Z. Angew. Math. Phys. (2020) 71:196

https://doi.org/10.1007/s00033-020-01420-7

Zeitschrift für angewandte Mathematik und Physik ZAMP

Characterizing geometrically necessary dislocations using an elastic–plastic decomposition of Laplace stretch

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Abstract. In this paper, the geometric dislocation density tensor and Burgers vector are studied using an elastic–plastic decomposition of Laplace stretch $\boldsymbol{\mathcal{U}}$. The Laplace stretch arises from a **QR** decomposition of the deformation gradient and is very useful, as one can directly and unambiguously measure its components by performing experiments. The geometric dislocation density tensor $\tilde{\mathbf{G}}$ is obtained using the classical argument of failure of a Burgers circuit in a suitable configuration $\tilde{\kappa}_p$ where the deformation of a body is solely due to the movement of dislocations. The geometric features of space $\tilde{\kappa}_p$ are explored. It is shown that the derived geometric dislocation tensor is related to the torsion of $\tilde{\kappa}_p$, which serves as a measure of incompatibility in this space. Additionally, $\tilde{\mathbf{G}}$ vanishes only when the space $\tilde{\kappa}_p$ is compatible. A balance law for geometric dislocations is derived taking into account the effect of the dislocation flux and source dislocations. The physical meaning of the plastic Laplace stretch, and consequently, of the derived geometric dislocation tensor proves to be particularly useful in the classification of dislocations. Finally, the significance of the dislocation density tensor is discussed. The derived geometric dislocation density tensor could be specifically useful in developing a strain-gradient and size-dependent theory of plasticity.

Mathematics Subject Classification. 53A17, 53A35, 53B05, 53C29, 53Z05, 74A05, 74C15.

Keywords. Dislocations, Incompatibility, Torsion, Gram-Schmidt factorization, Plasticity.

1. Introduction

The modern phenomenological theory of plasticity is based upon a multiplicative Kröner [28]–Lee [33] decomposition[1] where the deformation gradient is decomposed into elastic and plastic parts, viz., $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$. This decomposition involves an intermediate relaxed configuration κ_p in addition to an undeformed (reference) configuration κ_r and a deformed (current) configuration κ_t. $\mathbf{F}^p$ maps tangent vectors at a material point in κ_r to that at its corresponding point in an intermediate configuration, whereas $\mathbf{F}^e$ maps tangent vectors at a material point in κ_p to vectors in the tangent space of the current configuration κ_t. The plastic part of a deformation gradient is solely due to the lattice deformation resulting from defects, such as dislocations, whereas $\mathbf{F}^e$ represents a stretch and rotation imposed on the lattice in this intermediate configuration. It is important to note that such a decomposition is not unique (see Casey and Naghdi [8], Green and Naghdi [22], Naghdi [39]). In fact, one can have different intermediate configurations up to a finite rigid rotation. The issue of non-uniqueness of the intermediate configuration, however, is resolved at the constitutive level by imposing a requirement of invariance under rigid-body rotation (Simo [46] and Dafalias [13]).

In 2019, Freed et al. [17] proposed an alternative decomposition of the deformation gradient. This decomposition is based on a Gram-Schmidt factorization of a matrix representation for the deformation gradient. The Gram-Schmidt procedure is a well-known technique in the mathematics community that decomposes a matrix into an orthogonal matrix and an upper-triangular matrix (see Leon et al. [35] for

[1] Originally proposed by Bilby et al. [5].

Published online: 04 November 2020

a detailed review of the Gram-Schmidt process). McLellan [37,38] was the first to introduce it to the physics literature when he applied this decomposition to the matrix of a deformation gradient. A **QR** decomposition needs the specification of a coordinate system where the deformation gradient takes the form of an upper-triangular matrix, called Laplace stretch $\boldsymbol{\mathcal{U}}$ [17]. Srinivasa [47] showed that unlike the symmetric stretch tensor $\mathbf{U}$ arising from a traditional polar decomposition, the components of Laplace stretch $\boldsymbol{\mathcal{U}}$ can be measured unambiguously through experiments. **QR** kinematics have been further explored by Freed and Srinivasa [18], Lembo [34], Freed and Zamani [19] and Paul and Freed [43]. The upper-triangular decomposition was extended to elasto-plasticity when Ghosh and Srinivasa [21] used it in their work on shape-memory alloys. In this work, the plastic part of deformation gradient arising from a Kröner–Lee decomposition is further decomposed into a proper orthogonal matrix and an upper-triangular plastic stretch, while the elastic part of deformation gradient remains as a full matrix, thus $\mathbf{F} = \mathbf{F}^e \boldsymbol{\mathcal{R}} \boldsymbol{\mathcal{U}}^p$[2]. Freed et al. [17] used a different approach to employ an upper-triangular decomposition for elasto-plasticity. They first employed Gram-Schmidt factorization to the matrix of a deformation gradient with the resulting upper-triangular Laplace stretch being decomposed into elastic and plastic parts. The later decomposition is possible due to the fact that any upper-triangular matrix with positive determinant forms a group under multiplication. Moreover, this renders the elastic–plastic decomposition of Laplace stretch unique. Thus, the issue of non-uniqueness of the intermediate configuration is suppressed at the kinematics level when adopting their approach.

In this paper, we examine the geometrically necessary dislocations and Burgers [7] vector in the context of this alternative **QR** framework proposed by Freed et al. [17]. Characterization of the dislocations based on a Kröner–Lee decomposition of the deformation gradient has been the central aspect of many researchers' work in the past, starting with Nye [42] when he established a relation between the local rotation of a triad located at each point of an unstrained lattice with local dislocations. It is important to note that unlike the total deformation gradient, its elastic and plastic parts are not, in general, compatible and hence the intermediate configuration cannot be considered as an Euclidean space, i.e., a material manifold with a metric-compatible connection and with a vanishing torsion and curvature. This incompatibility of deformation is often associated with geometrically necessary dislocations—a lattice imperfection that causes plastic flow. Kondo [27] was the first among many researchers to identify this correspondence. Since then, many expressions for the dislocation density have been proposed in the literature (cf. Bilby et al. [4,6], Eshelby [30], Fox [29], Davini and Parry [14,15], Naghdi and Srinivasa [40], Le and Stumpf [32], Acharya and Bassani [2], Cermelli and Gurtin [9] and Gurtin [24], Gupta et al [23], Clayton [11,12] and Yavari and Goriely [49]). A detailed historical account of this field can be found in Acharya and Bassani [2] and Cermelli and Gurtin [9]. Dislocation theory is particularly useful when invoked to develop a strain-gradient and size-dependent theory of plasticity [2,16,20,31,41].

Like many other fundamental aspects of plasticity, a 'correct' definition for a dislocation density tensor has been a point of contention in the mechanics community for a long time. In fact, Acharya [10] pointed out that it is possible to have different physically valid measures of dislocation density based on different physically reasonable criteria. Keeping this in mind, we make yet another attempt to obtain a measure for the geometrically necessary dislocation (GND) density, this time using a **QR** framework to gain some more physical insights in the process. As mentioned earlier, a significant advantage of using a **QR** decomposition over the traditional Kröner–Lee decomposition is that one can directly measure the components of the plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$ from experiments (cf. Sect. 2) in an appropriate configuration $\tilde{\kappa}_p$. Because it is not possible to express $\mathbf{F}^e$ or $\mathbf{F}^p$ as the gradient of a deformation map owing to the incompatibility of its intermediate configuration, these fields clearly lack this physical interpretation. The primary motivation behind this work is to exploit this property of the plastic Laplace stretch to define a more physically intuitive measure for GND density. Since Laplace stretch is capable of *completely* capturing the deformation of a representative cube in all six degrees of freedom, it is certainly possible to

[2]Note that $\boldsymbol{\mathcal{R}}$ is different from the rotation tensor $\mathbf{R}$ obtained from polar decomposition of $\mathbf{F}$.

measure the GND density in an intermediate configuration $\tilde{\kappa}_p$ associated with $\boldsymbol{\mathcal{U}}^p$. Thus, a GND density measured in this configuration can be termed as the GND density due to plastic straining. Note that for the traditional measures of GND density that employ a Kröner–Lee decomposition, a different intermediate configuration κ_p is used. Configurations κ_p and $\tilde{\kappa}_p$ are related through a plastic rotation field $\boldsymbol{\mathcal{R}}^p$, which need not be homogeneous. Therefore, whenever a GND density is measured in configuration κ_p, the incompatibility of this plastic rotation field must be taken into account. A total GND density measured in configuration κ_p[3], thus, can be additively decomposed into a GND density due to plastic straining (measured in configuration $\tilde{\kappa}_p$) and a term representing the incompatibility of this plastic rotation field. The former is a more physically intuitive measure of GND density owing to the physical interpretations that the components of Laplace stretch have.

This article is organized as follows. In Sect. 2, pertinent kinematics of the **QR** decomposition are reviewed. The Laplace stretch $\boldsymbol{\mathcal{U}}$ arising from this decomposition can be further decomposed into an elastic part $\boldsymbol{\mathcal{U}}^e$ and a plastic part $\boldsymbol{\mathcal{U}}^p$. Using this decomposition, the Burgers vector and dislocation density tensor are obtained. Derivation of a dislocation density involves the traditional argument of closure failure of a Burgers circuit in an appropriate configuration where the body is subjected to only plastic deformation. Moreover, it has been shown that the dislocation density tensor also provides a measure for incompatibility in the deformation of a body in that configuration. In Sect. 6, an evolution equation for the dislocation density tensor and a balance law for geometrically necessary dislocations are derived. Different types of dislocations are characterized using the newly obtained dislocation density tensor in Sect. 7. Because $\boldsymbol{\mathcal{U}}^p$ has direct physical meaning, one can easily identify certain types of dislocations using this characterization. The paper is then summarized and drawn to conclusion.

2. Review of QR kinematics

Consider a simply connected body embedded in a three-dimensional Euclidean point space. Motion $\boldsymbol{\mathcal{X}}(\boldsymbol{X}, t)$ is a homeomorphism that maps points in an undeformed configuration κ_r into points in a current configuration κ_t. Position vectors of a material point in the undeformed and current configurations are denoted by $\boldsymbol{X}$ and $\boldsymbol{x}$, respectively. An assumption of simple-connectedness of the body ensures the applicability of Stokes' theorem. The deformation gradient $\mathbf{F} = \partial \boldsymbol{\mathcal{X}}(\boldsymbol{X}, t)/\partial \boldsymbol{X}$ is a linear transformation that maps tangent vectors at a point in the body in κ_r into tangent vectors at its corresponding point in κ_t.

We choose a Cartesian coordinate system $\tilde{\boldsymbol{e}}_I$ that aligns with our laboratory apparatus. In this coordinate system, one can decompose $\mathbf{F}$[4] into an orthogonal matrix $\boldsymbol{\mathcal{R}}$ and an upper-triangular matrix $\boldsymbol{\mathcal{U}}$ called the Laplace stretch [17] whose components are described by

$$\boldsymbol{\mathcal{U}} = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} \tag{1}$$

where a, b, c are three, independent extensions along the coordinate axes of our laboratory frame, and α, β, γ represent three, independent shears acting perpendicular to each other. Note that a, b, c are positive, whereas α, β, γ can be positive, zero or negative. The inverse of Laplace stretch is readily available

[3]This measure for GND density is same as the one derived in Cermelli and Gurtin [9].

[4]The Gram-Schmidt procedure does not specify the 1 coordinate direction nor the 12 coordinate plane, based upon which the other coordinate directions are determined. Therefore, one can potentially have a non-unique set of bases for an experimenter's frame of reference. This issue is resolved by re-indexing the deformation gradient using a strategy whereby the selected 1 direction undergoes the least amount of transverse shear, and the selected 12 coordinate plane experiences least amount of in-plane shear. This re-indexed deformation gradient is denoted by $\boldsymbol{\mathcal{F}}$, whose construction is developed in a paper soon to be published. In fact, the re-indexed deformation gradient $\boldsymbol{\mathcal{F}}$ is decomposed into $\boldsymbol{\mathcal{R}}$ and $\boldsymbol{\mathcal{U}}$. This is merely a problem of selecting the 'correct' set of bases. Deformation gradients $\mathbf{F}$ and $\boldsymbol{\mathcal{F}}$ essentially contain the same information.

