear, the scale of matter description of this section is named *continuum scale*.

2.1 Objective internal fields for the model description

The present mesoscopic theory is developed from the sole linear elastic strain, which itself is defined from the stress field (although the stress-strain relationship is not used in the sequel) and therefore is an objective internal field.

Assumption 1 ($2D$ mesoscopic elastic strain) *The linear strain $\mathcal{E}^\star$ is a given symmetric $L^1_{loc}(\Omega)$ tensor such that $\partial_z \mathcal{E}^\star = 0$. Moreover, $\mathcal{E}^\star$ is assumed as compatible on $\Omega_\mathcal{L} := \Omega \setminus \mathcal{L}$ in the sense that the incompatibility tensor defined by*

$$\text{INCOMPATIBILITY:} \qquad \eta^\star_{kl} := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathcal{E}^\star_{mn}, \tag{1}$$

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

In the following definition generalizing the concept of rotation and displacement gradients to dislocated media, the strain is considered as a distribution on Ω (i.e. as acting on $\mathcal{C}^\infty_c(\Omega)$ test-functions with compact support).

Definition 2.2 (Frank and Burgers tensors)

$$\text{FRANK TENSOR:} \qquad \overline{\partial}_m\omega^\star_k := \epsilon_{kpq}\partial_p\mathcal{E}^\star_{qm} \tag{2}$$

$$\text{BURGERS TENSOR:} \qquad \overline{\partial}_l b^\star_k := \mathcal{E}^\star_{kl} + \epsilon_{kpq}(x_p - x_{0p})\overline{\partial}_l\omega^\star_q, \tag{3}$$

where x_0 is a point where displacement and rotation are given[1].

Line integration of the Frank and Burgers tensors in $\Omega_\mathcal{L}$ (i.e., outside the defect set) provide the multivalued rotation and Burgers vector fields $\omega^\star$ and $b^\star$. These properties are summarized in the following theorem, whose proof is classical.

Theorem 2.3 (Multivalued displacement field) *From a symmetric smooth linear strain $\mathcal{E}^\star_{ij}$ on $\Omega_\mathcal{L}$ and a point x_0 where displacement and rotation are given, a multivalued displacement field $u^\star_i$ can be constructed on $\Omega_\mathcal{L}$ such that the symmetric part of the distortion $\partial_j u^\star_i$ is the single-valued strain tensor $\mathcal{E}^\star_{ij}$ while its skew-symmetric part is the multivalued rotation tensor $\omega^\star_{ij} := -\epsilon_{ijk}\omega^\star_k$. Moreover, inside $\Omega_\mathcal{L}$ the gradient ∂_j of the rotation and Burgers fields $\omega^\star_k$ and $b^\star_k = u^\star_k - \epsilon_{klm}\omega^\star_l(x_m - x_{0m})$ coincides with the Frank and Burgers tensors.*

For implications of multivaluedness in physics see also [16]. From Theorem 2.3, the Frank and Burgers vectors can be defined as invariants of any isolated defect line $L^{(i)}$ of $\mathcal{L}$.

Definition 2.4 (Frank and Burgers vectors) *The Frank vector of the isolated defect line $L^{(i)}$ is the invariant*

$$\Omega^{\star(i)}_k := [\omega^\star_k]^{(i)}, \tag{4}$$

while its Burgers vector is the invariant

$$B^{\star(i)}_k := [b^\star_k]^{(i)} = [u^\star_k]^{(i)}(x) - \epsilon_{klm}\Omega^{\star(i)}_l(x_m - x_{0m}), \tag{5}$$

with $[\omega^\star_k]^{(i)}, [b^\star_k]^{(i)}$ and $[u^\star_k]^{(i)}$ denoting the jumps of $\omega^\star_k, b^\star_k$ and $u^\star_k$ around $L^{(i)}$.

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[1]This point, which becomes crucial as soon as model variables are sought, is often overlooked in the literature. Though, Kleinert makes this dependance of the Burgers vector on an arbitrary point appear clearly in [15].

The three types of $2D$ defects are the screw and edge dislocations, and the wedge disclination. As an example, the distributional strain and Frank tensor of an isolated screw dislocation (see [35] for the other two) is given by the following $L^1_{loc}(\Omega)$ symmetric tensor and first-order distribution (remark that the Frank tensor is not a Radon measure [1])[2]:

$$[\mathcal{E}^\star_{ij}] = \frac{-B^\star_z}{4\pi r^2} \begin{bmatrix} 0 & 0 & y \\ 0 & 0 & -x \\ y & -x & 0 \end{bmatrix}$$

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

Besides their relationship with the multivalued rotation, Burgers and displacement fields, the Frank and Burgers tensors can be directly related to the strain incompatibility by use of (1), (2) & (3).

Theorem 2.5 *The distributional curls of the Frank and Burgers tensors are*

$$\epsilon_{ilj}\partial_l\overline{\partial}_j\omega^\star_k = \eta^\star_{ik} \tag{6}$$

$$\epsilon_{ilj}\partial_l\overline{\partial}_j b^\star_k = \epsilon_{kpq}(x_p - x_{0p})\eta^\star_{iq}, \tag{7}$$

with $\eta^\star_{ik}$ the incompatibility tensor.

From this theorem it results that single-valued rotation and Burgers fields $\omega^\star$ and $b^\star$ can be integrated on Ω if the incompatibility tensor vanishes.

To complete the model, two other objective internal fields are introduced: the dislocation and disclination densities.

Definition 2.6 (Defect densities)

DISCLINATION DENSITY: $\qquad \Theta^\star_{ij} := \sum_{k \in \mathcal{I} \subset \mathbb{N}} \Omega^{\star(k)}_j \tau^{(k)}_i \delta_{L^{(k)}} \ (i,j = 1 \cdots 3) \qquad$ (8)

DISLOCATION DENSITY: $\qquad \Lambda^\star_{ij} := \sum_{k \in \mathcal{I} \subset \mathbb{N}} B^{\star(k)}_j \tau^{(k)}_i \delta_{L^{(k)}} \ (i,j = 1 \cdots 3), \qquad$ (9)

where $\delta_{L^{(k)}}$ is used to represent the one-dimensional Hausdorff measure density [1] concentrated on the rectifiable arc $L^{(k)}$ with the tangent vector $\tau^{(k)}_i$ defined almost everywhere on $L^{(k)}$, while $\Omega^{\star(k)}_j$ and $B^{\star(k)}_j$ denote the Frank and Burgers vectors of $L^{(k)}$, respectively.

