Mesoscale Modeling of Microcrystalline Ceramics

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Abstract: Diffuse interface models and simulations capture deformation and failure of polycrystalline ceramics with multiple phases. Two heterogeneous ceramic solids are investigated. The first consists of a boron carbide matrix phase embedded with titanium diboride grains. The second consists of diamond crystals with a smaller fraction of silicon carbide grains, where the latter may encapsulate the former in a micro- or nano-crystalline matrix and/or may be interspersed as larger micro-crystals. A general constitutive framework suitable for representing behaviors of all phases of each material system is reported. This framework is implemented in three-dimensional (3D) finite element (FE) simulations of polycrystalline aggregates under compressive loading. Numerical results demonstrate effects of grain and phase morphology and activation or suppression of slip or twinning mechanisms on overall strength and ductility.

1 Introduction

Crystalline ceramics are important in technological applications requiring materials with high hardness, high stiffness, strong wear resistance, and relatively low mass density. This work invokes phase field theory [1,2] to study two heterogeneous ceramic materials. The first is composed by majority of crystalline boron carbide (B_4C, rhombohedral structure), with secondary grains of crystalline titanium diboride (TiB2, hexagonal). Boron carbide polycrystals demonstrate low mass density and extreme hardness but are brittle and may also undergo deformation twinning and a stress-induced crystal-to-glass transformation [2,3]. Titanium diboride, while of higher mass density and lower hardness, may be more ductile than boron carbide as a result of dislocation activity [4]. Secondary grains of the more ductile phase may improve overall fracture toughness and failure resistance by serving as obstacles to cleavage crack propagation. The second composite studied here is predominantly diamond (C, cubic structure) with secondary grains of silicon carbide (β-SiC, cubic). Diamond grains tend to be of equal or much larger size than SiC grains, and the latter may include layers of much smaller grains, perhaps even nano-structured, fully encapsulating the diamond. Silicon carbide is added to improved ductility and toughness; diamond is brittle and prone to cleavage failure. Stacking faults and twins are profuse in the SiC phase. In both material systems, residual stresses may be incurred during thermal processing.

2 Phase Field Theory

The phase field theory used here is a generalization of the framework first reported in [1], where, in addition to twinning and fracture, solid-solid phase changes and accumulation and slip of dislocations and stacking faults are addressed. Geometrically linear kinematics and a quasi-static model are implemented here; geometric nonlinearity [1,5,6] residual stresses, porosity, and tertiary phases are omitted.

Let $\boldsymbol{X}$ denote reference position of a material particle. Two scalar order parameters are introduced. The first, denoted by $\xi \in [0,1]$, is used to represent fracture, where

$\xi(\boldsymbol{X})=0 \forall \boldsymbol{X} \in$ undamaged material,

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$\xi(\boldsymbol{X}) \in (0,1) \forall \boldsymbol{X} \in$ partially degraded material, (1)

$\xi(\boldsymbol{X}) = 1 \forall \boldsymbol{X}$ fully failed material.

The second order parameter $\eta \in [0,1]$ describes the following material states:

$\eta(\boldsymbol{X}) = 0 \forall \boldsymbol{X} \in$ parent elastic crystal,

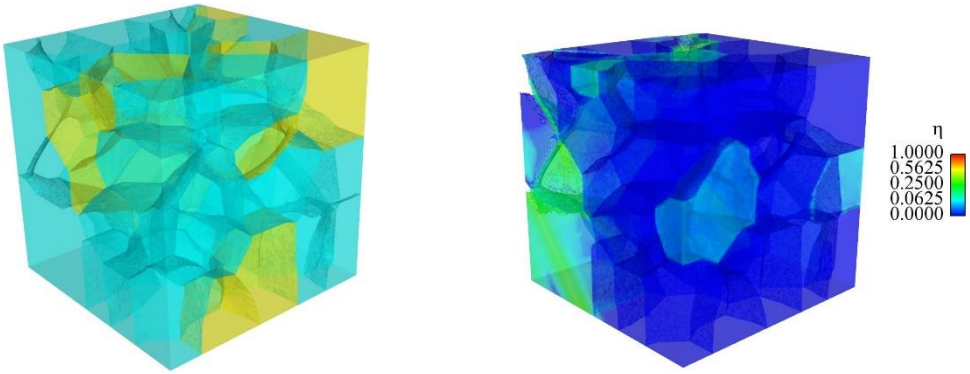
$\eta(\boldsymbol{X}) \in (0,1) \forall \boldsymbol{X} \in$ structural boundary zone, (2)

$\eta(\boldsymbol{X}) = 1 \forall \boldsymbol{X} \in$ structurally transformed state.

