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Finite element approximation of the fields of bulk and interfacial line defects

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ABSTRACT

A generalized disclination (g.disclination) theory (Acharya and Fressengeas, 2015) has been recently introduced that goes beyond treating standard translational and rotational Volterra defects in a continuously distributed defects approach; it is capable of treating the kinematics and dynamics of terminating lines of elastic strain and rotation discontinuities. In this work, a numerical method is developed to solve for the stress and distortion fields of g.disclination systems. Problems of small and finite deformation theory are considered. The fields of a single disclination, a single dislocation treated as a disclination dipole, a tilt grain boundary, a misfitting grain boundary with disconnections, a through twin boundary, a terminating twin boundary, a through grain boundary, a star disclination/penta-twin, a disclination loop (with twist and wedge segments), and a plate, a lenticular, and a needle inclusion are approximated. It is demonstrated that while the far-field topological identity of a dislocation of appropriate strength and a disclination-dipole plus a slip dislocation comprising a disconnection are the same, the latter microstructure is energetically favorable. This underscores the complementary importance of *all* of topology, geometry, and energetics in understanding defect mechanics. It is established that finite element approximations of fields of interfacial and bulk line defects can be achieved in a systematic and routine manner, thus contributing to the study of intricate defect microstructures in the scientific understanding and predictive design of materials. Our work also represents one systematic way of studying the interaction of (g.)disclinations and dislocations as topological defects, a subject of considerable subtlety and conceptual importance (Aharoni et al., 2017; Mermin, 1979).

1. Introduction

In the context of continuum mechanics, the distortion measure is similar to a deformation or a displacement gradient, except such a measure is not the gradient of a vector field in many situations involving material defects. Such a situation arises when the distortion represents, through a non-singular field, the 'gradient' of a field that contains a terminating discontinuity on a surface. If the discontinuity is in the displacement field, the terminating curve is called a dislocation; if the discontinuity is in the rotation field, the terminating curve is called a disclination. In some cases, the discontinuity can arise in the strain field as well, as for instance in the solid-to-solid phase transformation between austenite and

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martensite. In Acharya and Fressengeas (2012, 2015), the concept of the disclination is extended to the generalized disclination (g.disclination) to deal with general distortion-discontinuity problems. The g.disclination can be thought of as a discontinuity (along a curve or loop) of a distortion discontinuity (along a surface).

The strain and stress fields of dislocations and disclinations in a linear elastic isotropic body have been studied in Nabarro (1985), Nabarro (1967) and DeWit (1973a). Classical linear elasticity solutions for the stress and strain fields for these defects have singularities at the defect cores. Dislocation stress and strain singularities in classical linear theory predict infinite total energies for finite bodies which is a troublesome feature. The total energy of a disclination in a finite body, however, is bounded (Zhang and Acharya, 2016, Section 4). Nonlinear elastic solutions for wedge disclinations in cylindrical bodies of compressible *semi-linear* and *Blatz-Ko* materials are provided by Zubov (1997), and Yavari and Goriely (2013) provide the same for incompressible Ne-Hookean material response. In several such situations involving nonlinear elasticity, the stress fields are non-singular. In Acharya and Fressengeas (2012, 2015), a continuum model is introduced for the g.disclination static equilibrium as well as dynamic behaviors, where the singularities are well-handled. The Weingarten theorem for g.disclinations established in Acharya and Fressengeas (2015) is characterized further in Zhang and Acharya (2016), with the derivation of explicit formula for important topological properties of canonical g.disclination configurations. Relationships between the representations of the dislocation, disclination, and the g.disclination from the Weingarten point of view and in g.disclination theory are established therein. Concrete connections are also established between g.disclinations as mathematical objects and the physical ideas of interfacial and bulk line defects like defected grain and phase boundaries, dislocations, and disclinations. The papers (Acharya and Fressengeas, 2012; 2015; Zhang and Acharya, 2016) explain the theoretical and physical basis for the results obtained in the present work.