2.2 Kröner's formula

In this paper, only a simplified $2D$ mesoscopic distribution of defects in a tridimensional crystal is considered. Accordingly, the vectors $\eta^\star_k, \Theta^\star_k$ and $\Lambda^\star_k$ denote the tensor components $\eta^\star_{zk}, \Theta^\star_{zk}$ and $\Lambda^\star_{zk}$. Greek indices are used to denote the values $1, 2$ (instead of the Latin indices used in $3D$ to denote the values $1, 2$ or 3). Moreover, $\epsilon_{\alpha\beta}$ denotes the permutation symbol $\epsilon_{z\alpha\beta}$.

The contortion, introduced by Kondo [17], Nye [30] and Bilby et al. [6], will show a crucial defect density tensor. In fact, Kröner [21] was the first author to recognize the importance of this object in terms of modelling.

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[2]Consider a set of countable lines $\mathcal{L}$ and remark that the present distributional approach is subtle in the sense that the physical condition that $\sum_{L^{(i)} \in \mathcal{L}} |B^{\star(i)}_z|$ be finite appears as a consequence of the general assumptions allowing us [35] to prove the so-called Kröner's formula (cf. Section 2.2) for transfinite families of defect-lines clusters.

Definition 2.7 (2*D* **mesoscopic contortion**)

$$\text{CONTORTION:} \qquad \kappa^{\star}_{ij} := \delta_{iz}\alpha^{\star}_j - \frac{1}{2}\alpha^{\star}_z\delta_{ij} \quad (i,j = 1\cdots 3), \tag{10}$$

where

$$\alpha^{\star}_j := \Lambda^{\star}_j - \delta_{j\alpha}\epsilon_{\alpha\beta}\Theta^{\star}_z(x_\beta - x_{0\beta}). \tag{11}$$

Among several equivalent formulations, the formula relating strain incompatibility to the defect densities has been proposed in full generality by Kröner [21], and proved for a countable set of 2*D* lines (this meaning, replacing subscript i by z in the formula) by Van Goethem & Dupret [35]:

$$\text{KRÖNER'S FORMULA IN 2}D\text{:} \qquad \eta^{\star}_k = \Theta^{\star}_k + \epsilon_{\alpha\beta}\partial_\alpha\kappa^{\star}_{k\beta}. \tag{12}$$

For the expression of incompatibility for a set of skew isolated 3*D* lines, we refer to [36], while general 3*D* results can be found in [37].

3   Preliminar results at the macroscopic scale

Following Kondo [18], by calling a crystal "perfect", it is meant that the atoms form, in its stress-free configuration, a regular pattern proper to the prescribed nature of the matter. However, no real crystal is perfect, but rather filled with point and line defects which interact mutually. Each defect type is responsible for a particular geometric property, as will be described in this paper. In order to reach this crystal, we first need to provide a way from passing from the above scale to a scale where the fields have been smoothed.

3.1   Homogenization

Homogenization is obtained from the continuum scale by a limit procedure which will not be detailled here (cf. [37]), but whose effect is to erase the singularities (isolated ones or those resulting from accumulation) and hence to provide a smooth macroscopic crystal. Basically we postulate the following limits:

$$\Theta^{\star}, \Lambda^{\star}, \mathcal{E}^{\star} \to \Theta, \Lambda, \mathcal{E}, \tag{13}$$

where $\Theta, \Lambda, \mathcal{E}$ belong to $\mathcal{C}^{\infty}(\Omega)$ and where convergence is intended in the sense of measures [1]. The tensor $\mathcal{E}$ will be called macroscopic strain without claiming however that $\mathcal{E}$ is the elastic strain (i.e. as linearly related to the macroscopic stress σ). As a consequence of law (13) we directly obtain from (1), (12) and straightforward distribution properties, that

$$\text{MACROSCOPIC KRÖNER'S FORMULA:} \qquad \eta_k = \epsilon_{\alpha\beta}\partial_\alpha\overline{\partial}_\beta\omega_k = \Theta_k + \epsilon_{\alpha\beta}\partial_\alpha\kappa_{k\beta}, \tag{14}$$

where by (2) and (10), (11),

$$\text{MACROSCOPIC FRANK TENSOR:} \qquad \overline{\partial}_m\omega_k := \epsilon_{kpq}\partial_p\mathcal{E}_{qm} \tag{15}$$

$$\text{MACROSCOPIC CONTORTION:} \qquad \kappa_{ij} = \delta_{iz}\left(\Lambda^{\star}_j - \delta_{j\alpha}\epsilon_{\alpha\beta}\Theta_z(x_\beta - x_{0\beta})\right) - \frac{1}{2}\Lambda_z\delta_{ij}. \tag{16}$$

3.2   External and internal observers

The *external observer* analyzes the crystal actual configuration $\mathcal{R}(t)$ with the Euclidian metric $g^{ext}_{ij} = \delta_{ij}$. The internal observer, in turn, can only count atomic steps while moving in $\mathcal{R}(t)$, and parallelly transport a vector along crystallographic lines. According to Kröner [22], "in our universe we are internal observers who do not possess the ability to realize external actions on the universe, if there are such actions at all. Here we think

of the possibility that the universe could be deformed from outside by higher beings. A crystal, on the other hand, is an object which certainly can deform from outside. We can also see the amount of deformation just by looking inside it, e.g., by means of an electron microscope. Imagine some crystal being who has just the ability to recognize crystallographic directions and to count lattice steps along them. Such an *internal observer* will not realize deformations from outside, and therefore will be in a situation analogous to that of the physicist exploring the world. The physicist clearly has the status of an internal observer."

4 The macroscopic crystal

At time t, the defective crystal is a tridimensional body denoted by $\mathcal{R}(t)$. The crystal defectiveness is not countable anymore, as was the case in Section 2, since the fields have been smoothed by homogenization. However, defectiveness is recovered by the natural embedding of the crystal into a specific geometry which will be described in the two following sections.