Most generally, depending on the particular material, $\eta > 0$ is used to account for inelastic shearing from slip of full, partial, and/or twinning dislocations as well as localized slip in amorphous bands. It can also be used to account for densification (expansion) correlating with lower (higher) free volume. The displacement gradient $\nabla \boldsymbol{u}$ is decomposed additively into elastic and state-dependent parts. The total energy functional for an initially heterogeneous body Ω is

$$\Psi(\boldsymbol{u},\eta,\xi,\boldsymbol{X}) = \int_{\Omega} [W(\nabla u, \eta, \xi, \mathrm{X}) + f(\eta, \xi, \nabla\eta, \nabla\xi, \mathrm{X})] dV. \quad (3)$$

Strain energy density is W. Function f accounts for internal state and order parameter gradients. Stationary points of Ψ at fixed $\boldsymbol{X}$ produce the static Euler-Lagrange equilibrium equations via a variational derivation [1,6].



(a) Phases (B_4C-teal, TiB_2-yellow) (b) Fracture and structure changes (η)

Figure 1: Microstructure rendering (FE mesh) and η contours for B_4C-TiB_2 at compressive strain of 0.7% with fractured elements ($\xi > 0.8$) visually removed

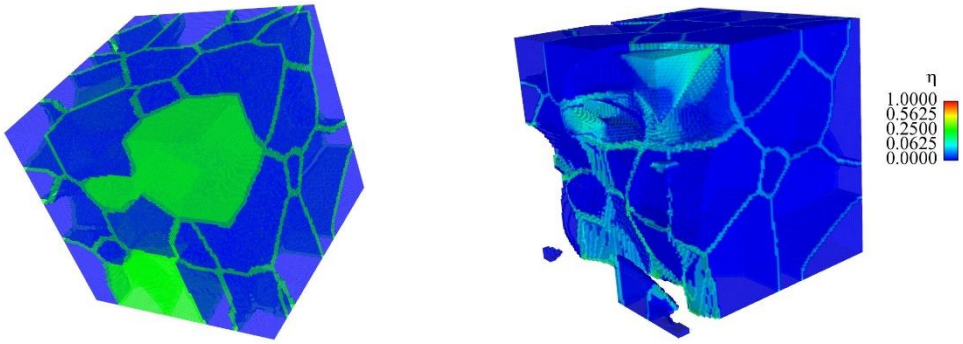
3 Boron Carbide-Titanium Diboride Composites

The constitutive model for B_4C crystals is similar to that in [2]. Twinning occurs on $\langle 10\bar{1}0 \rangle \{0001\}$, fracture on basal {0001} planes. Amorphous shear bands can form within twinned domains. The phase field constitutive model for TiB_2 is newly introduced here. The plane of minimum fracture energy is {0001}. Parameter η accounts for stacking fault energy from partial dislocation slip and stored line energy, and it interpolates from null to maximum single slip. A representative FE rendering and result are shown in Fig. 1. Results suggest that the less brittle TiB_2 phase can inhibit cleavage fractures and that suppression of localized inelastic deformation in B_4C improves overall strength and ductility.

4 Diamond-Silicon Carbide Composites

Diamond is modeled as an elastic-brittle material, where fracture corresponds to cleavage on {111} planes [7]. Silicon carbide is modeled as an elastic solid that may undergo fracture on {110} planes [8] and $\langle 11\bar{2} \rangle \{111\}$ deformation twinning whereby a very low stacking fault energy is observed [9]. A

representative FE mesh and computational result are shown in Fig. 2. Incorporation of the softer SiC phase in nano-crystalline layers along grain boundaries enhances overall strength and ductility relative to microstructures with less SiC in the form of larger grains. Twinning in SiC layers may improve ductility of the composite at the expense of lowered peak strength.



(a) Phases (C-blue, SiC-green) (b) Fracture (ξ>0.8) and twinning (η)

Figure 2: Microstructure and η contours for diamond-SiC at 0.6% strain

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