This paper focuses on the applications of the g.disclination model through computation. The goal is to show that the g.disclination model is capable of solving various material-defect problems, within both the small and finite deformation settings. Finite element schemes to solve for the stress and energy density fields of g.disclination distributions are proposed, implemented, and verified for the small and finite deformation settings, for a 'canonical' class of defect configurations (mentioned in the abstract). Our theoretical formalism allows for the description of non-singular cores leading to non-singular stress fields even in linear theory.

The paper is organized as follows. Section 2 contains notation and terminology. In Section 3, we briefly review elements of g.disclination theory from Acharya and Fressengeas (2012, 2015) that provide the governing equations for this work, rationalize a procedure for defining a g.disclination as data for computation of stress fields, and discuss the stress field of a disclination viewed as an Eshelby cut and weld problem. Section 4 proposes numerical schemes based on the Galerkin and Least Squares Finite Element methods to solve for the fields of g.disclinations at small and finite deformations. Section 5 contains results pertaining to twelve illustrative problems (with sub-cases), all modeled by appropriate combinations of g.disclinations, eigenwall fields, and dislocations as data. Section 6 makes contact between the g.disclination model and classical disclination theory of DeWit (1973a), under appropriate restriction on specified data. It is also shown here that for identical specified data, g.disclination theory predicts essentially the entire elastic distortion uniquely, while the classical theory uniquely predicts only the elastic strain field, a particularly clear distinction for the special case of both models in which the data specified is only a dislocation density field. Section 7 contains concluding remarks.

2. Notation and terminology

The condition that a is defined to be b is indicated by the statement $a := b$. The Einstein summation convention is implied unless specified otherwise. $\boldsymbol{Ab}$ is denoted as the action of a tensor $\boldsymbol{A}$ on a vector $\boldsymbol{b}$, producing a vector. A $\cdot$ represents the inner product of two vectors; the symbol $\boldsymbol{AD}$ represents tensor multiplication of the second-order tensors $\boldsymbol{A}$ and $\boldsymbol{D}$. A third-order tensor is treated as a linear transformation on vectors to second-order tensors.

The symbol *div* represents the divergence, *grad* represents the gradient. In this paper, all tensor or vector indices are written with respect to the basis $\boldsymbol{e}_i$, $\boldsymbol{i}$=1 to 3, of a rectangular cartesian coordinate system, unless stated otherwise. In component form,

$$
\begin{aligned}
(\boldsymbol{A}\times\boldsymbol{v})_{im} &= e_{mjk}A_{ij}v_k \\
(\boldsymbol{B}\times\boldsymbol{v})_{irm} &= e_{mjk}B_{irj}v_k \\
(\operatorname{div}\boldsymbol{A})_i &= A_{ij,j} \\
(\operatorname{div}\boldsymbol{B})_{ij} &= B_{ijk,k} \\
(\operatorname{curl}\boldsymbol{A})_{im} &= e_{mjk}A_{ik,j} \\
(\operatorname{curl}\boldsymbol{B})_{irm} &= e_{mjk}B_{irk,j}
\end{aligned}
$$

where e_{mjk} is a component of the alternating tensor $\boldsymbol{X}$.

The following list describes some of the mathematical symbols we use in this work:

$\boldsymbol{U}^e$: the elastic strain tensor (2nd-order).

$\boldsymbol{F}^e$: the elastic distortion tensor. In small deformation, $\boldsymbol{F}^e = \boldsymbol{I} + \boldsymbol{U}^e$ (2nd-order).

$\boldsymbol{W}$: the inverse-elastic (i-elastic) 1-distortion tensor. $\boldsymbol{W} = (\boldsymbol{F}^e)^{-1}$ (2nd-order).

$\hat{\boldsymbol{F}}^e$: the closest-well elastic distortion tensor (2nd-order).

$\hat{\boldsymbol{W}}$: the closest-well-inverse-elastic (cwi-elastic) 1-distortion tensor. $\hat{\boldsymbol{W}} = (\hat{\boldsymbol{F}}^e)^{-1}$ (2nd-order). $\boldsymbol{S}$: the eigenwall tensor (3rd-order).