4.1 Macroscopic strain and contortion as key physical fields

The macroscopic strain $\mathcal{E}$ and contortion κ have been defined by homogenization in Section 3.1. It turns out that the relevant physical fields are not the Frank and Burgers tensors but their completed counterparts [35]:

Definition 4.1

$$\text{COMPLETED FRANK TENSOR} \qquad \eth_j\omega_k \quad := \quad \overline{\partial}_j\omega_k - \kappa_{kj} \tag{17}$$

$$\text{COMPLETED BURGERS TENSOR} \qquad \eth_j b_k \quad := \quad \mathcal{E}_{kj} + \epsilon_{kpq}(x_p - x_{0p})\eth_j\omega_q. \tag{18}$$

The following result is a direct consequence of Definition 4.1 [35]:

Theorem 4.2

$$\text{MACROSCOPIC DISCLINATION DENSITY} \qquad \Theta_{ik} = \epsilon_{ilj}\partial_l\eth_j\omega_k \tag{19}$$

$$\text{MACROSCOPIC DISLOCATION DENSITY} \qquad \Lambda_{ik} = \epsilon_{ilj}\partial_l\eth_j b_k. \tag{20}$$

Vectors η_k, Θ_k and Λ_k denote the tensor components η_{zk}, Θ_{zk} and Λ_{zk}. With the above definitions and results, the Frank and Burgers vectors are physical measures of defect which are given in terms of the sole strain and contortion tensors:

Definition 4.3 *The Frank and Burgers vectors of surface S are defined as*

$$\text{MACROSCOPIC FRANK VECTOR} \qquad \Omega_k(S) \quad := \quad \int_S \Theta_k dS \tag{21}$$

$$\text{MACROSCOPIC BURGERS VECTOR} \qquad B_k(S) \quad := \quad \int_S \Lambda_k dS. \tag{22}$$

As a consequence of (19) and (21) and Stokes theorem, the relation between the completed Frank tensor and the rotation gradient appears clear. Moreover, it results from (20) and (22) that $(\eth b)_{jk} := \eth_j b_k$ appears in place of the displacement gradient.

In the crystal dislocation-free regions (i.e. where the contortion vanishes), it results from the classical integral relation of infinitesimal elasticity that the multiple-valued rotation and displacement fields read

$$\omega_k \quad = \quad \omega_{0k} + \int_{x_0}^{x} \eth_m\omega_k d\xi_m \tag{23}$$

$$u_i \quad = \quad u_{0i} - \epsilon_{ikl}\omega_k(x_l - x_{0l}) + \int_{x_0}^{x} \eth_m b_k(\xi)d\xi_m. \tag{24}$$

4.2 Bravais metric and nonsymmetric connection as key geometrical objects

A Riemannian metric is a smooth symmetric and positive definite tensor field g_{ij}. From its symmetry property, there is a smooth transformation a_i^j such that $g_{ij} = a_i^m a_j^n \delta_{mn}$. The metric of the "external observer" on $\mathcal{R}(t)$ is the Euclidian metric δ_{ij}. However, as soon as the macroscopic strain $\mathcal{E}_{ij}$ is given, another Riemannian metric can be defined on $\mathcal{R}(t)$, namely the

$$\text{BRAVAIS METRIC} \qquad\qquad g_{ij}^B = \delta_{ij} - 2\mathcal{E}_{ij}, \qquad\qquad (25)$$

where the term "Bravais" (from the notion of Bravais crystal [22]) is used to recall that it has not a purely elastic meaning.

The use of this metric on defect-free regions of $\mathcal{R}(t)$ implies the existence of a one-to-one coordinate change between $\mathcal{R}(t)$ and $\mathcal{R}_0$, whose deformation gradient writes as $a_{mi} = g_{mn}^B a_i^n = \delta_{mi} - \partial_i u_m$ where u_m denotes a displacement field. Let us remark that since small displacements are considered, no distinction is to be made between upper and lower indices.

In the presence of defects, the following object (which is said "of anholonomity" [33]) $\Omega_{ijk} := \partial_k a_{ji} - \partial_i a_{jk}$ is directly related to the strain incompatibility and hence does not vanish as soon as defects are present. This exactly signifies that there is no global system of coordinates $\{x_j^B(x_i)\}$ with a smooth transformation matrix $a_{ji} = \partial_i x_j^B$. In fact, such a smooth a_{ij} – or, equivalently, such a smooth displacement field only exist in the defect-free regions of the crystal.

Quoting Cartan [9], "the Riemannian space is for us an ensemble of small pieces of Euclidian space, lying however to a certain degree amorphously", while Kondo [18] suggests that "the defective crystal is, by contrast [with respect to the above by him given definition of perfect crystal], an aggregation of an immense number of small pieces of perfect crystals (i.e. small pieces of the defective crystal brought to their natural state in which the atoms are arranged on the regular positions of the perfect crystal) that cannot be connected with one other so as to form a finite lump of perfect crystals as an organic unity."

From the elastic metric, we define the compatible symmetric Christoffel symbols

$$\text{BRAVAIS CONNECTION} \qquad \Gamma_{k;ij}^B = \frac{1}{2}\left(\partial_i g_{kj}^B + \partial_j g_{ki}^B - \partial_k g_{ij}^B\right), \qquad (26)$$

whose torsion $\Gamma_{k;[ij]}^B := \Gamma_{k;ij}^B - \Gamma_{k;ji}^B$ vanishes, while its curvature

$$\text{BRAVAIS CURVATURE} \qquad R_{l;kmq}^B := \left(\partial_q \Gamma_{l;km}^B + \tilde{g}_{np}^B \Gamma_{n;km}^B \Gamma_{p;lq}^B\right)_{[mq]}, \qquad (27)$$

with $\tilde{g}_{np}^B = \delta_{np} + 2\mathcal{E}_{np}$ the inverse of g_{np}^B under the small strain assumption, and where symbol $[\cdot]$ denotes the skew-symmetric index commutation operator (i.e., $A_{[mn]} = A_{mn} - A_{nm}$).

Quoting Einstein, "to take into account gravitation, we assume the existence of Riemannian metrics. But in nature we also have electromagnetic fields, which cannot be described by Riemannian metrics. The question arises: How can we add to our Riemannian spaces in a logically natural way an additional structure that provides all this with a uniform character ?"

In the present case, it is sufficient to replace gravitation by strain, and electromagnetic fields by line defects to paraphrase Einstein and raise the question of the apropriate "connection" inside the defective crystal. To be complete we should add that in order for the theory of dislocations to be closed, it should be combined with the theory of point defects which play a crucial role at high temperatures (in the same way as Maxwell theory has to be combined with the theory of weak interactions, see Kröner [24]).

The Bravais geodesics are those lines whose tangent vector τ_i is parallelly transported, hence solutions to $\tau_j \nabla_j^B \tau_i = 0$, where ∇^B is the covariant derivative associated with Γ^B. It turns out that on these lines, the internal observer is not be able to recognize any defect line. Therefore, the above Bravais connection must be completed by a non-symmetric term.