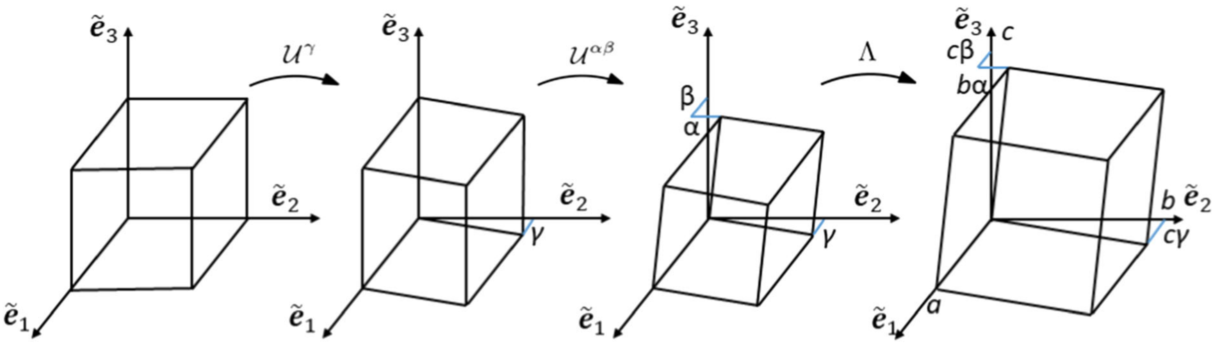

FIG. 1. The distortion of an unit cube into an oblique rectangular prism through various components of Laplace stretch $\boldsymbol{\mathcal{U}}$. Component γ causes a simple shear between X_1X_3 planar sheets in the $\tilde{\mathbf{e}}_1$ direction. Components α and β are the shearings along the $\tilde{\mathbf{e}}_1$ and $\tilde{\mathbf{e}}_2$ directions, respectively, between parallel X_1X_2 planes. Components a, b and c are projections of the vertices of this deformed parallelepiped onto a triad of base vectors $\tilde{\mathbf{e}}_1$, $\tilde{\mathbf{e}}_2$ and $\tilde{\mathbf{e}}_3$ whose lengths are referred to as elongations

and has components of

$$\boldsymbol{\mathcal{U}}^{-1} = \begin{bmatrix} \frac{1}{a} & -\frac{\gamma}{b} & -\frac{\beta - \alpha\gamma}{c} \\ 0 & \frac{1}{b} & -\frac{\alpha}{c} \\ 0 & 0 & \frac{1}{c} \end{bmatrix}. \tag{2}$$

Laplace stretch can be decomposed further into a diagonal matrix and two unit upper-triangular matrices [18]. This is a direct consequence of the Iwasawa matrix decomposition of a deformation gradient [19,25]:

$$\boldsymbol{\mathcal{U}} = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} \begin{bmatrix} 1 & 0 & \beta \\ 0 & 1 & \alpha \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \boldsymbol{\Lambda}\,\boldsymbol{\mathcal{U}}^{\alpha\beta}\,\boldsymbol{\mathcal{U}}^{\gamma} \tag{3}$$

where the physical meanings of $\boldsymbol{\Lambda}$, $\boldsymbol{\mathcal{U}}^{\alpha\beta}$ and $\boldsymbol{\mathcal{U}}^{\gamma}$ are explained through Fig. 1. Note that the final deformation of the unit cube is slightly different from the one described in Eq. (1). The reason behind this minor difference is that in Fig. 1, the deformation is shown in an oblique, convected bases [19], whereas in Eq. (1), the Laplace stretch is described in an orthonormal bases obtained from the Gram-Schmidt procedure.

In an experimenter's frame of reference, a body subjected to a deformation of $\boldsymbol{\mathcal{U}}^{\gamma}$ undergoes a simple shearing between parallel X_1X_3 planes along the $\tilde{\mathbf{e}}_1$ direction. $\boldsymbol{\mathcal{U}}^{\alpha\beta}$ causes a shearing between parallel X_1X_2 planes along the direction $\beta\tilde{\mathbf{e}}_1 + \alpha\tilde{\mathbf{e}}_2$. The deformation $\boldsymbol{\Lambda}$ denotes an extension of the body in all three directions. Thus, the deformation of a body in all six degrees of freedom is *completely* specified by Laplace stretch.

The right Cauchy–Green tensor $\mathbf{C} := \mathbf{F}^T\mathbf{F}$ is related to Laplace stretch through a Cholesky factorization of $\mathbf{C}$, and this factorization is unique, viz., [47]

$$\mathbf{C} = \boldsymbol{\mathcal{U}}^T\boldsymbol{\mathcal{U}} \quad \text{where} \quad \boldsymbol{\mathcal{U}} = \begin{bmatrix} \sqrt{C_{11}} & C_{12}/\mathcal{U}_{11} & C_{13}/\mathcal{U}_{11} \\ 0 & \sqrt{C_{22} - \mathcal{U}_{12}^2} & (C_{23} - \mathcal{U}_{12}\mathcal{U}_{13})/\mathcal{U}_{22} \\ 0 & 0 & \sqrt{C_{33} - \mathcal{U}_{13}^2 - \mathcal{U}_{23}^2} \end{bmatrix} \tag{4}$$

whose components can be found recursively.

Following the Kröner[28] – Lee[33] decomposition $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$, Freed et al. [17] proposed an extension of the upper-triangular decomposition to elasto-plasticity. In this work, first a **QR** decomposition of the deformation gradient is performed resulting in an orthogonal rotation tensor $\boldsymbol{\mathcal{R}}$ and the Laplace stretch $\boldsymbol{\mathcal{U}}$, and then this Laplace stretch is further decomposed into elastic and plastic parts such that

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p. \tag{5}$$

Both $\boldsymbol{\mathcal{U}}^e$ and $\boldsymbol{\mathcal{U}}^p$ are upper-triangular matrices. When written as matrices, the plastic part of Laplace stretch has components of

$$\boldsymbol{\mathcal{U}}^p = \begin{bmatrix} a^p & a^p\gamma^p & a^p\beta^p \\ 0 & b^p & b^p\alpha^p \\ 0 & 0 & c^p \end{bmatrix} \tag{6}$$

where a^p, b^p, c^p are three inelastic elongation ratios, and where $\alpha^p, \beta^p, \gamma^p$ are three magnitudes of shear that ideally remain upon a removal of traction.

Because the set of upper-triangular matrices with positive diagonal elements forms a group under multiplication, the elastic part of Laplace stretch also belongs to this group. In matrix form, the elastic part therefore has components of

$$\boldsymbol{\mathcal{U}}^e = \begin{bmatrix} a^e & a^e\gamma^e & a^e\beta^e \\ 0 & b^e & b^e\alpha^e \\ 0 & 0 & c^e \end{bmatrix} \tag{7}$$

where a^e, b^e, c^e are three elastic elongation ratios, and where $\alpha^e, \beta^e, \gamma^e$ are three magnitudes of elastic shear.

The components of Laplace stretch and its elastic and plastic parts are related through:

$$\begin{aligned} a &= a^e a^p \quad & \alpha &= c^p\alpha^e/b^p + \alpha^p \\ b &= b^e b^p \quad & \beta &= c^p\beta^e/a^p + b^p\gamma^e\alpha^p/a^p + \beta^p \\ c &= c^e c^p \quad & \gamma &= b^p\gamma^e/a^p + \gamma^p \end{aligned} \tag{8}$$

Similarly, components of $\boldsymbol{\mathcal{U}}^e$ and $\boldsymbol{\mathcal{U}}^p$ can be expressed in terms of their other corresponding counterparts. Upon unloading, $\boldsymbol{\mathcal{U}} \to \boldsymbol{\mathcal{U}}^p$ as $\boldsymbol{\mathcal{U}}^e \to \mathbf{I}$. Thus, the knowledge of any two kinematic quantities is sufficient to determine the third.

It is important to note that the rotation tensor $\boldsymbol{\mathcal{R}}$ is employed to transform the coordinate system. This fact has a greater consequence that will be discussed in the next section. In the new coordinate system $\tilde{\boldsymbol{e}}_i$, the deformation gradient takes on the form of an upper-triangular matrix that is capable of describing the deformations in all three degrees of freedom, as shown in Fig. 1. In this frame of reference, the crystal lattice vectors of a single crystal are deformed by the elastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^e$, whereas its plastic part $\boldsymbol{\mathcal{U}}^p$ is the remaining deformation due to the crystal defects; specifically, dislocation slip.

One key advantage of a **QR** decomposition of the deformation gradient is its utility in experiments. An experimentalist can, in principle, measure all components of the Laplace stretch $\boldsymbol{\mathcal{U}}$ in an experimenter's frame of reference. On the other hand, it is not possible to measure directly the components of symmetric stretch tensors **U** or **V** arising from a traditional polar decomposition; they lack physical meaning. The physical meaning of stretch tensors is unequivocally important, as they are commonly used in the construction of constitutive models. The inelastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ can also be measured from what would ideally be an homogeneous deformation in a configuration where all external tractions associated with $\boldsymbol{\mathcal{U}}$ have been removed, i.e., the body is subjected to an elastic unloading.

It is a common notion that the elastic components of a Kröner–Lee decomposition $\mathbf{F}^e$ for a single crystal can be measured from experiments using methods like high-resolution, electron backscatter diffraction (HR-EBSD), a common technique to measure the changes in length of a crystal along coordinate directions, and their crystallographic angles (e.g., Jiang et al. [26]). From these measurements, the components of an elastic deformation gradient $\mathbf{F}^e$ are determined. The components of a total deformation gradient $\mathbf{F}$ can be measured from techniques like digital image correlation (DIC), etc. Once these two quantities are measured, the inelastic component of $\mathbf{F}$ can be readily measured by employing $\mathbf{F}^p = \mathbf{F}^{e-1}\mathbf{F}$. However, such measurements suffer from a theoretical issue. By measuring changes in length along crystallographic directions, and crystallographic angles in a single crystal, what one really measures is the displacement field, and thereby, its gradient. The deformation gradient is eventually obtained by adding $\mathbf{I}$ to the measured displacement gradient. A similar technique is used to determine the total deformation gradient $\mathbf{F}$ from DIC experiments. In DIC measurement, this technique works because the total deformation is compatible, which enables one to define a global deformation map $\boldsymbol{x}(\boldsymbol{X}, t)$ between an undeformed configuration κ_r and a deformed configuration κ_t of a body. Hence, it is possible to define a displacement field by using the definition: $\boldsymbol{u}(\boldsymbol{X}, t) = \boldsymbol{x}(\boldsymbol{X}, t) - \boldsymbol{X}$. However, it is universally accepted that neither the elastic component $\mathbf{F}^e$ nor the inelastic component $\mathbf{F}^p$ of a deformation gradient $\mathbf{F}$ is compatible, which implies that it is not possible to define a global deformation map between the undeformed configuration κ_r and the intermediate configuration κ_p. In this case, such a definition for a displacement field becomes invalid. Therefore, such measurements for the components of $\mathbf{F}^e$ (and thus, $\mathbf{F}^p$) are unsound, from a theoretical point of view.

