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On the accessibility of the disclination tensor from spatially mapped orientation data

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ABSTRACT

Disclinations, defects that accommodate rotational incompatibilities in a crystal lattice, have been described in detail in the literature, but rarely observed in solid materials. Recently, a method has been described by which it is proposed that disclination densities can be estimated using spatially resolved orientation data generated from electron backscatter diffraction or precession electron diffraction. Herein, a rigorous evaluation of this approach is performed. In this work, a series of constructed and real data sets are used to evaluate the methodology for estimating disclination densities from spatially mapped orientation data and demonstrate the inherent error associated with this approach. It is shown that the outcome of this analysis is heavily dependent on the how numerical approximations are implemented. If a self-consistent method is used, then the disclination tensor will always be zero and if an inconsistent method is used then the error in the estimation of the disclination tensor is unbounded. Therefore, although the theory behind the disclination tensor is sound, the inputs needed to calculate it are not experimentally accessible through the application of numerical approximation methods to orientation maps and a different methodology is needed.

1. Introduction

1.1. Structure of disclinations

Disclinations are constructs that are used to describe rotational incompatibilities in the crystal lattice [1]. They are defined in terms of a relative rotation vector known as a Frank vector that describes the rotation of the lattice due to the presence of a disclination. This is analogous to the Burgers vector, which describes the translation of the lattice due to the presence of a dislocation. Two categories of disclinations exist: wedge disclinations, which have line directions parallel to their axis of rotation, and twist disclinations, which have line directions perpendicular to their axis of rotation [1–4]. Additionally, crystal disclinations can be divided into two types, perfect disclinations, which preserve the rotational symmetries of the lattice outside the disclination core, and partial disclinations, which do not [4]. Perfect disclinations are argued to not exist in bulk crystals due to the prohibitively high energy associated with them, a consequence of the large required Frank vector [4,5]. Partial disclinations, on the other hand, can exist in a bulk crystals and may play a role in plastic deformation but they must lie on the edge line of a planar defect that compensates for the disruption of rotational symmetry [1,4]. The topological nature of both perfect and partial disclinations have been described in detail [1,4,6]. Kroner and Anthony [4] detail how Frank circuits can be used to measure the Frank vector and line direction of a disclination analogously to how Burgers circuits are used to characterize dislocations.

Partial disclinations can theoretically exist either in a grain matrix at the edge line of a subgrain boundary or inside of a grain boundary or triple junction. Models have been developed to describe grain boundary structures in terms of disclination dipoles rather than dislocation structural units [7–9] and to describe how changes in grain boundaries occur during plastic deformation [10]. Several studies have reported structures that could be described as disclinations in heavily deformed metal samples examined using transmission electron microscopy (TEM) [11–14]. Three approaches have been used to attempt to characterize disclinations in TEM: direct observation of lattice plane curvature using high resolution

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TEM [11], Frank circuit construction at triple junctions and terminating subgrain boundaries [14], and bend extinction contour measurements [12,13]. The latter two techniques rely on the assumption that there is excess lattice curvature beyond what can be accommodated by the GND densities present that can be attributed to the presence of disclinations, but, since they are applied in heavily dislocated regions, it is almost impossible to determine without uncertainty. The former technique of direct atomic resolution imaging has been used to observe structures that could be described as disclinations inside of iron grains that have undergone severe plastic deformation [11]. In that case, a periodic array of dislocations was observed that resulted in a discontinuity in the rotation of the lattice, as shown schematically in Fig. 1a&b. It is important to note that this structure could be described either as a single partial wedge dislocation or as an array of geometrically necessary dislocations terminating inside the crystal lattice. The equivalency of such structures has been discussed in the literature [15,16]. At the continuum level, the disclination description can be more convenient because it reduces the system to being fully described by a single defect. At the atomistic level, however, describing the structure as an array of dislocations provides a more direct description of the phenomenon.