The following geometric objects are introduced from the sole dislocation density (or equivalently by (18) & (20) from the sole strain and contortion tensors):

Definition 4.4

$$
\begin{array}{llll}
\textit{DISLOCATION TORSION:} & T_{k;ij} & := & -\dfrac{1}{2}\epsilon_{ijp}\Lambda_{pk} & (28) \\[2mm]
\textit{CONNECTION CONTORTION:} & \Delta\Gamma_{k;ij} & := & T_{j;ik} + T_{i;jk} - T_{k;ji} & (29) \\[2mm]
\textit{NON SYMMETRIC CONNECTION:} & \Gamma_{k;ij} & := & \Gamma_{k;ij}^B - \Delta\Gamma_{k;ij}. & (30)
\end{array}
$$

According to Noll [29] $\Delta\Gamma_{k;[ji]}$ is the crystal *inhomogeneity tensor* which will be shown in the following sections to be directly related to the density of dislocations and disclinations.

5 The macroscopic crystal as a non-Riemannian manifold

By contrast with Kröner's presentation, the present approach shows geometrical objects as defined from homogenization of mesoscopic measurable, objective physical fields (20), (28) & (29) whose identification with their physical macroscopic counterparts follows as (proved) results.

5.1 Physical and geometrical torsions and contortions

The following lemma is easy to prove from the definitions.

Lemma 5.1 *The tensor g_{ij}^B defines a Riemannian metric. The symmetric Christoffel symbols $\Gamma_{k;ij}^B$ define a symmetric connection compatible with this metric, while $T_{k;ij}$ and $\Delta\Gamma_{k;ij}$ are skew-symmetric tensors w.r.t. i and j and i and k, respectively.*

The following results makes the link between internal motion of the observer by parallel transport and the deformation and defect internal variables as measured by an external observer.

Theorem 5.2 (Physical and geometrical torsions) *The Cristoffel symbols $\Gamma_{k;ij}$ define a nonsymmetric connection compatible with g_{ij}^B whose torsion writes as $T_{k;ij}$.*

It is easy to verify [12] that $\Gamma_{k;ij}$ is a connection since $\Gamma_{k;ij}^B$ is a connection and $\Delta\Gamma_{k;ij}$ is a tensor. Denoting by ∇_k (resp. ∇_k^B) the covariant gradient w.r.t. $\Gamma_{k;ij}$ (resp. $\Gamma_{k;ij}^B$), and recalling that a connection is compatible with the metric g_{ij}^B if the covariant gradient of g_{ij}^B w.r.t. this connection vanishes, we find by (30) that

$$
\nabla_k g_{ij}^B : = \partial_k g_{ij}^B - \Gamma_{l;ik} g_{lj} - \Gamma_{l;jk} g_{li}^B = \nabla_k^B g_{ij}^B + \Delta\Gamma_{l;ik} g_{lj}^B + \Delta\Gamma_{l;jk} g_{li}^B, \quad (31)
$$

where in the RSH, the 1st term vanishes by Lemma 5.1 while the 2nd and 3rd terms cancel each other since $\Delta\Gamma_{l;jk} g_{li} = \Delta\Gamma_{i;jk} = -\Delta\Gamma_{j;ik}$. It results that the connection torsion, i.e. the skew-symmetric part of $\Delta\Gamma_{j;ik}$ w.r.t. i and k, writes as

$$
\frac{1}{2}\left(\Delta\Gamma_{j;ik} - \Delta\Gamma_{j;ki}\right) = -\frac{1}{2}\left(\Delta\Gamma_{i;jk} - \Delta\Gamma_{k;ji}\right) = \frac{1}{2}\big((\Delta\Gamma_{k;ij} - \Delta\Gamma_{i;kj}) +
$$
$$
(\Delta\Gamma_{k;ji} - \Delta\Gamma_{k;ij}) - (\Delta\Gamma_{i;jk} - \Delta\Gamma_{i;kj})\big). \quad (32)
$$

Observing that the 1st term in the RHS side of (32) writes as $\Delta\Gamma_{k;ij}$ while, by Definition 4.4 (Eq. (29)), the LHS and the two remaining terms of the RHS of (32) are equal to $T_{j;ik}, T_{k;ji}$ and $-T_{i;jk}$, respectively, the proof is complete.

Theorem 5.3 (Physical and geometrical contortions) *The connection contortion tensor* $\Delta\Gamma_{k;ij}$ *writes in terms of the dislocation contortion* κ_{ij} *as*

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

For $k = z$, by Definition 4.4, the last statement of Lemma 5.1, and (16), it is found that $\Delta\Gamma_{z;ij} = \Delta\Gamma_{z;\alpha\beta}\delta_{i\alpha}\delta_{j\beta}$, with

$$\Delta\Gamma_{z;\alpha\beta} = T_{z;\alpha\beta} = -\frac{1}{2}\epsilon_{\alpha\beta}\Lambda_z = -\frac{1}{2}\epsilon_{\alpha\tau}\delta_{\tau\beta}\Lambda_z = \epsilon_{\alpha\tau}\kappa_{\tau\beta}.$$

For $k = \kappa$, by Definition 4.4 and the last statement of Lemma 5.1, it is found that

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

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

In conclusion, the non-Riemannian crystal is described from a physical viewpoint by $\mathcal{E}$ and κ, that is, by 15 degrees of freedom. From a geometrical viewpoint the 15 unknowns are the 6 components of the symmetric Bravais metric and the 9 (by (28) & (29)) nonvanishing components of the connection contortion.

5.2 The Bravais crystal

The following definition introduces two differential forms whose path integrations generalize (23) & (24) to the defective regions of the crystal.

Definition 5.4 (Bravais forms)

$$d\omega_j \quad := \eth_\beta\omega_j dx_\beta, \tag{33}$$

$$d\beta_{kl} \quad := -\Gamma_{l;k\beta}dx_\beta. \tag{34}$$

In the literature the existence of an elastic macroscopic distortion field is generally postulated together with the global distortion decomposition in elastic and plastic parts (for a rigorous justification of the latter, see [25]). The present approach renders however possible to avoid this a-priori decomposition. Nevertheless, the following theorem introduces rotation and distortion fields in the absence of disclinations (which must not be identified with the rotation and distortion as related to the macroscopic strain). As a consequence and in contrast with the classical literature where it is basically postulated that dislocation density is the distortion curl, this relationship is here proved.