This theoretical problem is resolved whenever an elastic–plastic decomposition of the Laplace stretch is used, owing to the physical meaning of the components of Laplace stretch. Note that one does not require to define a deformation map, and thereby, neither a displacement field, in order to provide a physical meaning for the components of Laplace stretch. The physical interpretation of the Laplace stretch and its components is valid irrespective of the compatibility of deformation. Therefore, *in an experimenter's frame of reference*, if one measures the changes in crystallographic lengths and angles, the measured quantities directly and unambiguously correspond to the components of elastic Laplace stretch $\boldsymbol{\mathcal{U}}^e$. The only caveat is: how can one obtain the crystallographic deformations in the experimenter's frame of reference? This can be done by performing the Gram-Schmidt procedure on a total deformation gradient $\mathbf{F}$ whose components are measured from DIC experiments, say. Therefore, the elastic Laplace stretch $\boldsymbol{\mathcal{U}}^e$ can be measured, in principle, by the following steps:

1. Measure the components of a total deformation gradient $\mathbf{F}$ from DIC experiments.
2. Perform the Gram-Schmidt procedure to find a rotation tensor $\boldsymbol{\mathcal{R}}$. This rotation tensor $\boldsymbol{\mathcal{R}}$ takes part in the coordinate transformation.
3. Fix a coordinate system and perform HR-EBSD experiments to measure changes in the crystallographic lengths along those coordinate directions, and their crystallographic angles.
4. Transform the measured elastic changes into crystallographic lengths and angles in the experimenter's frame of reference by applying $\boldsymbol{\mathcal{R}}$. The transformed elastic deformations correspond to the components of $\boldsymbol{\mathcal{U}}^e$.

The measurement of $\boldsymbol{\mathcal{U}}^e$ is unambiguous up to an homogeneous rotation field $\boldsymbol{\mathcal{R}}$.

Comparing with the traditional Kröner–Lee decomposition, one can express Lee's elastic and plastic deformation gradients in terms of $\boldsymbol{\mathcal{U}}^e$ and $\boldsymbol{\mathcal{U}}^p$, plus the elastic and plastic components of the rotation tensor, viz., $\boldsymbol{\mathcal{R}}^e$ and $\boldsymbol{\mathcal{R}}^p$ where $\boldsymbol{\mathcal{R}} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e$ with $\mathbf{F}^p = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{U}}^p$. Lee's elastic deformation gradient $\mathbf{F}^e$ can then be expressed as

$$\mathbf{F}^e = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{R}}^{pT} \tag{9}$$

and as such, the total deformation gradient can be expressed as

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p \tag{10}$$

where $\boldsymbol{\mathcal{R}} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e$ and $\boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p$.

3. Configurations relevant to plastic deformation

Before characterizing the Burgers vector and dislocation density tensor, we shall determine an appropriate configuration of the body where these two quantities will be measured. Note that unlike the total

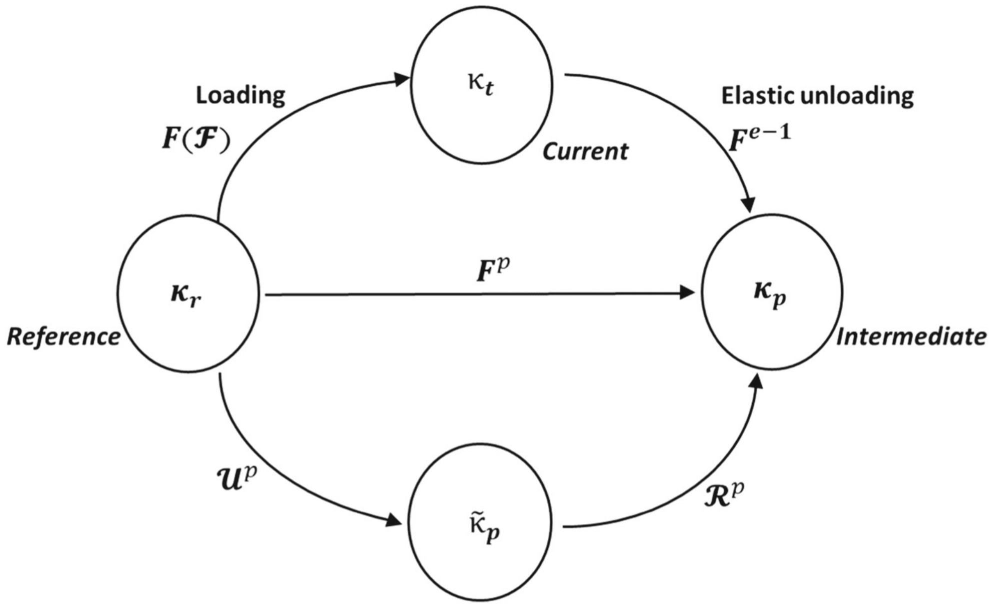

Fig. 2. Configurations of the body associated with plastic deformation, and the maps showing elastic–plastic loading and elastic unloading of the body

deformation, each of its components is incompatible. This leads to the fact that if the reference configuration κ_r is an Euclidean space, *only* the space κ_t is Euclidean. Therefore, it is possible to define different geometric dislocation tensors based on the incompatibility (torsion) of any of these non-Euclidean spaces. Cermelli and Gurtin [9] noted that the abundance of geometric dislocation tensors in the literature is a problem. They proposed a criteria to rule out most of these definitions, and then proposed a 'correct' definition for the geometric dislocation tensor. However, Acharya [1] noted that it is not reasonable to stipulate such a criteria to rule out other definitions for a geometric dislocation tensor. Indeed, all these definitions are valid, and some of them have advantages over the others. Keeping this in mind, we choose a configuration where the body is subjected to a deformation only due to the movement of dislocations.

Physically, it is not possible for a body in an undeformed or reference configuration κ_r to undergo only plastic deformation, and thereby reach an intermediate configuration κ_p.[5] However, if a body undergoes elasto-plastic deformation, i.e., goes from a reference configuration κ_r to the current configuration κ_t through $\mathbf{F}$ (or $\boldsymbol{\mathcal{F}}$), and then is subjected to an elastic unloading by applying $\mathbf{F}^{e-1}$, it is possible to measure a deformation of the body due to only plastic deformation. Hence, in this state of the body, closure failure of an arbitrary line integral provides the measure of lattice defects, i.e., dislocations in the sense of Burgers. This process is shown in Fig. 2.

Consider an infinitesimal fiber $\mathbf{d}\boldsymbol{X}$ in the reference configuration κ_r. The deformed fiber in a current configuration κ_t is denoted by $\mathbf{d}\boldsymbol{x}$ so that

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{\mathcal{F}}\,\mathrm{d}\boldsymbol{X} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p\,\mathrm{d}\boldsymbol{X}. \tag{11}$$

An elastic unloading of the fiber takes it from κ_t to an intermediate configuration κ_p. In this configuration, the deformation of the body is solely due to movement of dislocations. Here $\mathbf{d}\boldsymbol{x}^{\boldsymbol{p}}$ denotes an infinitesimal

[5]Although it is indeed possible for bodies made up of a rigid plastic material to undergo a plastic only deformation, such a constitutive relation is too restrictive.

fiber of the body subjected to an elastic unloading, i.e.,

$$\mathbf{d}\boldsymbol{x}^p = \mathbf{F}^{e-1}\,\mathbf{d}\boldsymbol{x} \tag{12}$$

where $\mathbf{F}^e$ denotes Lee's elastic deformation gradient. $\mathbf{F}^e$ is related to $\boldsymbol{\mathcal{U}}^e$ and a rotation tensor through Eq. (9). Using this relation, one can easily arrive at

$$\mathbf{d}\boldsymbol{x}^p = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{U}}^p\,\mathbf{d}\boldsymbol{X}. \tag{13}$$

At this point, it is important to understand the role of rotation tensor $\boldsymbol{\mathcal{R}}$. The inverse to this rotation tensor, i.e., $\boldsymbol{\mathcal{R}}^T$, rotates an Eulerian triad into the experimenter's frame of reference, and hence plays an important role in coordinate transformation. If $\mathbf{e}'_i$ and $\tilde{\mathbf{e}}_I$ denote Cartesian bases for the Eulerian and experimenter's frames of reference, respectively, then $\mathbf{e}'_i = \boldsymbol{\mathcal{R}}\tilde{\mathbf{e}}_I$ [18]. In view of the physical meaning of the components of Laplace stretch, it is clearly understood that deformation of a body in all six degrees of freedom is completely described by the six components of $\boldsymbol{\mathcal{U}}$, as shown in Sect. 2. However, the components of $\boldsymbol{\mathcal{U}}$ are not all independent, and their dependence has an important consequence in strain compatibility [43].

Therefore, plastic deformation of the body is completely described by the inelastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ in an experimenter's frame of reference, per Eq. (6). Let the configuration of a body, subjected only to $\boldsymbol{\mathcal{U}}^p$, be denoted by $\tilde{\kappa}_p$ with $\mathbf{d}\tilde{\boldsymbol{x}}^p$ denoting an infinitesimal fiber of the body in this configuration so that

$$\mathbf{d}\tilde{\boldsymbol{x}}^p = \boldsymbol{\mathcal{U}}^p\,\mathbf{d}\boldsymbol{X} = \boldsymbol{\mathcal{R}}^{pT}\,\mathbf{d}\boldsymbol{x}^p. \tag{14}$$

This configuration of the body is particularly important because it is in this configuration where the deformation of the body is purely due to the plastic component of Laplace stretch $\boldsymbol{\mathcal{U}}^p$. Due to the "deformation gradient-like" nature of the Laplace stretch, the plastic deformation caused by a movement of dislocations is *fully* characterized in this configuration.

Therefore, we shall compute a Burgers vector and a dislocation density tensor in our physical (experimenter's) frame of reference. Once computed, these quantities can be pushed forward or pulled back easily into the intermediate configuration κ_p or any other configuration by suitable field transfer formulae.

4. Geometric features of $\tilde{\kappa}_p$ and measure of incompatibility

Keeping with our communities' tradition of adopting a differential geometric approach to solve mechanics problems, we now explore some of the geometric features of space $\tilde{\kappa}_p$. This space is not compatible in the sense that the coefficient of a suitably defined metric-compatible connection in this space is not symmetric. It is instructive to discuss the different types of material manifolds that frequently appear in the literature. This classification of material manifolds is based on two geometric features, viz., curvature and torsion (the skew-symmetric part of the connection coefficient). A material manifold with a metric-compatible connection and a non-vanishing torsion and curvature is called a Riemann–Cartan manifold. If the torsion vanishes while maintaining a nonzero curvature tensor, then the manifold becomes Riemannian. On the other hand, a manifold with nonzero torsion and a vanishing curvature is known as a Weitzenböck manifold. The most commonly used manifold is an Euclidean (or flat) manifold where both the curvature tensor and torsion vanish [49].

Torsion of the connection coefficient is generally considered to be a measure of incompatibility in a deformation. In this section, we show that space $\tilde{\kappa}_p$ has a non-vanishing torsion expressed in terms of a spatial gradient for the plastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ with respect to referential coordinates. The dislocation density tensor that results in closure failure of a Burgers circuit involves a torsion of the space $\tilde{\kappa}_p$ in its definition, and it becomes zero when the torsion vanishes. This derivation closely follows Clayton's [11] approach for anholonomic deformation.

