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Slip-induced conservation laws for dislocation structures in the finite kinematic framework

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ABSTRACT

In the present paper we develop a general framework that captures topological, geometric, and energetic aspects of slip surfaces to provide conservation laws for dislocation structures. In this work, dislocations act as the boundary of active slip regions that support a finite displacement jump, while treating the material outside the slip regions with a continuum mechanic framework in the setting of large deformations. Within this semicontinuous description, it is shown that the condition of slip imposes an important restriction on the shape of the slip surfaces regardless of the material structure. This catalog of shapes for the slip surfaces can be further restricted for crystalline materials, providing a simple geometric description of common dislocation processes such as cross slip or dislocation loop glide. In this setting, the classical Kirchhoff-type rule for the conservation of the Burgers vector emanates directly from the formulation, while recent conservation laws designed for partial dislocations in face centered cubic crystals are also naturally captured.

1. Introduction

Dislocations are responsible for plastic slip in crystalline materials and have been the subject of many studies. From a theoretical and mathematical perspective, dislocations have been considered as discrete or isolated entities in linear (Volterra, 1907; Hirth and Lothe, 1982; Bacon et al., 1980) and nonlinear (Zubov, 1997) elastic bodies, as well as forming continuous distributions of defects (Nye, 1953; Bilby et al., 1955; Kroner, 1990; Puntigam and Soleng, 1997; Kleman and Friedel, 2008; Yavari and Goriely, 2012). The transition between both descriptions, discrete and continuous, has also been realized within the framework of calculus of variations (Ariza and Ortiz, 2005; Garroni et al., 2010; Scardia and Zeppieri). In terms of numerical methods, great advances have been made regarding both the atomistic scale (Yamakov et al., 2011; Chang et al., 2002; Zhou et al., 1998) and the continuum representation (Dao et al., 2007), each with their own set of time and length scale limitations. A successful intermediate approach germinated in the late 1980s with the development of dislocation dynamics (DD) simulations (Kubin et al., 1992). DD is based on the discretization of arbitrary dislocation networks into a finite collection of discrete segments embedded in a liner elastic medium. Segments interact according to the laws of elasticity and use atomistic input to define dislocation-core-based properties.

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The topology of a discrete set of dislocation segments can be described by enforcing the conservation of the Burgers vector at dislocation nodes (Hirth and Lothe, 1982). As well, more complex crystallographic defects can be tracked by recourse to additional conservation rules, such as partial dislocations in face centered cubic metals within DD (Martínez et al., 2008). These *Kirchhoff*-type laws allow for an efficient and self-consistent treatment of relatively complex line topologies, enabling large-scale simulations of dislocation ensembles. The goal of the present work is to provide a general framework for the study of conservation laws in dislocation networks, differentiating between topological, geometric and energetic conditions.

In this work, we describe line defects by two of their most general features: (i) they are boundaries of surfaces of displacement discontinuity, (ii) the surfaces leave, after deformation, a material with equivalent elastic behavior.[1] These two properties are material independent and suffice to determine, by means of the mathematical formalism of Reina and Conti (2014), that slip surfaces are necessarily orientable and that their geometry is highly constrained. These topological and geometric features of slip surfaces will then enable us to define general conservation laws in dislocation ensembles, to recover the well-known conservation of the Burgers vector and set the limits of applicability of the recently formulated Kirchhoff-type law for partial dislocations (Martínez et al., 2008). Furthermore, we will show that the two premises used as starting point deliver the six elementary distortions defined by Volterra without any necessary assumptions on the smoothness of the associated deformations.

The paper is organized as follows. We begin in Section 2 by discussing two commonly used definitions of dislocations and introducing the definition that is used in this work. Next, in Section 3, we review the ingredients of the mathematical formalism of Reina and Conti (2014) needed for this paper, and derive important topological and geometric properties of slip surfaces. These properties of slip surfaces are then translated in Section 4 into general conservation laws in dislocation ensembles. We finalize in Section 5 with the conclusions.

2. Dislocations as linear defects

The precise definition of a dislocation is not universal and depends on the type of material considered (Cermelli, 1999). Two common definitions of dislocations emanate from kinematic (Volterra dislocations Volterra, 1907) and topological (Mermin, 1979; Kleman and Friedel, 2008) considerations. In what follows, we touch on the most important aspects of these definitions and proceed to describe the definition that will be used in the remainder of the paper.

2.1. Volterra dislocation

In solid continuum mechanics, dislocations are commonly viewed as the boundary of a cut surface in a translational Volterra process (Volterra, 1907), cf. Fig. 1. These consist on cutting the body along a reference surface and displacing the two lips of the cut with respect to each other with a constant rigid translation. If such process results in an interpenetration of matter, then the extra matter is removed. Conversely, if a void results from the rigid body motion, material is added to fill it. The two lips are then glued together and the material is allowed to relax elastically.

This characterization of dislocations goes back to the mathematical analyses of elasticity in multiply connected bodies (Volterra, 1907; Weingarten, 1901), which were performed before dislocations were observed experimentally or even associated to plastic distortions in materials. Particularly, the displacement field in multiply connected elastic bodies subjected to prescribed boundary conditions, cannot be uniquely determined from the boundary data. To render it unique, it is necessary to provide six constants per cut necessary to transform the domain into a simply connected one. Each of these six constants precisely corresponds to the six elementary distortions represented in Fig. 1.

2.2. Dislocations as topological defects in crystalline materials

For the purpose of the discussion we look at the material in terms of the atoms that form it and the connectivities between them. With this considerations in mind, an elastic distortion leaves the topology (connectivities) invariant. However, if dislocations appear in the body during the deformation process, topological changes occur that can be characterized by recourse to the so-called Burgers circuit.

Consider a close atomic path in the deformed configuration that encloses a dislocation, c.f. Fig. 2. Starting from an arbitrary atom in this path, one can follow identical connectivities in a reference perfect crystal. Such operations are possible, since far away from the dislocation, the structure is locally identical to a perfect crystal from a topological perspective. Performing this operation to the entire closed loop results into an open circuit in the reference configuration. The path required to close it quantized in terms of atomic connections (*topological Burgers vector*) is independent of the initial closed circuit as long as the same dislocation is enclosed.[2] As a result, the (topological) Burgers vector is often an attribute that is used to characterize the linear defect. However, it is important to point out that, from this topological

[1] In the case of partial dislocations, a surface defect remains the slip surface (stacking fault), with an associated energy per unit area. Its effect on the volumetric elastic behavior is typically small and will be neglected in this work.

[2] To illustrate this, it suffices to add any small loop in a perfect region of the ordered structure. Due to the fact that such region is isomorphic to the dislocation-free material it will not affect the closing path.