Theorem 5.5 *If the macroscopic disclination density vanishes, there exists rotation and distortion fields defined as*

BRAVAIS ROTATION $$\omega_j(x) := \omega_j^0 + \int_{x_0}^x d\omega_j, \tag{35}$$

BRAVAIS DISTORTION $$\beta_{kl}(x) := \mathcal{E}_{kl}(x^0) - \epsilon_{klj}\omega_j^0 + \int_{x_0}^x d\beta_{kl}, \tag{36}$$

$$= \mathcal{E}_{kl}(x) - \epsilon_{klj}\omega_j(x) \tag{37}$$

where ω_j^0 *is arbitrary and the integration is made on any line with endpoints* x_0 *and* x. *Moreover,*

$$\partial_\alpha\beta_{k\beta} = \partial_\alpha\mathcal{E}_{k\beta} + \epsilon_{kp\beta}\eth_\alpha\omega_p \quad and \quad \epsilon_{\alpha\beta}\partial_\alpha\beta_{k\beta} = \Lambda_{zk}. \tag{38}$$

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By Definition 4.4, the symmetric part of the connection writes as

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

while, by Definition 4.4 and Theorem 5.3, the skew-symmetric part writes as

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

Observing, by (17) and Definition 5.4 and Theorem 5.3, that $d\omega_j = \eth_\beta \omega_j dx_\beta = -\frac{1}{2}\epsilon_{lkj}\Gamma_{[l;k]\beta}dx_\beta$, it results that $d\beta_{kl} = d\mathcal{E}_{kl} - \epsilon_{klj}d\omega_j$. Under the assumption of a vanishing macroscopic disclination density, the existence of single-valued Bravais rotation and distortion fields follows from (33), (19) & (21). Moreover, since $\partial_\alpha \beta_{k\beta} = \partial_\alpha \mathcal{E}_{k\beta} - \epsilon_{k\beta j}\eth_\alpha \omega_j$, Eq. (38) is satisfied by (19) & (20).

Remark 1 *Eq. (35) indicates that symbol $\eth$ in (33) becomes a true derivation operator in the absence of disclinations.*

Remark 2 *Referring to "Bravais" instead of "elastic" rotation and distortion fields is devoted to highlight that these quantities do not have a purely elastic meaning. In fact, the Bravais metric is not even needed since the internal observer only requires the prescription of the connection, and subsequent path integration of the forms*

$$d\mathcal{E}_{kl} = -\Gamma_{(l;k)\beta}dx_\beta, \quad d\omega_j := -\frac{1}{2}\epsilon_{lkj}\Gamma_{[l;k]\beta}dx_\beta \quad and \quad d\beta_{kl} := -\Gamma_{l;k\beta}dx_\beta.$$

Remark 3 *The Bravais distortion does not derive from any "Bravais displacement" in the presence of dislocations. In fact, around a closed loop C, even if the disclination density vanishes, the differential of the displacementas $du_k := \beta_{k\alpha}dx_\alpha$ verifies by Theorem 5.5:*

$$\int_C du_k = \int_S \epsilon_{\alpha\beta}\partial_\alpha \beta_{k\beta}dS = \int_C \eth_\beta b_k dx_\beta = \Lambda_k(S) = \int_S \epsilon_{\alpha\beta}\partial_\alpha \eth_\beta b_k dS. \tag{39}$$

Remark 4 *Theorem 5.2 defines an operation of parallel displacement according to the Bravais lattice geometry. The parallel displacement of any vector v_i along a curve of tangent vector $dx_\alpha^{(1)}$ is such that $dx_\alpha^{(1)}\nabla_\alpha v_i = 0$ and hence that the components of v_i vary according to the law $d^{(1)}v_i = -\Gamma_{i;j\beta}v_j dx_\beta^{(1)}$ [12]. This shows the macroscopic Burgers vector and dislocation density together with the Bravais rotation and distortion fields as reminiscences of the defective crystal properties at the atomic, mesoscopic and continuum scales. In fact, if $dx_\nu^{(1)}, dx_\xi^{(2)}$ are two infinitesimal vectors with the associated area $dS := \epsilon_{\nu\xi}dx_\nu^{(1)}dx_\xi^{(2)}$, it results from Eq. (28) and the skew symmetry (in α,β) of $\Gamma_{k;\alpha\beta}$ that, in the absence of disclinations,*

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

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

$$dB_k = \epsilon_{\alpha\beta}\partial_\alpha \eth_\beta b_k dS = -\epsilon_{\alpha\beta}d^{(\alpha)}(dx^{(\beta)}).$$

5.3 Motion of the internal observer

The internal observer will be represented by the $\mathbf{k}^{th}$ geodesic basis element $\mathbf{e_k}(x)$ solution to

$$(\mathbf{e_k})_j \nabla_j (\mathbf{e_k})_l = 0 \quad \text{(with no summation on } \mathbf{k}), \tag{40}$$

where ∇ is the covariant derivative associated with Γ as given by (30). We have seen in the above two sections that it was sufficient to provide him with a connection, i.e. with

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a law of parallel transport inside the crystal. In fact at this stage the internal observer is not able to measure distances, while he can measure the disclination (resp. dislocation) content of a surface S by boundary measurements of $\eth_\beta b_k$ (resp. $\eth_\beta \omega_k$) on the curve C enclosing S (which depend merely on Γ – cf. Remarks 2-4).

The notion of metric connection can be explained as follows. Let the external observer be equipped with the Bravais metric and Cartesian coordinate system $\{x_i\}$. Since $\Gamma_{l;km} = \nabla_m(\mathbf{e_k})_l$, we have on a portion $A - B$ of geodesic $\mathbf{k}$,

$$(\mathbf{e_k})_l(B) - (\mathbf{e_k})_l(A) = \int_A^B \Gamma_{l;km} dx_m = \lim_{N \to \infty} \sum_{1 \leq i \leq N} \Gamma_{l;km}(x^i)(\mathbf{e_k})_m(x^i)\Delta s^i,$$

where x^i are discretization points on the curve with endpoints $x^1 = A$ and $x^N = B$, and Δs^i a tending to zero element of the geodesic. Moreover, if the connection is compatible with the metric g^B, the angles between these lattice vectors and their (unit) length remain invariant during parallel transport. So, we understand Kröner [23] when he says: "when a lattice vector is parallelly displaced using Γ along itself, say 1000 times, then its start [say, A] and goal [say, B] are separated by 1000 atomic spacings, as measured by g^B. Because the result of the measurement by parallel displacement and by counting lattice steps is the same, we say that the space is metric with respect to the connection Γ."