Let us choose a set of Cartesian base vectors $\tilde{\mathbf{e}}_a$ in the configuration $\tilde{\kappa}_p$, i.e., the bases of an experimenter's frame. In view of Eq. (14), the plastic part of Laplace stretch can be written in this coordinate frame as

$$\boldsymbol{\mathcal{U}}^p = \mathcal{U}^{pa}_A\left(\boldsymbol{X}, t\right)\ \tilde{\mathbf{e}}_a \otimes \boldsymbol{E}^A\left(\boldsymbol{X}\right) \tag{15}$$

where $\boldsymbol{E}^A$ denotes a Cartesian basis for the reference configuration κ_r. Convected basis vectors and their reciprocals in $\tilde{\kappa}_p$ are defined as

$$\boldsymbol{E}'^A\left(\tilde{\boldsymbol{x}}^p, t\right) = \mathcal{U}^{p-1A}_a\left(\tilde{\boldsymbol{x}}^p, t\right)\ \tilde{\mathbf{e}}^a \quad \text{and} \quad \boldsymbol{E'}_A\left(\boldsymbol{X}, t\right) = \mathcal{U}^{pa}_A\left(\boldsymbol{X}, t\right)\ \tilde{\mathbf{e}}_a. \tag{16}$$

We are now able to compute the metric of space $\tilde{\kappa}_p$ by using the convected basis vectors defined above, specifically

$$\boldsymbol{E}'_A \cdot \boldsymbol{E}'_B = \mathcal{U}^{p\,a}_{\ \ A}\,\mathcal{U}^{p\,a}_{\ \ B} := C^p_{AB}. \tag{17}$$

Equation (17) uses the fact that $\tilde{\mathbf{e}}_a \cdot \tilde{\mathbf{e}}_b = \delta_{ab}$ for Cartesian basis $\tilde{\mathbf{e}}_a$. Note that the Cauchy–Green tensor $\mathbf{C}$ can be written as

$$\mathbf{C} = \boldsymbol{\mathcal{U}}^{pT}\mathbf{C}^e\boldsymbol{\mathcal{U}}^p \tag{18}$$

where an elastic Cauchy–Green tensor is given as $\mathbf{C}^e = \boldsymbol{\mathcal{U}}^{eT}\boldsymbol{\mathcal{U}}^e$. During an elastic unloading, $\boldsymbol{\mathcal{U}}^e \to \mathbf{I}$, thus, $\mathbf{C} \to \mathbf{C}^p = \boldsymbol{\mathcal{U}}^{pT}\boldsymbol{\mathcal{U}}^p$.

We now define a suitable linear connection associated with the metric $\mathbf{C}^p$ and its associated covariant derivative. For a general space, the covariant derivative ∇ is defined in terms of its action on a vector field $\boldsymbol{W}$ with respect to another vector field $\boldsymbol{V}$. In reference coordinates, i.e., in the configuration κ_r, the covariant derivative of $\boldsymbol{W}$ with respect to $\boldsymbol{V}$ is given as

$$\nabla_{\boldsymbol{V}}\boldsymbol{W} = \left(V^B\,\partial_B W^A + \Gamma^A_{BC}W^C V^B\right)\boldsymbol{E_A} \tag{19}$$

where $\boldsymbol{\Gamma}$ is the connection coefficient of the space κ_r, and where $\boldsymbol{E}_A = \partial_A\boldsymbol{X}$ is the basis vector of that space. It can be shown that the connection coefficient follows the identity

$$\Gamma^A_{BC}\partial_A = \nabla_{\partial_B}\partial_C. \tag{20}$$

Therefore, to determine the connection coefficient, we need to find a gradient of the convected basis vector with respect to the referential coordinates, in particular

$$\partial_B\,\boldsymbol{E'}_A = \partial_B\,\mathcal{U}^{pa}_{\ \ A}\,\tilde{\mathbf{e}}_a = \mathcal{U}^{p-1\,D}_{\ \ \ \ a}\partial_B\,\mathcal{U}^{pa}_{\ \ A}\,\boldsymbol{E'}_D. \tag{21}$$

Let $\overset{\mathbf{C}^p}{\boldsymbol{\Gamma}}$ represent the connection coefficient associated with metric $\mathbf{C}^p$. The last part of Eq. (21) is obtained by using the interrelation (16) between basis vectors of $\tilde{\kappa}_p$ and its convected basis vectors. Using the property of connection coefficient $\partial_B\,\boldsymbol{E'}_A = \overset{\mathbf{C}^p}{\Gamma}\,\boldsymbol{E}'^D$, we define

$$\overset{\mathbf{C}^p}{\Gamma}{}^{D}_{BA} = \mathcal{U}^{p-1\,D}_{\ \ \ \ a}\,\partial_B\,\mathcal{U}^{pa}_{\ \ A}. \tag{22}$$

The connection coefficient is clearly not symmetric because $\boldsymbol{\mathcal{U}}^p$ is an upper-triangular matrix. The torsion of this connection, i.e., the skew-symmetric part of its connection coefficient, is therefore defined as

$$T^D_{AB} = \frac{1}{2}\left(\overset{\mathbf{C}^p}{\Gamma}{}^{D}_{BA} - \overset{\mathbf{C}^p}{\Gamma}{}^{D}_{AB}\right) = \frac{1}{2}\,\mathcal{U}^{p-1\,D}_{\ \ \ \ a}\left(\,\partial_B\,\mathcal{U}^{pa}_{\ \ A} - \,\partial_A\,\mathcal{U}^{pa}_{\ \ B}\right). \tag{23}$$

A non-vanishing torsion of a connection is a natural measure of incompatibility. Clearly, a non-vanishing torsion makes the associated space $\tilde{\kappa}_p$ non-Euclidean and, therefore, the geometry is definitely non-Riemannian. Nevertheless, it is still possible to construct a local, Cartesian, coordinate system in this space.

In view of Eq. (23), one can conclude that $\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)$ provides a measure for the local incompatibility of deformation for a body in configuration $\tilde{\kappa}_p$. This is due to the fact that the plastic part of Laplace stretch is always nonzero. Therefore, for a connection to be symmetric, i.e., for the configuration $\tilde{\kappa}_p$ to be compatible, one must have $\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p) = \mathbf{0}$. In Sect. 5, we show that the dislocation density tensor vanishes only when $\mathbf{T}$ is zero, i.e., the deformation $\boldsymbol{\mathcal{U}}^p$ is compatible.

Herein the incompatibility (torsion) is determined in the context of inelasticity. In a later section, it will be shown that the derived measure of incompatibility is directly related to what is traditionally called the *geometric dislocation tensor*. However, the derived measure of incompatibility is not limited to elasto-plasticity and has a much wider range of application. In fact, one can derive similar measures of incompatibility whenever the deformation gradient is multiplicatively decomposed into two or more kinematic variables. Such decompositions are abundant in the literature [36]. For instance, Vujosevic and Lubarda [48] decomposed the total deformation gradient into isothermal deformation gradient $\mathbf{F}^e$ and thermal deformation gradient $\mathbf{F}^\theta$ in the context of thermoelasticity; Rodriguez et al. [44] decomposed $\mathbf{F}$ into an elastic component $\mathbf{F}^e$ and a growth component $\mathbf{F}^g$ while modeling the growth in soft elastic tissues. In all these cases, the intermediate configuration is incompatible, and hence, a measure of incompatibility can be computed following the procedure described in Sect. 4. Needless to say, the measures of incompatibility in these cases will bear different physical interpretations.

5. Burgers vector and dislocation density tensor

5.1. Closure failure of a Burgers circuit

Consider a curve ζ in configuration $\tilde{\kappa}_p$ that was initially a closed loop before deformation in some reference configuration κ_r. The path integral of a spatial variable along a curve physically represents the distance between its two ends. Therefore, when calculated in an Euclidean space, say the reference configuration κ_r or the current configuration κ_t, the path integral of a spatial variable along the closed loop ζ will be zero. However, this is not the case when the path integral is calculated in an intermediate configuration. In fact, in this configuration, the path integral represents the closure failure of the initially closed loop ζ. Therefore, if ζ is considered as a Burgers circuit, this path integral, calculated in an intermediate configuration $\tilde{\kappa}_p$, represents the Burgers vector, as understood in the materials science literature. Hence, the cumulative Burgers vector of all dislocations inside the surface enclosed by ζ is given as

$$\tilde{\boldsymbol{b}} = \oint_\zeta \mathrm{d}\tilde{\boldsymbol{x}}^p = \oint_\zeta \boldsymbol{\mathcal{U}}^p \,\mathrm{d}\boldsymbol{X}. \tag{24}$$

Let $\tilde{\boldsymbol{n}}$ be the unit normal to a surface $\tilde{S}$ whose boundary is curve ζ, and let S be the surface corresponding to $\tilde{S}$ in the undeformed configuration. When transferred into the reference configuration κ_r, $\boldsymbol{n}_R$ denotes the unit normal to the surface S. Now applying Stokes' theorem to Eq. (24), we get

$$\tilde{\boldsymbol{b}} = \int_S \left(\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)\right)^T \boldsymbol{n}_R \,\mathrm{d}A_R. \tag{25}$$

Here 'Curl' represents the curl operator taken with respect to reference coordinates. Upon transforming the referential vector area $\boldsymbol{n}_R\,\mathrm{d}A_R$ to configuration $\tilde{\kappa}_p$ by $\boldsymbol{n}_R\,\mathrm{d}A_R = J_p\,\boldsymbol{\mathcal{U}}^{p-T}\,\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a}$ with $J_p = \det(\boldsymbol{\mathcal{U}}^p) = a^p b^p c^p$, we obtain

$$\tilde{\boldsymbol{b}} = \int_{\tilde{S}} \frac{1}{J_p} (\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p))^T \boldsymbol{\mathcal{U}}^{pT}\,\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a}. \tag{26}$$

Equation (26) represents the cumulative Burgers vector of all dislocations threading an arbitrary surface $\tilde{S}$ in configuration $\tilde{\kappa}_p$. If $\tilde{\mathbf{G}}_p$ denotes the geometric dislocation tensor, then $\tilde{\mathbf{G}}_p^T\tilde{\boldsymbol{n}}$ represents the local Burgers vector, given as $\frac{1}{J_p}(\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p))^T\boldsymbol{\mathcal{U}}^{pT}\,\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a}$, for a surface $\tilde{S}$ in $\tilde{\kappa}_p$. Thus, a dislocation density tensor in configuration $\tilde{\kappa}_p$ obtains the form

$$\tilde{\mathbf{G}}_p = \frac{1}{J_p}\boldsymbol{\mathcal{U}}^p\,\mathrm{Curl}\left(\boldsymbol{\mathcal{U}}^p\right). \tag{27}$$

Physically, $\tilde{\mathbf{G}}_p$ provides a measure of the local Burgers vector per unit area of a body in configuration $\tilde{\kappa}_p$. Note that $\tilde{\mathbf{G}}_p^T \tilde{\boldsymbol{n}}$ represents the local Burgers vector measured *per unit area*. It is also common to assign the term *dislocation density* to the total length of dislocation lines *per unit volume* of the material.

In terms of the components of $\boldsymbol{\mathcal{U}}^p$, the components of this dislocation density tensor $\tilde{\mathbf{G}}_p$ can be written as

$$
\begin{aligned}
\tilde{G}_{p11} &= \frac{1}{b^p c^p}\left[(a^p\beta^p)_{,2} - (a^p\gamma^p)_{,3}\right] + \frac{\gamma^p}{b^p c^p}\left[a^p_{,3} - (a^p\beta^p)_{,1}\right] + \frac{\beta^p}{b^p c^p}\left[(a^p\gamma^p)_{,1} - a^p_{,2}\right]\\
\tilde{G}_{p12} &= \frac{1}{b^p c^p}\left[(b^p\alpha^p)_{,2} - b^p_{,3}\right] - \frac{\gamma^p}{b^p c^p}(b^p\alpha^p)_{,1} + \frac{\beta^p}{b^p c^p} b^p_{,1}\\
\tilde{G}_{p13} &= \frac{1}{b^p c^p} c^p_{,2} - \frac{\gamma^p}{b^p c^p} c^p_{,1}\\
\tilde{G}_{p21} &= \frac{1}{a^p c^p}\left[a^p_{,3} - (a^p\beta^p)_{,1}\right] + \frac{\alpha^p}{a^p c^p}\left[(a^p\gamma^p)_{,1} - a^p_{,2}\right]\\
\tilde{G}_{p22} &= -\frac{1}{a^p c^p}(b^p\alpha^p)_{,1} + \frac{\alpha^p}{a^p c^p} b^p_{,1}\\
\tilde{G}_{p23} &= -\frac{1}{a^p c^p} c^p_{,1}\\
\tilde{G}_{p31} &= \frac{1}{a^p b^p}\left[(a^p\gamma^p)_{,1} - a^p_{,2}\right]\\
\tilde{G}_{p32} &= \frac{1}{a^p b^p} b^p_{,1}\\
\tilde{G}_{p33} &= 0
\end{aligned}
\tag{28}
$$

Here '$_{,i}$' represents the derivative of a quantity with respect to referential coordinate X_i. This obtained dislocation density tensor clearly remains invariant under a superposed compatible elastic deformation.

