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# Nonlinear continuum dislocation theory revisited

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ABSTRACT

The present paper provides the definition of resultant Burgers' vector and the related dislocation density tensor in terms of the plastic deformation, regarded as that creating dislocations without deforming the crystal lattice. Based on this kinematics the thermodynamic framework of the finite strain continuum dislocation theory is developed. The proposed theory is then applied to the problem of antiplane constrained shear admitting an analytical solution.



## 1. Introduction

In view of a huge number of dislocations appearing in plastically deformed crystals (which typically lies in the range $10^8 \div 10^{15}$ dislocations per square meter) the necessity of developing the continuum dislocation theory (CDT) to describe the evolution of dislocation network in terms of mechanical and thermal loading conditions becomes clear to all researchers in crystal plasticity. However, the development of such a theory requires two questions to be clarified: (i) what are kinematically independent and dependent quantities characterizing the deformed state of crystals with dislocations and the rate of change of the dislocation network, (ii) how to specify energy and dissipation as functions of these kinematic quantities.

Among the above two questions the first one is the most crucial. To be able to answer it let us analyze the dislocation density tensor which is the key kinematic quantity in CDT. Tracing back the whole literature on finite strain CDT (Kondo, 1952; Bilby et al., 1955, 1957; Kröner, 1958, 1960; Berdichevsky, 2006a, 1967; Naghdi and Srinivasa, 1993; Le and Stumpf, 1996a,b,c; Ortiz and Repetto, 1999; Ortiz et al., 2000; Cermelli and Gurtin, 2001; Acharya and Bassani, 2001; Gurtin, 2006; Clayton et al., 2006; Yavari and Goriely, 2012) we could not find the commonly accepted and convincing definition of this quantity. The majority of past and contemporary authors (see, e.g. Le and Stumpf, 1996b; Acharya and Bassani, 2001; Yavari and Goriely, 2012), following the original idea of Kondo (1952) and Bilby et al. (1955), adopted the following definition of the resultant Burgers vector

$$\mathbf{b}_r = \mathbf{F}^e \cdot \oint_c \mathbf{F}^{e-1} \cdot d\mathbf{y}, \tag{1}$$

with $\mathbf{F}^e$ being the elastic deformation and $c$ any close and piecewise smooth contour in the current configuration along which the integral is taken. As we will see later, the vector defined in this way is related to, but does not represent the true closure failure in dislocated crystals induced by the macroscopic plastic deformation. Ortiz and Repetto (1999) defined the resultant Burgers vector in a completely different way

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[1] This paper is dedicated to the memory of Huy Duong Bui who was my mentor.

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$$\mathbf{b}_r = \oint_{\mathcal{C}} \mathbf{F}^p \cdot d\mathbf{x}, \tag{2}$$

with $\mathbf{F}^p$ being the plastic deformation and $\mathcal{C}$ any close and piecewise smooth contour in the reference configuration along which the integral is taken. Formula (2) turns out to be valid for single crystals having one active slip system. However, it will be shown that (2) is not invariant with respect to an arbitrary superimposed uniform plastic deformation which does not produce additional dislocations inside the crystal. Cermelli and Gurtin (2001) formulated three requirements which must be fulfilled by the true Burgers vector (see also Gurtin (2006) as well as the discussions of that paper in Acharya (2008) and Ozakin and Yavari (2013)). Their first and most important requirement was that the true Burgers vector should measure the local closure failure per unit area of the so-called "intermediate" or relaxed configuration. Cermelli–Gurtin's first requirement seems quite questionable due to the following reason: the inverse "elastic" deformation, based on Kröner's "thought experiment" of cutting the representative volume element and releasing dislocations to the boundary to have the stress- and dislocation-free crystal, is not elastic because it moves dislocations to the boundary and changes the dislocation content inside the specimen. Thus, the concept of "intermediate" configuration originating from Kröner's thought experiment is misleading and consequently Cermelli–Gurtin's first requirement is open to doubt. Berdichevsky (2006a) introduced the proper measure of the resultant closure failure leading to the dislocation density tensor