Moreover, as long as $(\mathbf{e_k})_l(A)$ (that is, the internal observer) is parallely transported along a closed curve C with start- and endpoint A, the gap as created when he comes back to his origin can be measured by the external observer, since by Stokes theorem we have

$$(\mathbf{e_k}^{''})_l - (\mathbf{e_k})_l = \int_C \Gamma_{l;km} dx_m = \int_S \epsilon_{pqm} \partial_q \Gamma_{l;km} dS_p$$

$$= \int_S \epsilon_{pqm} \left(\nabla_q \Gamma_{l;km} + (\Gamma_{l;pm}\Gamma_{p;kq} + \Gamma_{l;pq}\Gamma_{p;km}) + \Gamma_{l;kp}\Gamma_{p;mq}\right) dS_p,$$

where $(\mathbf{e_k}^{''})_l$ denotes the base $(\mathbf{e_l})_k$ after being parallely transported along C. Since the term inside the parenthesis is symmetric in m and q, we have [12]:

$$= \int_S \epsilon_{pqm} \frac{1}{2} \left(\nabla_{[q}\nabla_{m]}(\mathbf{e_k})_l + \nabla_p(\mathbf{e_k})_l T_{p;mq}\right) dS_p = \int_S \epsilon_{pqm} \frac{1}{2} R_{l;nmq}(\mathbf{e_k})_n dS_p, \qquad (41)$$

with the definition of the Riemannian curvature tensor

$$R_{l;kmq} := R^B_{l;kmq} + \Delta R_{l;kmq}, \qquad (42)$$

where by (27) & (30), R^B and ΔR denote the Riemann curvature tensors associated to Γ^B and $\Delta\Gamma$, respectively. So, by (41), the internal observer is convinced to have returned to his startpoint while the external observer however can see the gap as created by the crystal curvature, itself resulting from the presence of defects.

5.4   Geometric and physical curvatures

Let us remark that in the absence dislocations ($T = \Delta R = \Lambda = 0$), the gap is merely due to curvature effects with a curvature tensor directly related by (14) to the disclination density by $R_{l;kmq} = -\epsilon_{lki}\epsilon_{mqj}\Theta_{ij}$. It should however be noted that in the absence of disclinations, the curvature is not vanishing but depends on the sole contortion, since from (14) & (42),

$$R_{l;kmq} = -\epsilon_{lki}\epsilon_{mqj}\epsilon_{ipn}\partial_p\kappa_{jn} + \Delta R_{l;kmq}, \qquad (43)$$

where by Theorem 5.3, ΔR is linearly related to the contortion. It is computed from (43) that the Ricci and Gauss curvatures [12] read

RICCI CURVATURE	R^B_{kq} :=	$R^B_{l;kmq} = R^B_{p;kpq} = \eta_{kq} - \delta_{kq}\eta_{pp}$	(44)
GAUSS CURVATURE	R^B :=	$\frac{1}{2}R^B_{pp} = -\eta_{pp},$	(45)

while Einstein tensor reads

$$-\frac{1}{4}\epsilon_{lki}\epsilon_{mqj}R^B_{l;kmq} = \eta_{ij} = R^B_{ij} - \delta_{ij}R^B \tag{46}$$

in the presence of dislocations and disclinations[3], thereby contradicting Kröner who identified Einstein tensor with the disclination density in [23].

Moreover, since the macroscopic strain can be decomposed into (symmetric) compatible and (symmetric) solenoidal parts (see, eg., [35]), where only the second one as denoted by $\mathcal{E}^s$ is relevant for the incompatibility tensor, it results that its trace $\mathcal{E}^s_{pp}$ satisfies by (45) $-\Delta\mathcal{E}^s_{pp} = R^B$, thereby showing how the Gauss curvature is related to the variation of matter density.

5.5 Summary of the non-Riemannian metric crystal

The crystal equiped with $\{g^B, \Gamma\}$ as given by (25) and (30) has the following properties: (i) the geodesics of Γ are the crystallographic lines; (ii) the effect of parallel displacement of the internal observer (equiped with Γ) along a crystallographic line is equivalent to counting the lattice steps; (iii) the defect content, i.e. disclination and/or dislocation densities can be computed from the values of Γ only; (iv) the torsion of Γ is merely due to the presence of dislocations, while its curvature is due to the presence of both disclinations and dislocations; (v) in the absence of disclinations, there exists a single-valued rotation and distortion field; (vi) if and only if there are no defect lines, Γ is Euclidean and there exists a holonomic coordinate system. In the latter case only, one can properly speak of a reference configuration, of single-valued rotation, displacement and distortion fields, with the macroscopic strain compatible with the displacement field.

Figure 1 illustrate the inseparable link between physics and geometry. On the one hand, the physical fields can be set apart: the deformation and defect internal variables are shown in rectangular and hexagonal boxes, respectively. On the other hand, the purely geometrical object are in oval boxes. The interrelation between fields is represented by an arrow. The double (resp. triple) boundary lines mean that the quantity contains differential combinations of order 1 (resp. 2), while single lines mean algebraic combinations only.[4]

The main deformation field is the strain, while the distortion and rotation are only obtained in the absence of disclinations (see Theorem 5.5). Because the latter two depend on an arbitrary point where their value is assumed known, they are considered inappropriate as model variables. Concerning defect internal variables, one could indifferently chose the dislocation torsion or contortion. Let us mention that since strain instead of distortion is chosen, the deformation and defect variables should be considered as independent physical fields.

5.6 Nonmetricity, teleparallelism and the paradox of the flat crystal

Let us first remark that the notions of metric and of connection must be considered as distinct. This has been emphasized in [7] where it is recalled that historically it has not been so for a long time (including Einstein literature). Here, we have seen that the metric is attached to the notion of external observer, while the connection is attached to the notion of parallel displacement of the internal observer inside the crystal. We have seen that parallel displacement with Γ^B and counting-step measurements are the same in a

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[3]Proving (46) at the macroscale by homogenization of its mesoscopic counterpart can be found in [36], [37].

[4]As an example, the Bravais metric is algebraically obtained from the elastic strain, whereas the nonsymmetric connection is obtained by one differentiation of the Bravais metric.
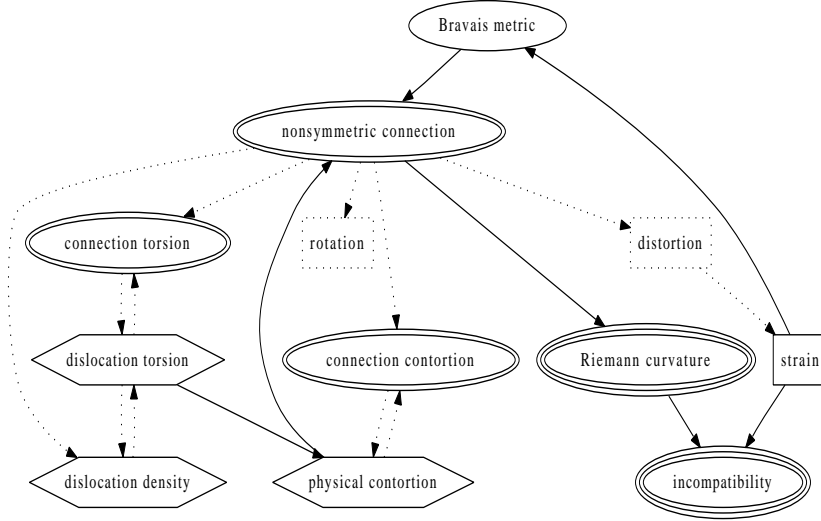
Figure 1: Link between physics and geometry of defects

crystal filled with line defects. This was true because Γ^B was compatible with g^B and hence crystallographic basis elements remain crystallographic as transported along the crystallographic lines.