One can express the derived dislocation density tensor $\tilde{\mathbf{G}}_p$ in terms of the torsion $\mathbf{T}$ of space $\tilde{\kappa}_p$ and its plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$. A deformation in $\tilde{\kappa}_p$ is compatible whenever $\mathbf{T}$ is zero. Because $\boldsymbol{\mathcal{U}}^p$ is always nonzero and invertible, a vanishing of $\mathbf{T}$ implies that the Curl($\boldsymbol{\mathcal{U}}^p$) is zero. By similar argument, one can easily realize that the dislocation density tensor vanishes only when the Curl($\boldsymbol{\mathcal{U}}^p$) vanishes. Thus, *the dislocation density tensor becomes zero if and only if the torsion* $\mathbf{T}$ *vanishes and the plastic deformation field* $\boldsymbol{\mathcal{U}}^p$ *is compatible.*

In view of the physical meaning of $\boldsymbol{\mathcal{U}}^p$, one can realize that the geometric dislocation tensor $\tilde{\mathbf{G}}_p$ measures the incompatibility of the plastic deformation field due to the distortion (straining) of the crystal lattice caused by the movement of dislocations. In that sense, $\tilde{\mathbf{G}}_p$ is equivalent to the traditional definition of dislocation tensor, viz., $\mathbf{F}^p$Curl($\mathbf{F}^p$) [9,45], derived using a Kröner–Lee decomposition of the deformation gradient.

It is important to note that the scalar quantity $\rho = \boldsymbol{l} \cdot \tilde{\mathbf{G}}\boldsymbol{b}$ is often referred to as dislocation density in the literature [9,31]. Herein vectors $\boldsymbol{l}$ and $\boldsymbol{b}$ denote the line direction and Burgers vector of a dislocation per unit area. Consequently, ρ is just another measure for $\tilde{\mathbf{G}}$, and one can easily understand which measure is in use from the context.

5.2. Burgers vector and dislocation density tensor in terms of $\boldsymbol{\mathcal{U}}^e$

Because the elastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^e$ can be expressed in terms of the total Laplace stretch $\boldsymbol{\mathcal{U}}$ and its plastic part $\boldsymbol{\mathcal{U}}^p$ [17], one can also determine the Burgers vector and dislocation density tensor in terms of $\boldsymbol{\mathcal{U}}^e$, starting from a deformation analysis done in configuration κ_t. Because Laplace stretch is capable of describing deformation in all six degrees of freedom, one can define a deformed configuration $\tilde{\kappa}_t$ for the experimenter's frame of reference such that if $\mathrm{d}\tilde{\boldsymbol{x}}$ denotes an infinitesimal fiber of the body in this configuration, then

$$\mathrm{d}\tilde{\boldsymbol{x}} = \boldsymbol{\mathcal{U}}\,\mathrm{d}\boldsymbol{X} = \boldsymbol{\mathcal{R}}^T\,\mathrm{d}\boldsymbol{x}. \tag{29}$$

The inverse elastic Laplace stretch $\boldsymbol{\mathcal{U}}^{e-1}$ maps the infinitesimal fiber $\mathrm{d}\tilde{\boldsymbol{x}}$ in $\tilde{\kappa}_t$ to $\tilde{\kappa}_p$, where the Burgers vector per unit area and dislocation density tensor are measured. These configurations and associated maps are shown in Fig. 3.

An infinitesimal fiber $\mathrm{d}\tilde{\boldsymbol{x}}_p$ in configuration $\tilde{\kappa}_p$, where a deformation of the body is caused solely by the movement of dislocations, is related to its corresponding fiber in the current configuration κ_t through

$$\mathrm{d}\tilde{\boldsymbol{x}}^p = \boldsymbol{\mathcal{U}}^{e-1}\mathrm{d}\tilde{\boldsymbol{x}} = \boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\mathrm{d}\boldsymbol{x}. \tag{30}$$

Using a similar argument as above, we find that

$$\tilde{\boldsymbol{b}}_e = \oint_\zeta \mathrm{d}\tilde{\boldsymbol{x}}^p = \oint_{\tilde{S}} \frac{1}{\det\left(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\right)} \left(\mathrm{curl}\left(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\right)\right)^T . \left(\boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}^{e-T}\right)\, \tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a} \tag{31}$$

where 'curl' denotes the curl operator taken with respect to spatial coordinates, and where $\tilde{\boldsymbol{b}}_e$ denotes the cumulative Burgers vector per unit area represented in terms of $\boldsymbol{\mathcal{U}}^e$. If $\tilde{\mathbf{G}}_e$ denotes the dislocation density tensor, represented in terms of $\boldsymbol{\mathcal{U}}^e$, then

$$\tilde{\mathbf{G}}_e = \frac{1}{\det\left(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\right)}\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\mathrm{curl}(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T) = \det(\boldsymbol{\mathcal{U}}^e)\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\mathrm{curl}\left(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\right). \tag{32}$$

The last part of Eq. (32) is obtained by employing the fact that $\det(\boldsymbol{\mathcal{R}}) = 1$. Therefore, the geometrically necessary dislocation density tensor, expressed in the experimenter's frame of reference, is defined as

$$\tilde{\mathbf{G}} = \frac{1}{J_p}\boldsymbol{\mathcal{U}}^p\,\mathrm{Curl}\,(\boldsymbol{\mathcal{U}}^p) = \det(\boldsymbol{\mathcal{U}}^e)\;\boldsymbol{\mathcal{U}}^{e-1}\;\boldsymbol{\mathcal{R}}^T\;\mathrm{curl}(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T) \tag{33}$$

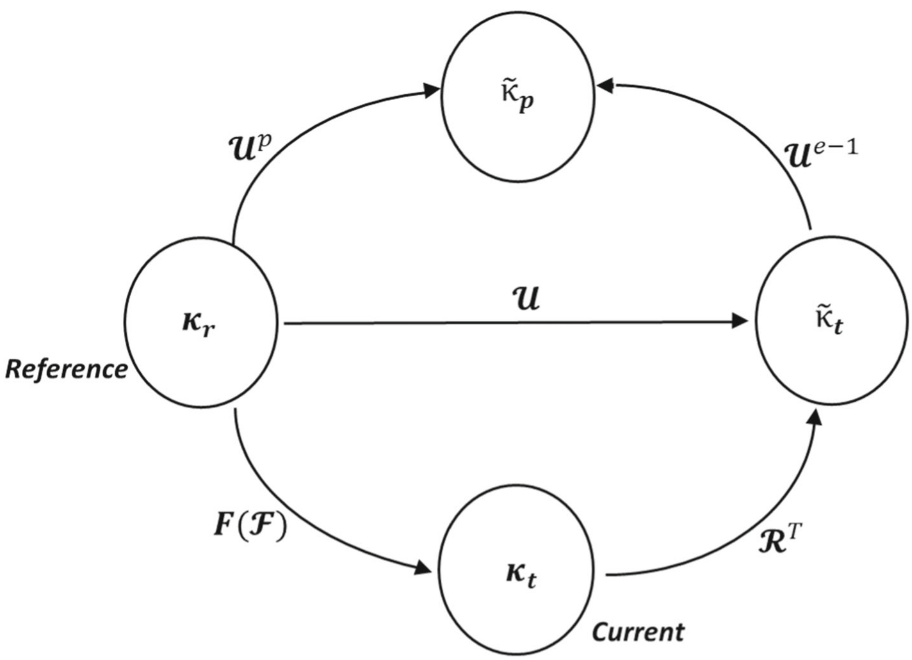

FIG. 3. Deformation maps showing a transformation of tangent vectors between different configurations of the body

or $\tilde{\mathbf{G}} = \tilde{\mathbf{G}}_e = \tilde{\mathbf{G}}_p$. Note that $\tilde{\mathbf{G}}$ denotes the geometric dislocation tensor *due to 'permanent' distortion or straining of the crystal lattice.*

In the literature, $\tilde{\mathbf{G}}$ is sometimes referred to as Burgers tensor or the geometric dislocation tensor. Although the dislocation density tensors $\tilde{\mathbf{G}}, \tilde{\mathbf{G}}_e$ and $\tilde{\mathbf{G}}_p$ obtained herein are defined in terms of upper-triangular stretch tensors, none of them are upper-triangular. Because the dislocation density tensor transforms as a second-order tensor, when pushed forward into the intermediate configuration κ_p, it takes the form:

$$\mathbf{G} = \boldsymbol{\mathcal{R}}^p \, \tilde{\mathbf{G}} \, \boldsymbol{\mathcal{R}}^{pT} \tag{34}$$

where $\mathbf{G}$ denotes the dislocation density tensor in the intermediate configuration κ_p, which arises in a traditional Kröner–Lee decomposition. Similarly, the derived dislocation density tensor can be pulled back or pushed forward to any other configurations by suitable field transfer formulae.

Note that the definition for a dislocation density tensor presented here is significantly different from the ones found in literature; most of which involve $\mathbf{F}^{e-1}$ or $\mathbf{F}^p$ and, in some cases, the rotation tensor $\mathbf{R}$. This is due to the fact that in the literature a polar decomposition is applied to the elastic and plastic parts of the deformation gradient arising from its Kröner-Lee decomposition. However, in our definition, a $\mathbf{QR}$ decomposition is applied first to the deformation gradient with the resulting Laplace stretch being decomposed into elastic and plastic components, which is assured because of the closure property of a group. The derived expression for the dislocation density tensor is also consistent with our definition of a plastic velocity gradient $\boldsymbol{\mathcal{L}}^p$, defined as $\boldsymbol{\mathcal{L}}^p := \dot{\boldsymbol{\mathcal{U}}}^p \boldsymbol{\mathcal{U}}^{p-1}$ instead of $\dot{\mathbf{F}}^p \mathbf{F}^{p-1}$ [17].

5.3. Incompatibility of plastic rotation field

The geometric dislocation tensor $\tilde{\mathbf{G}}_p$ (or $\tilde{\mathbf{G}}$) measures the incompatibility of a deformation field that causes plastic straining to a crystal lattice in a rotated configuration $\tilde{\kappa}_p$. In general, to measure the geometric dislocation density tensor, based on a Kröner–Lee decomposition, a different intermediate configuration κ_p is used. This configuration κ_p is related to our physical configuration $\tilde{\kappa}_p$ through the plastic rotation field $\boldsymbol{\mathcal{R}}^p$ which is not, in general, homogeneous. Therefore, it is important to account for the incompatibility of a plastic rotation field.

As mentioned earlier, the rotation tensor $\boldsymbol{\mathcal{R}}$ acts as a coordinate transformation matrix. Specifically, $\boldsymbol{\mathcal{R}}^T$ rotates an Eulerian triad into the set of base vectors belonging to our physical frame of reference, $\tilde{\mathbf{e}}_I$. In the absence of an elastic rotation field, the rotation tensor $\boldsymbol{\mathcal{R}}$ becomes $\boldsymbol{\mathcal{R}}^p$. Therefore, physically $\boldsymbol{\mathcal{R}}^p$ denotes the local rotation of the crystal lattice vectors in the absence of elastic deformation. In general, this rotation field is not homogeneous and therefore, the spatial variation of the rotation $\boldsymbol{\mathcal{R}}^p$ measures the incompatibility of the plastic rotation field. Let us define the geometric dislocation tensor due to a plastic rotation field $\tilde{\mathbf{G}}_r$ in a way that it has the same structure as $\tilde{\mathbf{G}}_p$. Thus, $\tilde{\mathbf{G}}_r$ is defined as

$$\tilde{\mathbf{G}}_r = \boldsymbol{\mathcal{R}}^p \, \mathrm{Curl}\,(\boldsymbol{\mathcal{R}}^p)\,. \tag{35}$$

This definition is consistent with Nye's dislocation tensor. Nye [42] assumed that the crystal lattice is unstrained, but the local rotation between the director vectors varies in spatial direction. Therefore, this assumption is perfectly in sync, in view of the physical meaning of $\boldsymbol{\mathcal{R}}^p$. The spatial variation of $\boldsymbol{\mathcal{R}}^p$ effectively determines the spatial variation of the coordinate frame (lattice director vectors) in which the components of plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$ is measured. Thus, $\tilde{\mathbf{G}}_r$ is nothing but an analogue of Nye's dislocation tensor in our framework.

