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Phase field modeling and simulation of coupled fracture and twinning in single crystals and polycrystals☆

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Abstract

A phase field theory incorporating both fracture and deformation twinning behaviors in crystalline solids is described and implemented in finite element calculations. A variational approach is used to derive governing equations for quasi-static loading. The constitutive theory accounts for possible anisotropy of surface energy of fracture, enabling preferential cleavage on intrinsically weak crystallographic plane(s). Both linear elastic and nonlinear elastic models for bulk material behavior are addressed, the latter via compressible neo-Hookean elasticity. Numerical implementation is undertaken via the finite element method, wherein nodal degrees of freedom are displacement components and order parameters associated with twinning shear and local elastic stiffness reduction from fracture. Three dimensional simulations are reported, with solutions obtained via incremental energy minimization subjected to appropriate boundary and irreversibility constraints. Two sets of calculations are considered: a single crystal with a geometric notch, from which a crack and/or twin may extend upon mode I or mode II loading, and simple tension of a polycrystal consisting of grains with various lattice orientations. Results from the first set of calculations demonstrate a tendency for fracture before twinning when surface energies of the two mechanisms are equal, and a tendency for twinning to delay fracture when the fracture energy substantially exceeds the twin boundary energy. Results from the second set demonstrate effects of relative orientations of cleavage planes to habit planes (parallel or perpendicular), effects of initial orientation distributions, and effects of secondary grain boundary phases differing in strength and stiffness from surrounding crystals.
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Keywords: Phase field; Fracture; Twinning; Elasticity; Crystals; Finite strain

1. Introduction

Crystalline solids may demonstrate cleavage fracture and/or deformation twinning when subjected to loading that exceeds some elastic limit. Of particular interest in the present work is cleavage fracture, which tends to occur on planes of lowest surface energy [1]. Deformation twinning or mechanical twinning is induced by mechanical stress and

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involves isochoric inelastic deformation as well as a reflection of the crystal lattice across a habit plane associated with the twin boundary [2,3]. Stress concentrations resulting from crack tip geometry can induce localized twinning [4,5], or obstruction of twin propagation due to grain boundaries or other heterogeneities may lead to fracture [2]. Predictive models allowing for the possibility of both phenomena are needed for a comprehensive representation of inelasticity in classes of materials with limited other plasticity mechanisms, such as ceramics, rocks, minerals, and some metals with restricted dislocation slip modes, e.g. those of low crystallographic symmetry.

Modern computer simulations permit consideration of fracture in solids under complicated loading protocols and for nonlinear and anisotropic material behaviors, difficult, if not impossible, to model via analytical methods based on linear elastic fracture mechanics. Finite Element (FE) simulations most often rely on continuum damage mechanics theories, wherein the stiffness of a material element degrades as an internal state variable, typically labeled "damage", increases in magnitude. Conventional continuum damage models [6,7] require user-prescribed kinetic equations specifying damage accumulation; associated parameters in such equations must be tuned to experiments similar to those simulated numerically, and numerical solutions often are sensitive to mesh size. Cohesive finite element models [8–10] enable interactions and branching among discrete cracks, but crack paths are constrained to follow element boundaries. Extended finite element methods (e.g., XFEM) [11] allow displacement jumps to penetrate elements, but crack propagation direction(s) are user-specified. Alternative incremental crack growth laws [12] require specification of criteria for crack extension such as maximum energy release [13].

Somewhat analogously to continuum damage theories, crystal plasticity-type models with internal state variables have been developed and implemented in numerical simulations of deformation twinning. The volume fraction of a local material element occupied by variants belonging to one or more twin systems evolves with loading via a user-supplied kinetic law. Transformation kinetics are controlled by driving (i.e., resolved shear) stress in a mechanical setting. Such models can describe texture evolution [14], macroscopic stress–strain behavior [15,16], and in some cases subgrain twin morphology [17].

The present paper invokes phase field theory to address fracture and twinning. In comparison to standard continuum approaches such as those mentioned above, phase field models exhibit some noteworthy features: structural transformations may be modeled naturally via energy minimization [18] or Ginzburg–Landau type kinetics [19], without the need for user-supplied evolution criteria; relatively few material parameters may be needed; and numerical solutions can become regularized, i.e., mesh-size independent, with respect to a length parameter associated with interface structure. Regularized variational models may demonstrate so-called gamma convergence towards the Griffith theory of fracture as the regularization length is reduced [20].

Phase field theories have been invoked elsewhere for separate/distinct simulations of fracture and deformation twinning. Phase field theories for fracture [21–29], or variational gradient-type theories based on energy minimization similar to phase field approaches [30–32], have witnessed ongoing development since the early 2000s. Other theories with distinct order parameters for fracture and electric polarization have been reported [33,34]; the latter can be physically related to formation of twinned domains in ferroelectrics, though electromechanical twinning differs from deformation twinning associated with partial dislocations considered herein. Though most theories are couched in the context of small strains, a few do address nonlinear elasticity [29,31]. Phase field models of deformation twinning have been developed over the previous five years, with most again based on linear elasticity [35–37]. Geometrically nonlinear models include those of the present authors [5,18,38] as well as [39].

The theory implemented in the preset paper, in contrast to those listed above, may be the first that simultaneously addresses both cleavage fracture and deformation twinning phenomena, in the same simulation or analysis, with distinct order parameters for twinned and fractured domains (though a coupled fracture-martensitic transformation theory was recently reported in [40]). The geometrically nonlinear coupled theory has been described in a recent publication by the co-authors [41], wherein analytical and simple numerical solutions to a one-dimensional shear problem were obtained, and wherein theoretical aspects of stability were analyzed mathematically. The first numerical implementation (e.g., in a finite element setting) and computational results of three dimensional simulations resulting from this coupled phase field theory are the major new contributions of the present work. The general theory combines aspects of prior work on isolated twinning [18,38] and fracture [29,42] behaviors. Necessary material parameters are the twinning habit plane and twinning eigen-shear, the twin boundary surface energy, the crack plane normal (if fracture is anisotropic), the surface energy of fracture, and elastic constants. A numerical parameter is also needed for regularization of the twin boundary/crack width. The energy functional implemented in the model accounts for coupling between fracture and twin evolution. Dislocation mediated plasticity – a primary inelasticity mechanism in

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