Suppose now that the crystal also contains point defects. According to Kröner [25], "nonmetricity means that length measurements are disturbed. It is easy to see that this just occurs in the presence of point defects. In fact, when counting atomic steps along crystallographic lines to measure distance between two atoms, [the internal observer] feels disturbed when suddenly a vacancy or an intersticial emerges instead of another atoms [of the perfect crystal]."

Let C_V and C_I be the scalar vacancy (resp. interstitial) concentration, that is the number of vacancies (resp. interstitials) per unit volume of crystal. Then, the following metric as proposed by Kröner [22]:

$$g' = (1 + C_I - C_V)^2 g^B, \tag{47}$$

verifies $dV = \sqrt{\det g'}dV_0 = (1 + \Delta C)\sqrt{\det g^B}dV_0$, with dV_0 the volume element of the stress-free crystal and dV that of the actual one, and where $\Delta C = C_I - C_V$ is the excess atomic content of dV. An evolution equation for C_V and C_I (and hence for ΔC and g') will be given in Section 6.

It is clear that the non-metricity defined as $Q_{j;ik} := \hat{\nabla}_j g'_{ik} \neq 0$ [33, 23] must now enter the geometric point- and line-defect model. Differentiation $\hat{\nabla}$ is here intended with respect to connection $\hat{\Gamma}$, as defined by

CONNECTION WITH POINT DEFECTS: $\qquad \hat{\Gamma}_{k;ij} := \Gamma'_{k;ij} - \Delta\Gamma_{k;ij} - \dfrac{1}{2}\delta\Gamma_{k;ij}$ (48)

with $\Delta\Gamma_{k;ij}$ given by (28) & (29) and where $\Gamma'_{k;ij} := \frac{1}{2}\left(\partial_i g'_{kj} + \partial_j g'_{ki} - \partial_k g'_{ij}\right)$ and

NONMETRIC CONTORTION: $\qquad \delta\Gamma_{k;ij} := Q_{j;ik} + Q_{i;jk} - Q_{k;ji}.$ (49)

Since Q is a tensor quantity, it is expected to play a role for the physical description of the crystal (and to obey an evolution equation as related to the other defects).

The paradox of the flat crystal is the fact that a defective solids with in addition to defect lines a certain amount of point defects can recover a vanishing curvature[5] if the following balance holds:

TELEPARALLELISM ASSUMPTION: $$\delta R_{l;kmq} = -(R'_{l;kmq} + \Delta R_{l;kmq}), \qquad (50)$$

where the three terms are the curvature of $\delta\Gamma, \Gamma'$ and $\Delta\Gamma$, respectively. This is what Kröner (and Bilby et al [6]) calls teleparallelism, by this meaning that the global connection curvature vanishes and hence that the internal observer ends up parallel when travelling along a loop. It should be emphasized that teleparallelism is often considered as a working assumption [6, 25].

However, we rather follow Kröner [22] when he says that "curved crystals are possible only if the curvature is, in some sense, compatible with the considered crystal structure", which means that instead of a flat crystal given by (50), the connection curvature $\hat{R}$ of the actual crystal should be such that point and line defects accomodate to satisfy

$$\hat{R}_{l;kmq} = \delta R_{l;kmq} + (R'_{l;kmq} + \Delta R_{l;kmq}). \qquad (51)$$

Particularizing (51) we learn from identity $\hat{R}_{(l;k)mq} + \hat{\nabla}_{[m}Q_{q];lk} + T_{p:mq}Q_{p;lk} = 0$ [33, 23] that point defects and dislocations must be geometrically related, which phenomena is well known from solid-state physicist: "dislocations moving perpendicular to their Burgers vector produce point defects, and similar processes occur when dislocations cut each other" [22] (concerning non metricity, see also [4]).

6 Concluding remarks: the choice of model variables

Let us conclude by attempting to answer Kröner's question of the Introduction. To the knowledge of the author, this question has not been answered yet, or to say the least, there is still no agreement on the answer.

In fact it depends of the physics which one wants to capture. If motion of dislocations is modelled, then not only the conservative glide but also the non-conservative climb mode must be taken into account. Non conservation is due to the presence, creation, anihilation and motion of point defects, and these processes require high temperatures and non-negligible temperature gradients [34, 32]. Therefore a complete model of dislocation motion must be thermodynamical, away from thermal equilibrium (i.e. irreversible), and coupled with the motion of point defects. In [34] the following set of PDEs showed very good results to model point defects:

$$\frac{DC_K}{Dt} \quad = \quad \nabla \cdot \left(D_K \nabla C_K + \tilde{D}_K C_K \nabla T \right) - P, \qquad (52)$$

with the Lagrangian derivative D/Dt, and where $C_K, D_K, \tilde{D}_K$ and P mean (scalar) concentration, (tensorial) equilibrium diffusion, thermodiffusion and (scalar) recombination ($K = I$ for interstitials and $K = V$ for vacancies).

Concerning the motion of dislocations (we assume here that disclinations are negligible), a similar equation as (52) should be proposed, with an inter-dislocation recombination term and a term of interaction with point defects, collectively denoted by $\tilde{P}$ (and hence also appearing in (52)). However, the dislocation density cannot be scalar (which is the

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[5]In the terminology of Wang [38] and Noll [29] a connection $\hat{\Gamma}_{k;ij}$ such that its curvature $\hat{R}_{l;kmq}$ vanishes is called *a (flat) material connection*, while for such a connection, $\hat{\Gamma}_{k;[ij]}$ is denoted as *inhomogeneity tensor*.

case in most of the current models available in the literature) but must be the tensorial Λ (or equivalently the contortion κ). The PDE could read

$$\frac{D\kappa}{Dt} \;\;=\;\; \nabla \cdot \left(D\nabla\kappa + \tilde{D}\kappa\nabla T \right) - \tilde{P}, \tag{53}$$

with appropriate boundary condition and where D and $\tilde{D}$ are tensor diffusivities of order 4. Moreover the contortion verifies the conservation law [35] $\nabla \cdot \kappa = \nabla(\texttt{tr}\ \kappa)$, meaning that the mesoscopic dislocations are loops or end at the crystal boundary, in such a way that Eq. (53) amounts to a system of 6 coupled PDEs. Moreover the expression of $\tilde{P}$ must somehow satisfy the geometric interaction between defects as given by (51).