In this definition, the space $\tilde{\kappa}_p$ is considered as a reference. The primary issue with defining a physically meaningful dislocation tensor is that it should be measured with respect to the undeformed configuration κ_r or the deformed configuration κ_t. In case of $\tilde{\mathbf{G}}_r$, however, it is impossible to measure it with respect to κ_r without bypassing the plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$. Nevertheless, one can define a physically meaningful dislocation tensor due to plastic rotation by computing the incompatibility in the space κ_p with κ_r as a reference, and then show that it is equivalent to $\tilde{\mathbf{G}}_r$.

If one chooses to measure the dislocation tensor in the configuration κ_p with the undeformed configuration κ_r considered as a reference, then following the procedure in Sect. 5.1, it can be easily shown that the geometric dislocation tensor in this configuration takes on the form

$$\mathbf{G}_{\kappa_p} = \boldsymbol{\mathcal{R}}^p \boldsymbol{\mathcal{U}}^p \, \mathrm{Curl} \left(\boldsymbol{\mathcal{R}}^p \boldsymbol{\mathcal{U}}^p \right). \tag{36}$$

Writing the equation in indicial notation with respect to a Cartesian coordinate system E_i, and doing some algebraic manipulation, we obtain

$$G_{\kappa_p}{}^{ij} = \epsilon^{ABM} \, \mathcal{R}^{pi}_{s} \, \mathcal{U}^{ps}_{M} \, \mathcal{R}^{pj}_{q,A} \, \mathcal{U}^{pq}_{B} \; + \; \mathcal{R}^{pi}_{r} \, \tilde{G}_p{}^{rq} \, \mathcal{R}^{pj}_{q}. \tag{37}$$

Here 'p' is not a dummy index; it represents the plastic component. Let us define the geometric dislocation tensor $\mathbf{G}_r$ measured in configuration κ_p such that $\mathbf{G}_r{}^{ij} := \epsilon^{ABM} \mathcal{R}^{pi}_{s} \mathcal{U}^{ps}_{M} \mathcal{R}^{pj}_{q,A} \mathcal{U}^{pq}_{B}$. Therefore, substituting in Eq. (37), we obtain

$$\mathbf{G}_{\kappa_p} = \mathbf{G}_r \; + \; \boldsymbol{\mathcal{R}}^p \, \tilde{\mathbf{G}}_p \, \boldsymbol{\mathcal{R}}^{pT}. \tag{38}$$

When *only* a rotation field is applied to the body, i.e., $\boldsymbol{\mathcal{U}}^p \to \mathbf{I}$, then $\mathbf{G}_r$ becomes equal to $\tilde{\mathbf{G}}_r$. This is also evident because, in this case, the reference configuration κ_r and the intermediate configuration $\tilde{\kappa}_p$ coincide. Because the dislocation tensor due to straining of the crystal lattice is zero in this case, the total dislocation tensor measured in κ_p, viz., $\mathbf{G}_{\kappa_p}$, also reduces to $\tilde{\mathbf{G}}_r$. Similarly, when the rotation field is homogeneous, then $\mathbf{G}_r \to \mathbf{0}$ and $\mathbf{G}_{\kappa_p} \to \boldsymbol{\mathcal{R}}^p \tilde{\mathbf{G}}_p \boldsymbol{\mathcal{R}}^{pT}$. In view of Eq. (34), it is easy to understand that the reduced dislocation tensor $\mathbf{G}_{\kappa_p}$ under the condition of a homogeneous rotation field is the dislocation tensor $\tilde{\mathbf{G}}_p$ pushed forward to the configuration κ_p. Note that only in the presence of $\tilde{\mathbf{G}}_r$ will the coordinate frame in which a **QR** decomposition is performed spatially vary, and thus, in that case, a measurement of the components for $\boldsymbol{\mathcal{U}}^p$ becomes ambiguous.

It is instructive that the plastic part of Laplace stretch is related to Lee's plastic deformation gradient through the relation $\mathbf{F}^p = \boldsymbol{\mathcal{R}}^p \, \boldsymbol{\mathcal{U}}^p$. Therefore, the expression for the total geometric dislocation density tensor $\mathbf{G}_{\kappa_p}$, measured in the configuration κ_p, is the same as the one derived in Cermelli and Gurtin [9], and can be shown to relate to other measures of the dislocation density tensor found in the literature. However, the additive decomposition of this field into dislocation density due to plastic straining and an incompatible rotation field provides a more physical understanding of this expression.

6. Balance law for geometrically necessary dislocations in the configuration $\tilde{\kappa}_p$

Let us consider an arbitrary surface $\tilde{S}$ enclosed by a curve ζ in configuration $\tilde{\kappa}_p$. Let $\tilde{A}$ and $\tilde{\boldsymbol{n}}$ denote the surface area and unit normal to the surface, respectively. Let f be a dislocation flux that measures the inflow of dislocations into surface $\tilde{S}$ through its boundary ζ, measured per unit length. Let $\tilde{\mathbf{G}}_s$ be a dislocation source density that accounts for the rate of dislocation generation per unit area inside surface $\tilde{S}$. The dislocation tensor due to plastic rotation must be pulled back to the configuration $\tilde{\kappa}_p$ through appropriate formulae. We assume that $\tilde{\mathbf{G}}$, $\mathbf{G}_r$, f and $\tilde{\mathbf{G}}_s$ are continuous functions and that the dislocation flux f is continuously differentiable. Although it is reasonable to consider the dislocation flux and the source dislocation in our physical frame of reference (i.e., the configuration $\tilde{\kappa}_p$), one must take into account the incompatibility of the plastic rotation field, which appears in the expression for the dislocation density tensor when measured in configuration κ_p. Therefore, the dislocation density tensor $\mathbf{G}_r$ due to an incompatibility of the plastic rotation field should be pulled back into the configuration $\tilde{\kappa}_p$ in the derivation of this balance law. Now, a balance law for dislocations can then be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\tilde{S}} \left(\tilde{\mathbf{G}}^T \; + \; \boldsymbol{\mathcal{R}}^{pT} \, \mathbf{G}_r^T \, \boldsymbol{\mathcal{R}}^p \right) \, \tilde{\boldsymbol{n}} \, \mathrm{d}\tilde{a} = \int_{\zeta} f \, \mathrm{d}\tilde{\boldsymbol{x}}_p + \int_{\tilde{S}} \tilde{\mathbf{G}}_s^T \tilde{\boldsymbol{n}} \, \mathrm{d}\tilde{a}. \tag{39}$$

Using Eq. (14) and applying Stokes' theorem to Eq. (39),[2] we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\tilde{S}}\left(\tilde{\mathbf{G}}^T + \boldsymbol{\mathcal{R}}^{pT}\,\mathbf{G}_r^T\,\boldsymbol{\mathcal{R}}^p\right)\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a} = \int_S (\mathrm{Curl}(f\,\boldsymbol{\mathcal{U}}^p))^T\boldsymbol{n}_R\,\mathrm{d}A_R + \int_{\tilde{S}}\tilde{\mathbf{G}}_s^T\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a} \tag{40}$$

where S is the corresponding surface in the reference configuration κ_r with unit normal $\boldsymbol{n}_R$ and area A_R. The vector area of $\tilde{S}$ can be transferred into κ_r by the formula $\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a} = \dfrac{1}{J_p}\boldsymbol{\mathcal{U}}^{pT}\,\boldsymbol{n}_R\,\mathrm{d}A_R$.

Note that the dislocation source tensor $\tilde{\mathbf{G}}_s$ contains the source of dislocations that cause plastic distortion (straining) in a crystal lattice, while the dislocation density is responsible for incompatibility in a plastic rotation field; the latter of which is pulled back into the configuration $\tilde{\kappa}_p$. The same is true for the dislocation flux f. A similar calculation can be carried out in the configuration κ_p using appropriate pull back and push forward operations to suitable quantities.

At this point, we need to transfer the surface integrals in Eq. $(40)^{1,3}$ into the reference configuration by using its area transformation formula. For the term in Eq. $(40)^1$, it is possible to move the time-derivative inside the integral sign after transferring it into reference configuration, hence we get

$$\int_S\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{J_p}\left(\tilde{\mathbf{G}}^T + \boldsymbol{\mathcal{R}}^{pT}\,\mathbf{G}_r^T\,\boldsymbol{\mathcal{R}}^p\right)\boldsymbol{\mathcal{U}}^{pT}\right) - (\mathrm{Curl}(f\boldsymbol{\mathcal{U}}^p))^T - \frac{1}{J_p}\tilde{\mathbf{G}}_p^T\boldsymbol{\mathcal{U}}^{pT}\right]\boldsymbol{n}_R\,\mathrm{d}A_R = 0. \tag{41}$$

In order to use the arbitrary nature of the chosen curve $\tilde{S}$, we need to get back to configuration $\tilde{\kappa}_p$ via the area transformation formula $\boldsymbol{n}_R\,\mathrm{d}A_R = J_p\,\boldsymbol{\mathcal{U}}^{p-T}\,\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{A}$. Thus, Eq. (41) becomes

$$\int_{\tilde{S}}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{J_p}\boldsymbol{\mathcal{U}}^p\left(\tilde{\mathbf{G}}^T + \boldsymbol{\mathcal{R}}^{pT}\,\mathbf{G}_r^T\,\boldsymbol{\mathcal{R}}^p\right)\right) - (\mathrm{Curl}(f\boldsymbol{\mathcal{U}}^p)) - \frac{1}{J^p}\boldsymbol{\mathcal{U}}^p\tilde{\mathbf{G}}\right]^T J_p\,\boldsymbol{\mathcal{U}}^{p-1}\,\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a} = 0. \tag{42}$$

Note that the integrand is continuous and that Eq. (41) holds for any arbitrary surface S, plus f is considered to be continuously differentiable. Moreover, J_p is always positive and $\boldsymbol{\mathcal{U}}^p$ is an invertible, upper-triangular matrix with positive diagonal elements (hence, nonsingular). Thus, upon taking all these conditions into account, we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{J_p}\boldsymbol{\mathcal{U}}^p\tilde{\mathbf{G}}\right) + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{J_p}\boldsymbol{\mathcal{U}}^p\boldsymbol{\mathcal{R}}^{pT}\,\mathbf{G}_r\,\boldsymbol{\mathcal{R}}^p\right) = \mathrm{Curl}(f\,\boldsymbol{\mathcal{U}}^p) + \frac{1}{J_p}\boldsymbol{\mathcal{U}}^p\tilde{\mathbf{G}}_s \tag{43}$$

which is the evolution equation governing the geometrically necessary dislocation tensors $\tilde{\mathbf{G}}$ and $\mathbf{G}_r$.