Partial disclinations have also been reported to occur in five-fold twin configurations in FCC metal nanostructures [1,17,18]. There is a 7.35° incompatibility in a five-fold twin structure due to the 70.53° angle between {111} planes in the FCC structure, as shown in Fig. 1c. It has been hypothesized that the extra rotation to close this gap is achieved through the presence of a positive wedge disclination with a 7.35° Frank vector lying on the shared axis of the twins. Experimental measurements of the strain and rotation fields of a five-fold twinned gold nanoparticle performed via analysis of atomic resolution TEM images showed that small elastic shear strains account for some of the missing rotation by altering the crystal lattice such that there is an additional 0.60° between {111} planes, while the rest is accommodated by a uniform elastic rotation of 4.3° across the entire structure that is indicative of a disclination (see Fig. 7c) [19], as shown schematically in Fig. 1d. Unlike disclinations observed in the matrix, disclinations residing in boundaries cannot be adequately described using only dislocations as there is a uniform elastic rotation about the boundary in which the disclination exists that cannot otherwise be explained. This method works well for measuring the effects of an isolated disclination in a nanostructured material, but is difficult and labor-intensive to apply experimentally (e.g. using atomic resolution TEM).

Disclinations are typically excluded from conventional, dislocation-based elasto-plastic continuum theory of deformation. By including the possibility of the presence of rotational incompatibilities described by disclinations, a more complete description of plastic deformation can be achieved [4,15]. This expanded continuum defect theory, often referred to as disclination theory, (although it includes descriptions of both dislocations and disclinations) is well described in the literature [4,6,15,20–24] extending other work [25,26]. There are a variety of ways to describe disclinations in continuum defect theory, depending on the point of view: a continuous distribution of defects, discrete defect lines, a continuous distribution of infinitesimal defect loops, and the so-called dislocation model of discrete disclinations [15]. This last approach details how a discrete disclination line can be equivalently described as a discrete dislocation line in the same place bounding a uniform distribution of dislocations along a surface (see Fig. 1b).

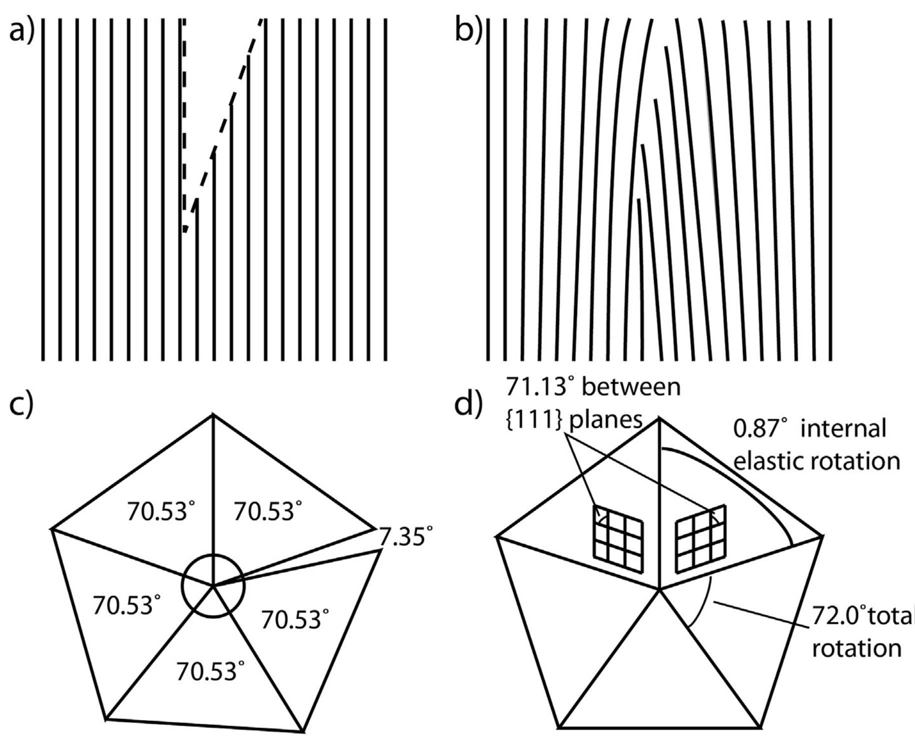

Fig. 1. a & b) schematic representation of a partial wedge disclination in the interior of a crystal lattice, where the lines represent the lattice planes. If the wedge of material missing from a) is accommodated by local rotations in the adjacent lattice planes in order to maintain compatibility, this results in a series of evenly spaced dislocations, as shown in b). The terminus of these dislocations can be described as a partial wedge disclination with a line direction perpendicular to the schematic [11]. C) Closure failure of FCC five-fold twin structure. D) Schematic showing how the presence of a partial wedge disclination at the center of the structure, combined with elastic shear strain in the lattice, results in the closure of the structure shown in C), as described in Ref. [19].