Concerning the deformation variables, let us first observe Figure 2. Incompatibility is
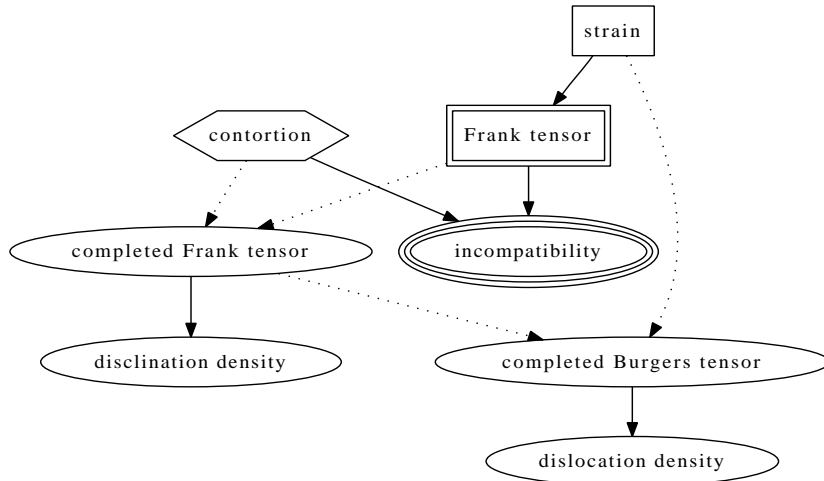

Figure 2: The deformation and defect state variables

the final quantity as obtained by recursive differentiation of either the strain (twice), or the contortion (once). It hence shows the ultimate convergence (in the sense of *agreement*) of the initially set apart deformation and defect variables. The other oval boxes denote defect variables obtained from the two key model variables: strain and contortion.

It should be observed that all relations between strain $\mathcal{E}$, Frank tensor $\overline{\partial}\omega$, contortion κ and incompatibility are obtained by means of recursive application of the curl operator (either $\nabla\times$ or $\times\nabla$).

As a first step, Kröner proposed an ("athermal") Gibbs free energy reading $W = \tilde{W}(F^e, \Lambda)$ with F^e the elastic deformation gradient. Restricting hence to statics, he thereby attempted to answer his question [24]: "what are the independent (extensive) [explicit state] variables entering the free energy (at constant temperature)?" However in [25], he recognizes that the use of F^e is inevitably ambiguous because the elasto-plastic decomposition is not unique.

According to our theory, the free energy naturally reads from the diagram on Fig. 2 as a first strain gradient (see [10, 27]) model $W = W_1(\mathcal{E}, \overline{\partial}\omega; \kappa)$ where the strain gradient is however replaced by its curl. Equivalently it could read $W = W_2(\mathcal{E}, \eth\omega, \Lambda)$ by combination of the last two variables of W_1, or even $W = W_3(\mathcal{E}, \eth b, \Lambda)$ by combination of the first two variables of W_2. Let us observe that according to Theorem 5.5, W_3 can nevertheless be compared with $\tilde{W}$ as soon as $\eth b$ is identified with a distortion (i.e. a deformation

gradient), although not becessarily the elastic one (cf. Remark 2). Moreover, a curl differential relation is also observed between W_3 last two variables (cf. Remark 3). A recent thermodynamic analysis with W_3 has been remarkably reported by Berdichevsky [5] where $\eth b$ is identified with the plastic distortion. Let us remark however that by (17) & (18), $\eth b$ is not, because of the prescription of the arbirary x_0, an unambiguous state variable, as opposed to $\eth \omega$.

They are however reasons to be tempted by the choice $W = W_1$ because (i) all variables are explicit state variables defined by objective fields (which do not appeal to reference configurations, arbitrary plastic parts, or points x_0), (ii) there is a distinction between (strain-like) deformation and (internal) defect variables, (iii) all variables have clear and unambiguous physical and a geometrical meanings. If needed, all other variables (such as $\nabla \mathcal{E}, \eth \omega, \eth b, \Lambda, \eta$) can be recovered as implicit state variables of the model [24]. Moreover, if applying the curl operator twice to the strain and once to the contortion, then the only additional model variable naturally appearing is the incompatibility, of both deformation and defect nature. This sounds like a closure on the recursive iteration for (higher-order) models.

Nonetheless, we rather prefer to introduce incompatibility through Kröner's formula (14) as a constraint to the Gibbs energy with 6 degrees of freedom as coupling strain, Frank tensor and contortion:

$$\nabla \times \mathcal{E} \times \nabla = \nabla \times \overline{\eth}\omega = \kappa \times \nabla, \tag{54}$$

while the equilibrium law[6] writes as the following equation with 3 d.o.f.:

$$-\nabla \cdot \sigma = f \quad \text{with} \quad \sigma := \frac{\partial W}{\partial \mathcal{E}} \quad \text{and} \quad W = \mathcal{W}(T, \nabla T; \mathcal{E}, \overline{\eth}\omega; \kappa), \tag{55}$$

where f is the sum of external forces and of configurational (internal) pseudo-forces directly related to κ and to the derivative of the so-called dislocation moment stress $\partial W_1/\partial \kappa$ [25, 5]. Let us also mention that the additional constraint of incompressibility must be added in order to avoid climb and point defects [24]. Also, a remarkable discussion on the nature of $W = W_4(\eth b)$ (with identification of $\eth b$ with the distortion) in a nonlinear and variational setting can be found in [31].

Summarizing, an athermal model of dislocations requires to solve equations (53)-(55) which involve a total of 15 degrees of feedom. This number is exactly the number of d.o.f. required by the internal observer to parallel displace inside the crystal (through the nonsymmetric connection). Moreover, to be closed the theory must involve point and line defects, and hence must consider high temperature and temperature gradients. So, as recognized by Kröner [25], the dislocation model must be cast within the general frame of irreversible thermodynamics because the time variations of the internal variables create thermal dissipation.

This is the main reason why a huge work remains to be done in order to determine, e.g., the stress-strain relation, all other constitutive laws, the diffusion coefficients (which depend on the crystal internal symmetries, glide planes, etc), and the defect interaction/production terms.

The author is unable to answer definitely any of these questions but will pursue research on the topic. This paper aims at recalling Ekkehart Kröner's legacy, and in particular the fundamental questions he raised which are still open and crucial nowadays. It is also aimed at stressing that solutions to dislocation modelling will most probably arise from a strong interplay between mathematics and physics, as remarkably done by Kröner along his papers [19]-[26].

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[6]See also Wang [38] on this question.

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