Now, let us consider a special case where the body is subjected to a homogeneous rotation field, i.e., $\mathbf{G}_r = \mathbf{0}$. Under this condition, we now compute the left-hand side of Eq. (43). To do so, we require the material derivative of J_p and of the dislocation density tensor $\tilde{\mathbf{G}}$. Derivation of the material derivative of J_p is straightforward and, hence, it is stated here without proof, i.e.,

$$\frac{\mathrm{d}J_p}{\mathrm{d}t} = \det\left(\boldsymbol{\mathcal{U}}^p\right)\,\mathrm{tr}\left(\dot{\boldsymbol{\mathcal{U}}}^p\boldsymbol{\mathcal{U}}^{p-1}\right) = J_p\,\mathrm{tr}\left(\boldsymbol{\mathcal{L}}^p\right). \tag{44}$$

Now we derive the material derivative of dislocation density tensor $\tilde{\mathbf{G}}$ starting from its definition (27). The plastic velocity gradient $\boldsymbol{\mathcal{L}}^p$ is defined as $\boldsymbol{\mathcal{L}}^p := \dot{\boldsymbol{\mathcal{U}}}^p\boldsymbol{\mathcal{U}}^{p-1}$. In terms of the components of $\boldsymbol{\mathcal{U}}^p$, $\boldsymbol{\mathcal{L}}^p$ takes on the form

$$\mathcal{L}_{ij}^p = \begin{bmatrix} \dfrac{\dot{a}^p}{a^p} & \dfrac{a^p\dot{\gamma}^p}{b^p} & \dfrac{a^p}{c^p}\left(\dot{\beta}^p - \alpha^p\dot{\gamma}^p\right) \\ 0 & \dfrac{\dot{b}^p}{b^p} & \dfrac{b^p\dot{\alpha}^p}{c^p} \\ 0 & 0 & \dfrac{\dot{c}^p}{c^p} \end{bmatrix}. \tag{45}$$

Note that the operation 'Curl' is with respect to referential coordinates, and as such, the differentiation operators with respect to t and $\boldsymbol{X}$ can be interchanged. Hence, $\dot{\overline{\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)}} = \mathrm{Curl}(\dot{\boldsymbol{\mathcal{U}}}^p)$. Taking the time derivative of Eq. (27) while keeping $\boldsymbol{X}$ fixed therefore produces

$$\dot{\tilde{\boldsymbol{G}}} = -\mathrm{tr}\left(\boldsymbol{\mathcal{L}}^p\right)\ \tilde{\mathbf{G}} + \boldsymbol{\mathcal{L}}^p \tilde{\mathbf{G}} + \frac{1}{J_p} \boldsymbol{\mathcal{U}}^p\ \mathrm{Curl}\left(\boldsymbol{\mathcal{L}}^p \boldsymbol{\mathcal{U}}^p\right). \tag{46}$$

Equation (46)[1] follows from Eq. (44), while Eq. (46)[2,3] follows from the definition of $\boldsymbol{\mathcal{L}}^p$. Using Eqs. (6), (27) and (45), one can compute the material derivative of $\tilde{\mathbf{G}}$.

Substituting the above material derivative of $\tilde{\mathbf{G}}$ into Eq. (43), we obtain

$$J_p\left(\mathrm{Curl}\left(f\,\boldsymbol{\mathcal{U}}^p\right)\right) + \boldsymbol{\mathcal{U}}^p \tilde{\mathbf{G}}_s = -2\,\mathrm{tr}\left(\boldsymbol{\mathcal{L}}^p\right) \boldsymbol{\mathcal{U}}^p \tilde{\mathbf{G}} + \left(\boldsymbol{\mathcal{L}}^p \boldsymbol{\mathcal{U}}^p + \boldsymbol{\mathcal{U}}^p \boldsymbol{\mathcal{L}}^p\right)\tilde{\mathbf{G}} + \frac{1}{J_p} \boldsymbol{\mathcal{U}}^p \boldsymbol{\mathcal{U}}^p \mathrm{Curl}\left(\boldsymbol{\mathcal{L}}^p \boldsymbol{\mathcal{U}}^p\right) \tag{47}$$

for establishing the right-hand side of the evolution Eq. (43). Therefore, for a given $\boldsymbol{\mathcal{U}}^p$ and $\dot{\boldsymbol{\mathcal{U}}}^p$, one can compute the combined effect of incoming dislocation flux and internal dislocation source for any arbitrary surface. Computation of the dislocation flux is particularly important in, e.g., the development of a gradient based theory for plasticity where it is considered as one of its degrees of freedom.

7. Classification of dislocations

As mentioned earlier, the **QR** decomposition is particularly useful for a homogeneous rotation field[6] as one can, in theory, measure the components of $\boldsymbol{\mathcal{U}}^e$ (and thus, $\boldsymbol{\mathcal{U}}^p$) in that case. In this section, we show that for a homogeneous rotation field, with the aid of physical meaning of $\boldsymbol{\mathcal{U}}^p$, one can immediately classify the dislocations.

The dislocation density tensor $\tilde{\mathbf{G}}$ in configuration $\tilde{\kappa}_p$ can be expressed as

$$\tilde{\mathbf{G}} = \boldsymbol{l} \otimes \boldsymbol{b} \tag{48}$$

where $\boldsymbol{l}$ and $\boldsymbol{b}$ are vectors representing the dislocation line direction and the principal Burgers vector per unit area, respectively. When written in the Cartesian basis $\tilde{\mathbf{e}}_i$, components of $\tilde{\mathbf{G}}$ become

$$\tilde{G}_{IJ} = \begin{bmatrix} l_1 b_1 & l_1 b_2 & l_1 b_3 \\ l_2 b_1 & l_2 b_2 & l_2 b_3 \\ l_3 b_1 & l_3 b_2 & l_3 b_3 \end{bmatrix} \tag{49}$$

where l_i and b_i, $i = 1, 2, 3$, are the components of $\boldsymbol{l}$ and $\boldsymbol{b}$, respectively, expressed in basis $\tilde{\mathbf{e}}_i$. Based upon these two characterizing vector quantities, the dislocations found in a crystal are mainly classified into three categories.

7.1. Pure-edge dislocation

In a pure-edge dislocation, the line direction $\boldsymbol{l}$ and the principal Burgers vector $\boldsymbol{b}$ are perpendicular to each other. In other words, $\boldsymbol{b}$ acts parallel to the plane $\boldsymbol{l}^{\perp}$– plane with a normal along the line direction. Therefore, the condition imposed upon this dislocation line and principal Burgers vector is that

$$\boldsymbol{b} \cdot \boldsymbol{l} = 0 \implies l_1 b_1 + l_2 b_2 + l_3 b_3 = 0. \tag{50}$$

Consequently, Eq. (50) implies that for a pure-edge dislocation the trace of $\tilde{\mathbf{G}}$ must vanish. Because $\tilde{\mathbf{G}}$ is expressed in terms of plastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ through Eq. (33), the condition for a dislocation to be pure-edge takes on the form of

$$\frac{1}{J_p}\,\epsilon_{PQK}\,\mathcal{U}^{pi}_{K}\,\mathcal{U}^{pi}_{Q,P} = 0. \tag{51}$$

[6]Such cases appear whenever the deformation gradient is upper-triangular, e.g., a uniaxial or a biaxial tension.

Here $\boldsymbol{\mathcal{U}}^p$ is expressed in the Cartesian basis $\tilde{\mathbf{e}}_i$ and ϵ_{PQR} is the alternator with properties

$$\begin{aligned} \epsilon_{PQR} &= 0 && \text{when any two indices are repeated} \\ \epsilon_{PQR} &= +1 && \text{when } PQR = 123, 231, 312 \\ \epsilon_{PQR} &= 7-1 && \text{when } PQR = 132, 213, 321. \end{aligned} \tag{52}$$

When expressed in terms of components of $\boldsymbol{\mathcal{U}}^p$, Eq. (51) becomes

$$\begin{aligned} &\frac{1}{b^p c^p}\left((a^p\beta^p)_{,2} - (a^p\gamma^p)_{,3}\right) + \frac{\gamma^p}{b^p c^p}\left(a^p_{,3} - (a^p\beta^p)_{,1}\right) \\ &\quad + \frac{\beta^p}{b^p c^p}\left((a^p\gamma^p)_{,1} - a^p_{,2}\right) - \frac{1}{a^p c^p}\left(b^p\alpha^p\right)_{,1} + \frac{\alpha^p}{a^p c^p}\left(b^p_{,1}\right) = 0. \end{aligned} \tag{53}$$

Because the components of $\boldsymbol{\mathcal{U}}^p$ can be measured by performing experiments, one can readily identify if the dislocations present in a crystal are pure-edge by using Eq. (53).

7.2. Pure-screw dislocation

A pure screw dislocation is characterized by a line direction and principal Burgers vector that are parallel to one another, i.e., $\boldsymbol{b} = \boldsymbol{l}$. Thus, the Burgers vector $\boldsymbol{b}$ acts perpendicular to the slip plane $\boldsymbol{l}^{\perp}$. Now expressing $\tilde{\mathbf{G}}$ in terms of $\boldsymbol{l}$ and $\boldsymbol{b}$ through Eq. (48), one gets

$$\tilde{\mathbf{G}} = \begin{bmatrix} l_1^2 & l_1 l_2 & l_1 l_3 \\ l_2 l_1 & l_2^2 & l_2 l_3 \\ l_3 l_1 & l_3 l_2 & l_3^2 \end{bmatrix}. \tag{54}$$

Note that Eq. (54) renders $\tilde{\mathbf{G}}$ as being symmetric, therefore

$$\epsilon_{PQK}\left(\mathcal{U}^{pi}_K \mathcal{U}^{pj}_{Q,P} - \mathcal{U}^{pj}_K \mathcal{U}^{pi}_{Q,P}\right) = 0. \tag{55}$$

Characterization of pure-screw dislocations is slightly more complicated than that of pure-edge dislocations. In view of Eq. (54), a pure-screw dislocation is manifested by the following conditions.

- Because $\tilde{G}_{33} = 0$ for all deformations due to the upper-triangular nature of $\boldsymbol{\mathcal{U}}^p$, $l_3^2 = 0$ which in turn implies that $l_1 l_3 = l_3 l_1 = l_2 l_3 = l_3 l_2 = 0$. This leads to the following 4 conditions:

$$\frac{1}{b^p c^p}\left(c^p_{,2}\right) - \frac{\gamma^p}{b^p c^p}\left(c^p_{,1}\right) = 0 \tag{56a}$$

$$-\frac{1}{a^p b^p}\left((a^p\gamma^p)_{,1} - a^p_{,2}\right) = 0 \tag{56b}$$

$$c^p_{,1} = 0 \tag{56c}$$

$$b^p_{,1} = 0 \tag{56d}$$

- Recalling that $\tilde{\mathbf{G}}$ is symmetric, and the only remaining off-diagonal terms in $\tilde{\mathbf{G}}$ are $\tilde{G}_{12}$ and $\tilde{G}_{21}$, consequently

$$\begin{aligned} \tilde{G}_{12} = \tilde{G}_{21} \implies &\frac{1}{b^p c^p}\left((b^p\alpha^p)_{,2} - b^p_{,3}\right) - \frac{\gamma^p}{b^p c^p}\left(b^p\alpha^p\right)_{,1} \\ &+ \frac{\beta^p}{b^p c^p}\left(b^p_{,1}\right) - \frac{1}{a^p c^p}\left(a^p_{,3} - (a^p\beta^p)_{,1}\right) - \frac{\alpha^p}{a^p c^p}\left((a^p\gamma^p)_{,1} - a^p_{,2}\right) = 0 \end{aligned} \tag{56e}$$

- The final condition for a dislocation to be pure screw comes from the structure of $\tilde{\mathbf{G}}$ itself. It is evident from Eq. (54) that $\tilde{G}_{11}\tilde{G}_{22} = \tilde{G}_{12}\tilde{G}_{21}$, hence,

$$\begin{aligned}&\left[\left((a^p\beta^p)_{,2} - (a^p\gamma^p)_{,3}\right) + \gamma^p\left(a^p_{,3} - (a^p\beta^p)_{,1}\right) + \beta^p\left((a^p\gamma^p)_{,1} - a^p_{,2}\right)\right]\\ &\quad\times\left[-(b^p\alpha^p)_{,1} + \alpha^p b^p_{,1}\right] = \left[((b^p\alpha^p)_{,2} - (b^p)_{,3}) - \gamma^p\left(b^p\alpha^p\right)_{,1} + \beta^p\left(b^p\right)_{,1}\right]\\ &\quad\times\left[\left((a^p)_{,3} - (a^p\beta^p)_{,1}\right) + \alpha^p\left((a^p\gamma^p)_{,1} - (a^p)_{,2}\right)\right]\end{aligned} \tag{56f}$$

Using Eqs. (56a)–(56f), one can readily realize if the dislocations present in a crystal lattice are pure-screw in nature. Note that for a dislocation to be pure-screw, all six of the above equations must be satisfied.

