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Kröner's formula for dislocation loops revisited

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ABSTRACT

In this communication, our aim is to respond to open questions which arose from a previous publication (Van Goethem, N., 2011. Strain incompatibility in single crystals: Kröner's formula revisited. Journal of Elasticity 103 (1), 95–111) where a new Kröner's formula was proved for a set of skew dislocation and disclination lines: (i) Does the new formula hold for a dislocation loop? (ii) Which new terms appear due to the line curvature? In this work we validate by complete calculation of distributional type a general Kröner's formula for two classical examples of dislocation loops.

1. Introduction

Several dislocation theories coexist in the literature and in general each emphasizes a particular aspect of the physics of dislocations and disclinations. For a physical approach let us refer to Kröner (1980), Dascalu and Maugin (1994), Hehl and Obukhov (2007), Lazar (2007), and Lazar and Hehl (2010). In engineering practice, empirical models are for instance used in the context of single crystal growing from the melt (Müller and Friedrich, 2004; Müller et al., 2004). These models are in general rather crude extensions of models available for polycrystals, whereas the physics of single crystals which we here consider is radically different for one main reason. Since the dislocations satisfy a conservation law and since there are no internal boundaries, dislocation may form curves which are comparable with the characteristic length of the crystal. So, separation of scales can hardly be done, and one is forced to analyze the properties of dislocations and/or disclination curves, even if a macroscopic thermomechanical model is adopted.

As soon as the mesoscale is considered[1] (thus also at the macroscale, cf. Van Goethem, 2012), one crucial governing equation holding for both static and dynamic descriptions of dislocations, is what we called in previous contributions (Van Goethem and Dupret, 2012a; Van Goethem, 2010, 2011b) the "Kröner's formula". This formula relates the linear elastic strain incompatibility to dislocation and disclination density tensors. This means that as soon as these densities are known, the strain $\mathcal{E}^\star$ must satisfy a geometrical constraint, which can roughly be stated as follows: the Ricci (i.e., curvature) tensor associated to the elastic metric $g = I - 2\mathcal{E}^\star$ is directly related to the contortion curl, being the contortion $\kappa^\star$ an alternative tensorial expression of the dislocation density. For a discussion on the non-Riemannian nature of the dislocated crystal, see Kröner (1980) and the recent contributions (Maugin, 2003; Hehl and Obukhov, 2007; Kleinert, 2010; Van Goethem, 2010; Lazar and Hehl, 2010). Let us emphasize that in, e.g., Kröner (1980) and Kleinert (1989) the mesoscopic "Kröner's formula", namely $\mathrm{inc}\,\mathcal{E}^\star = -\kappa^\star \times \nabla$, follows in a straightforward manner from an "elastic–plastic" displacement gradient (or distortion) decomposition postulate, which itself requires the selection of a particular reference configuration.[2] Therefore, it is not admissible in our approach which avoids any such arbitrary reference body prescription.

In Van Goethem (2011b) a new "Kröner's formula" was proven in the absence of disclinations and under precise field assumptions for a finite set of skew isolated (i.e., with no accumulation sets) rectilinear defects. It turned out that the formula we proved was not the formula classically reported in the literature (Kröner, 1980; Kleinert, 1989), since an additional term generated by the edge segments of a dislocation curve happens to be directly related to the scalar curvature of g, or, equivalently, to the trace of $\kappa^\star$.

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[1] In our approach, mesoscopic fields are identified with a $\star$-superscript, which is removed as their macroscopic counterparts are considered.

[2] Elastic and plastic decomposition of the strain can classically be considered. However, no rigorous such decomposition holds for the distortion since in the absence of a well-defined *privileged* reference configuration, there is no constitutive law which would define the elastic and plastic parts of the rotation tensor.

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In this communication, our aim is to respond to open questions which arose from Van Goethem (2011b):

(1) does the new formula hold for a dislocation loop?
(2) which new terms appear due to the line curvature?

Therefore, the main part of the present work is devoted to verify by complete calculation of distributional type that a general Kröner's formula (i.e., an extension of that proven in Van Goethem (2011b), which we here state as Conjecture 1) holds true for two classical examples of dislocation loops.

Let us emphasize that Kröner's formulae are crucial since they relate the *mechanical* to the *defect internal variables* in any complete thermodynamic model of dislocations. Whereas it could seem artificial to consider sets of rectilinear dislocation lines, as in Van Goethem and Dupret (2012a,b), and Van Goethem (2011b), this is no more the case for dislocation loops, which are the most common type of dislocations observed in single crystal growing from the melt. So, the topic of this paper has a potential scientific impact for engineer and technology-oriented applications (Müller et al., 2004).