$$\mathbf{T} = -\mathbf{F}^{p-1} \cdot (\mathbf{F}^p \times \nabla). \tag{3}$$

Unfortunately, he did not provide arguments or examples of the macroscopic plastic deformation[2] supporting formula (3). The example of crystal with one dislocation, traditionally considered in the physics of dislocations when its Burgers vector is defined (Hirth and Lothe, 1982; Nabarro, 1967; Friedel, 1964; Weertman and Weertman, 1966), does not shed light on the definition of resultant Burgers vector for macroscopic plastic deformation as the deformation creating a large number of dislocations.

The aim of this paper is twofold. First, we want to critically examine the kinematics of finite elastoplastic deformation based on the multiplicative resolution of the deformation gradient into its elastic and plastic parts (Bilby et al., 1957). Attributing the active role to the plastic deformation as that creating dislocations without deforming the crystal lattice, we will show how the closure failure arises naturally from inhomogeneous macroscopic plastic deformation having a large number of dislocations. Then, the resultant Burgers vector must be defined in such a way that it is invariant with respect to a superimposed homogeneous plastic deformation which does not create additional dislocations inside the volume element of the crystal. With this firmly established kinematics of finite elastoplastic deformation, the whole machinery of small strain CDT which is well understood (Nye, 1953; Bilby, 1955; Kröner, 1955, 1992; Gurtin, 2002; Berdichevsky, 2006a,b; Berdichevsky and Le, 2007; Kochmann and Le, 2008a,b, 2009; Le and Sembiring, 2008a,b, 2009; Kaluza and Le, 2011; Le and Nguyen, 2010, 2012, 2013) can be extended to the finite strain CDT, which is done in the second part of this paper. We then illustrate the application of the theory to the problem of finite antiplane constrained shear which admits an exact analytical solution in terms of the elliptic functions.

The paper is organized as follows. After this short introduction we develop in Section 2 the kinematics of finite elastoplastic deformation. Section 3 represents the thermodynamic framework of the nonlinear CDT. Sections 4 and 5 are devoted to the problem of antiplane constrained shear. Finally, Section 6 concludes the paper.

## 2. Kinematics

One of the fundamental, and at the same time most difficult, feature of plastic deformation is that Cauchy–Born's rule is not applicable to it even for small strains. To clarify this matter let us consider the resolution of the deformation gradient $\mathbf{F} = \partial\mathbf{y}/\partial\mathbf{x}$ into elastic and plastic parts

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p. \tag{4}$$

In general, the elastic and plastic deformations $\mathbf{F}^e$ and $\mathbf{F}^p$ cannot be gradients of global maps (they are therefore called incompatible). Nevertheless, we may suppose that they are orientation preserving so that

$$J_p = \det \mathbf{F}^p > 0, \quad J_e = \det \mathbf{F}^e > 0.$$

This means, $\mathbf{F}^p$ and $\mathbf{F}^e$ have inverse deformations, denoted correspondingly by $\mathbf{F}^{p-1}$ and $\mathbf{F}^{e-1}$. The resolution (4) was first introduced by Bilby et al. (1957) as a basic assumption to develop the kinematics of elastoplastic bodies with continuously distributed dislocations. In that paper $\mathbf{F}, \mathbf{F}^e$, and $\mathbf{F}^p$ are called the shape deformation, the lattice deformation, and the dislocation deformation, respectively. We keep close to the point of view of Bilby et al. (1957) by attributing an active role to the plastic deformation: $\mathbf{F}^p$ is the deformation *creating* dislocations (either inside or at the boundary of the volume element) or *changing* their positions in the crystal without deforming the crystal lattice. In contrary, the elastic deformation $\mathbf{F}^e$ deforms the crystal lattice having *frozen* dislocations. Note that this physical interpretation differs essentially from that of Kröner (1958), who introduced first the inverse elastic deformation $\mathbf{F}^{e-1}$ as the deformation *releasing* all dislocations in the current state to

[2] This critisism applies to all the above cited papers.