7.3. Mixed dislocations

Dislocations in which the line direction and the principal Burgers vector are neither perpendicular nor parallel are called mixed dislocations. This kind of dislocation possesses features of both pure-edge and pure-screw dislocations and, therefore, it is possible to decompose the dislocation density tensor for mixed dislocations into those representing pure-edge dislocations and those representing pure-screw dislocations.

Vectors $\boldsymbol{l}$ and $\boldsymbol{b}$ denote the line direction and principal Burgers vector and the angle between them φ is established via $\boldsymbol{l}\cdot\boldsymbol{b} = \cos\varphi$. The conditions $\varphi = 0$ and $\varphi = \frac{\pi}{2}$ represent pure-screw and pure-edge dislocations, respectively. One can decompose the principal Burgers vector $\boldsymbol{b}$ into components $\boldsymbol{b}^{\parallel}$ and $\boldsymbol{b}^{\perp}$ such that $\boldsymbol{b}^{\parallel} = \delta\boldsymbol{l}$ and $\boldsymbol{b}^{\perp}\cdot\boldsymbol{l} = 0$. Using the projection operator of $\boldsymbol{b}$ onto $\boldsymbol{l}$, we find $\delta = \boldsymbol{l}\cdot\boldsymbol{b}$, and as such

$$\boldsymbol{b}^{\parallel} = (\boldsymbol{l}\cdot\boldsymbol{b})\, l; \quad \boldsymbol{b}^{\perp} = \boldsymbol{b} - (\boldsymbol{l}\cdot\boldsymbol{b})\,\boldsymbol{l}. \tag{57}$$

One can additively decompose the dislocation density tensor $\tilde{\mathbf{G}}$ into edge $\tilde{\mathbf{G}}_e$ and screw $\tilde{\mathbf{G}}_s$ tensors representing their pure-edge and pure-screw dislocations so that

$$\tilde{\mathbf{G}} = \tilde{\mathbf{G}}_e + \tilde{\mathbf{G}}_s. \tag{58}$$

The pure-edge and pure-screw components of the dislocation density tensor are therefore given as

$$\tilde{\mathbf{G}}_s = (\boldsymbol{l}\cdot\boldsymbol{b})\,(\boldsymbol{l}\otimes\boldsymbol{l}) \quad \text{and} \quad \tilde{\mathbf{G}}_e = \boldsymbol{l}\otimes\boldsymbol{b}^{\perp} = (\boldsymbol{l}\otimes\boldsymbol{b}) - (\boldsymbol{l}\cdot\boldsymbol{b})\,(\boldsymbol{l}\otimes\boldsymbol{l}) \tag{59}$$

recalling that $\mathrm{tr}(\tilde{\mathbf{G}}_e) = \boldsymbol{l}\cdot\boldsymbol{b}^{\perp} = 0$.

7.4. Examples of pure-edge and pure-screw dislocations: strict plane strain and strict anti-plane shear

Cermelli and Gurtin [9] showed that the dislocation density tensors for strict plane strain and strict anti-plane shear represent pure-edge and pure-screw dislocations, respectively. In this section, we reproduce these deformations in our framework ignoring the contribution from $\mathbf{G}_r$ and show that dislocations for these deformations satisfy the conditions mentioned earlier and, thus, provide an example for pure-edge and pure-screw dislocations. The term 'strict' implies that Laplace stretch $\boldsymbol{\mathcal{U}}$ and its plastic part $\boldsymbol{\mathcal{U}}^p$ have the same form for these deformations.

Strict plane strain. For a strict plane-strain deformation, if the deformation takes place in the X_1X_2 plane, then the plastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ becomes

$$\boldsymbol{\mathcal{U}}^p = \begin{bmatrix} a^p & a^p\gamma^p & 0\\ 0 & b^p & 0\\ 0 & 0 & 1\end{bmatrix} \tag{60}$$

with a restriction that a^p, γ^p and b^p do not vary with the out-of-plane direction X_3. The form of $\boldsymbol{\mathcal{U}}^p$ along with the restriction on variation of a^p, b^p and γ^p make the diagonal terms of $\tilde{\mathbf{G}}$ given in Eq. (28)

identically zero and, hence, it ensures that Eq. (53) is automatically satisfied. Thus, the finding of Cermelli and Gurtin [9] is corroborated. In fact, Eq. (53) is a more general and simpler representation of pure-edge dislocations.

Strict anti-plane shear. For an anti-plane shear, we choose a displacement $u = u(X_2, X_3)$ to be along the X_1 direction such that

$$x_1 = X_1 + u(X_2, X_3), \quad x_2 = X_2, \quad x_3 = X_3 \tag{61}$$

Herein the chosen plane of shear is different from that used by Cermelli and Gurtin [9]. The reason for choosing a displacement u to be in the X_1 direction is for computational simplicity. The chosen deformation map produces an upper-triangular deformation gradient $\mathbf{F}$. Hence, this deformation gradient is the same as Laplace stretch $\boldsymbol{\mathcal{U}}$ and the rotation tensor $\boldsymbol{\mathcal{R}}$ is an identity tensor. For a strict anti-plane shear, the plastic part of Laplace stretch takes the form

$$\boldsymbol{\mathcal{U}}^p = \begin{bmatrix} 1 & \gamma^p & \beta^p \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{62}$$

When the total Laplace stretch, consisting of both elastic and plastic parts, is considered the off-diagonal elements of Laplace stretch are given as $\gamma = \partial u(X_2, X_3)/\partial X_2$ and $\beta = \partial u(X_2, X_3)/\partial X_3$[7] (cf. Barber [3]). The only nonzero element in the dislocation density tensor calculated from Eq. (62) is $\tilde{\mathbf{G}}_{11}$. Vanishing of all other elements of $\tilde{\mathbf{G}}$ ensures that Eqs. (56a)–(56f) are identically satisfied and, hence, this $\tilde{\mathbf{G}}$ tensor represents pure-screw dislocations. Note that even though anti-plane shear represents pure-screw dislocations, this deformation is too restrictive to use as the general representation for a dislocation density tensor for pure-screw dislocations.

8. Significance of the derived dislocation density tensor

Dislocation density tensors found in the literature are constructed using a traditional Kröner–Lee decomposition of the deformation gradient, and involve its elastic or plastic parts, their spatial derivatives and, in some cases, the rotation tensor $\mathbf{R}^e$ arising from a polar decomposition of $\mathbf{F}^e$. A detailed account of these dislocation density tensors is provided in Acharya and Bassani (2000) [2] and Cermelli and Gurtin (2001) [9]. Although these geometric dislocation tensors are extensively used, their definitions are often questionable. In fact, the disagreements over an appropriate definition produced this myriad of geometric dislocation tensors. The dislocation density tensor $\tilde{\mathbf{G}}$ derived herein overcomes some of these disagreements, and hence, we believe will be more useful. Some of these utilities are mentioned below.

- It is widely accepted that Kröner–Lee decomposition, the foundation of the previously defined dislocation density tensors, is not unique [8,22], at least at the kinematic level. Naghdi [39] also mentioned that the existence of such a decomposition is somewhat dubious. Because the dislocations are measured at the kinematic level, this issue of a non-unique intermediate configuration is prevalent. This problem, however, is easily resolved in the case of an elastic–plastic decomposition of Laplace stretch. The uniqueness of this decomposition is attributed to the fact that the set of upper-triangular matrices with positive determinant is closed under multiplication [17]. Therefore, a dislocation density tensor $\tilde{\mathbf{G}}$, built upon this decomposition, is free from such non-uniqueness issues.
- Components of the plastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ are physically meaningful. An experimentalist can, in principle, directly and unambiguously measure all of its components in the $\tilde{\kappa}_p$ configuration of a body, at least, for a homogeneous rotation field. It is in this configuration that our geometric dislocation density tensor $\tilde{\mathbf{G}}_p$ is measured. Therefore, the derived dislocation density tensor is physically meaningful and finds its utility in the context of experiments. In comparison, because

[7] Note that in this case, elongation along the 1 direction is $a = 1$.

the plastic deformation gradient $\mathbf{F}^p$ is not compatible, $\mathbf{F}^p$ cannot be expressed as the gradient of a deformation map, unlike the total deformation gradient $\mathbf{F}$. In other words, it is not possible to define a deformation map between the undeformed and intermediate configurations. On the other hand, the components of plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$ denote a specific deformation of the body (e.g., a^p denotes the elongation along the X_1 direction) in a particular coordinate system. Thus, classifying dislocations using this decomposition has an inherent advantage over that using the measures of GND's found in literature, at least from the continuum kinematics point of view. Moreover, the upper-triangular nature of Laplace stretch eliminates complications regarding computation of $\tilde{\mathbf{G}}$. Even though it is possible to derive a simpler balance law for geometric dislocations (e.g., the one derived by Cermelli and Gurtin [9]), the balance law derived in Sect. 6 is much more precise and reasonable.

- With the help of the derived dislocation density tensor, one has a means to readily characterize the different types of dislocations, at least for a homogeneous rotation field. Because it is possible to measure the components of $\boldsymbol{\mathcal{U}}^p$ directly from experiments, one can plug these measured components into Eqs. (53) and (56a)–(56f) to check if the dislocations present in a crystal are pure-edge, pure-screw or a mixture thereof, wherefore the dislocation density tensor becomes decomposed into pure-edge and pure-screw components according to Eq. (58). In this way, characterization of dislocations is much simpler.

9. Summary

In this article, the geometrically necessary dislocation density tensor and Burgers vector are studied using an elastic–plastic decomposition of Laplace stretch $\boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p$ arising from a Gram-Schmidt factorization of the deformation gradient $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}$. The derived dislocation density tensor has the form of $\tilde{\mathbf{G}} = J_p^{-1}\,\boldsymbol{\mathcal{U}}^p\,\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)$. The term $\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)$ is related the to torsion of configuration $\tilde{\kappa_p}$, where deformation of the body is caused solely by the movement of dislocations. Thus, it provides a measure for incompatibility in the plastic deformation of that configuration. This incompatibility prevents space $\tilde{\kappa}_p$ from being Euclidean, and vanishes only when $\tilde{\mathbf{G}}$ becomes zero. The dislocation density tensor has also been derived in terms of the elastic components of Laplace stretch and the associated rotation tensor. When the dislocation tensor is measured in configuration κ_p, it can be decomposed into two physically meaningful components: a dislocation tensor due to an incompatibility of plastic rotation, and a dislocation tensor due to a plastic 'straining' of the crystal lattice. An evolution equation for $\tilde{\mathbf{G}}$ in the form of a balance law for geometrically necessary dislocations has been derived. We also developed conditions for different types of dislocations in terms of $\boldsymbol{\mathcal{U}}^p$. Finally, the significance of the obtained dislocation density tensor is discussed.

In view of the physical meanings associated with the components of $\boldsymbol{\mathcal{U}}^p$, the derived quantities are particularly important, and are expected to be very useful in the development of new theories for plasticity; in particular, for strain-gradient and size-dependent theories of plasticity.

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(Received: December 24, 2019; revised: August 20, 2020; accepted: October 20, 2020)