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 (Van Goethem and Dupret, 2012a,b), 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 set of points in the plane. These two introductory works paved the way for the first application of the theory to 3D dislocations and disclinations in an elastic medium (Van Goethem, 2011b), where the lines were not assumed parallel anymore and where in addition to the 3 above-mentioned families of defects, we included the twist disclination. The main results of these three papers are first recalled.

Let us emphasize that in the present work, disclinations, which is a rarer kind of defects in single crystals growing from the melt, are not considered.

Notations 1. For a second-order tensor E, we introduce the left (resp. right) curl operator $\nabla\times$ (resp. $\times\nabla$), i.e., $(\nabla \times E)_{ij} = \epsilon_{ikl}\partial_k E_{lj}$ and[3] $(E \times \nabla)_{ij} = \epsilon_{lkj}\partial_k E_{il}$ (otherwise written, $(E \times \nabla)^T = -\nabla \times E^T$), where E^T denotes the transpose of E.

The incompatibility tensor associated to the symmetric second-order tensor E writes as

$$\operatorname{inc} E := -\nabla \times E \times \nabla = \nabla \times (\nabla \times E)^T,$$

i.e., written componentwise, $(\operatorname{inc} E)_{ij} = \epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l E_{mn}$.

The assumed open and connected domain is denoted by Ω, the dislocation(s) are indicated by $\mathcal{L} \subset \Omega$, and $\Omega_{\mathcal{L}}$ stands for $\Omega \setminus \mathcal{L}$.

In the sequel, we say that a symmetric tensor E_{mn} is compatible on $U \subset \Omega$ if $\epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q E_{mn}$ vanishes in U. Moreover, as soon as $E \in L^1_{loc}(\Omega^\star, \mathbb{R}^{3\times 3})$, the incompatibility of E, $\operatorname{inc} E$ is a distribution (Schwartz, 1957), that is, a linear and continuous form on the space of test functions $\mathcal{C}^\infty_c(\Omega)$.

Assumption 1 *(Planar loop).* Let $\mathcal{L} \subset \Omega$ be a torsion-free dislocation loop with is assumed homoeomorphic to the circle[4] and has a Lipschitz continuous tangent vector.[5]

Assumption 2 *(3D elastic strain).* The linear strain $\mathcal{E}^\star_{mn}$ is a given symmetric $L^s_{loc}(\Omega)$-tensor compatible on $\Omega^\star_{\mathcal{L}}$, with $1 \le s < 2$. In other words, the incompatibility tensor, as defined by the distribution $\eta^\star_{kl} := \epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathcal{E}^\star_{mn}$, vanishes everywhere on $\Omega^\star_{\mathcal{L}}$.

Definition 1 *(Dislocation densities).*

$$\text{Dislocation density:} \quad \alpha^\star := \tau\delta_{\mathcal{L}} \otimes B^\star \quad (\alpha^\star_{ij} := \tau_i B^\star_j \delta_{\mathcal{L}}) \tag{2.1}$$

$$\text{Mesoscopic contortion:} \quad \kappa^\star := \alpha^\star - \frac{I}{2}\operatorname{tr}\alpha^\star \quad (\kappa^\star_{ij} := \alpha^\star_{ij} - \frac{1}{2}\delta_{ij}\alpha^\star_{kk}), \tag{2.2}$$

where $\delta_{\mathcal{L}}$ denotes the 1-dimensional Hausdorff measure concentrated on $\mathcal{L}$, and τ the unit tangent vector to $\mathcal{L}$.

The following classical theorem is easily proven from the relation $\nabla \cdot \alpha^\star = 0$ (see, e.g. Kleinert, 1989).

Theorem 1 (Conservation laws). *Isolated dislocations are either closed or end at the boundary of Ω.*

It has been proven in Van Goethem and Dupret (2012a,b) that at the mesoscale and for a set parallel rectilinear defects, strain incompatibility satisfies the following theorem.

Theorem 2 (Incompatibility of Volterra dislocations). *For a set of isolated parallel dislocations $\mathcal{L}$, incompatibility is the following first-order symmetric tensor distribution,*

$$\text{Kröner's formula:} \quad \tilde{\eta} = \operatorname{inc}\mathcal{E}^\star = -\kappa^\star \times \nabla = \nabla \times (\kappa^\star)^T. \tag{2.3}$$

This result correspond to the Kröner's formula as reported in, e.g., Kröner (1980) and Kleinert (1989).

Moreover, it turns out that this formula is no longer true without a correction term if the lines are not parallel. It has been proven in Van Goethem (2011b) that at the mesoscale and for a set of skew rectilinear defects, strain incompatibility satisfies the following theorem.

[3] This notation is preferred to the other as found in Van Goethem (2011a,b) with the opposite sign convention for the $\times\nabla$ operator.
[4] That is, is represented by a continuous stretching and bending of the circle.
[5] Therefore its curvature exists almost everywhere and is bounded.