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Study of crack propagation behavior in single crystalline tetragonal zirconia with the phase field method

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ABSTRACT

The tetragonal to monoclinic phase transformation and its toughening effect on the Mode I crack propagation in single crystalline zirconia is investigated by a coupled phase field model. The developed phase field model can simulate the evolution of the tetragonal to monoclinic phase transformation and crack propagation simultaneously. Two tetragonal lattice orientations: 0° and 90°, are studied and compared with the case that the material is untransformable. The numerical results show that the phase transformation always initiates from the crack tip. The phase transformation dramatically reduces the normal stress near the crack tip and slows down the crack growth speed for both orientation angles. A closure of the crack tip may even be observed shortly after the phase transformation, which is caused by the transformation stain and the stress re-distribution at the junction of the monoclinic phase and the crack phase. The lattice orientations have great influences on the final monoclinic microstructure and the transformation toughening effect. This work shows the validity of the phase field method to simulate the microstructure evolution during the crack propagation and it can serve as a robust tool to investigate the transformation toughening behavior of Zirconia ceramics.

1. Introduction

Zirconia ceramics possess excellent mechanical properties, such as high strength and toughness, dimensional and chemical stability, biocompatibility and wear resistance. They have received intensive applications in various engineering fields such as thermal barrier coatings, biomedical implants [1]. The main mechanism responsible for their high fracture toughness is the stress-induced tetragonal monoclinic phase transformation ($T \rightarrow M$ transformation) during crack propagation. Considerable amount of research work has been carried out in the past decades since the discovery of the transformation toughening capabilities of zirconia in the mid-1970s [2–11]. Our own work on this topic can be found in Luo and Xiao [12]. Thorough reviews on this topic can be found in the monographs given by Hannink et al. [13] and Kelly and Rose [14]. Most of the research work shares an emphasis on the development of a transformation process zone associated with an advancing crack. A phase transformation criterion or a constitutive relation is adopted to determine the shape and size of the phase transformation zone around the advancing crack tip. Two different approaches are generally adopted to study the toughening

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Nomenclature

η_p	content of monoclinic variant
$\mathbf{r}$	position vector of the material point
t	time
F	free energy in the phase field model for phase transformation
L	mobility parameter for phase transformation
ς	Langevin-noise
$\beta_{ij}(p)$	the positively defined gradient energy coefficient tensor
f	bulk chemical free energy density
ΔG	chemical driving force
A, B, C	expansion coefficients of the Landau polynomial at a fixed temperature
ε_{ij}^{tot}	total strain
ε_{ij}^{00}	transformation strain
ε_{ij}^{el}	elastic strain
C_{ijkl}	elastic tensor
$\tilde{E}$	free energy in the phase field model for crack propagation
ϕ	the crack phase
M	mobility parameter of crack propagation
λ	mixing energy density
γ	half of the fracture energy
G_c	fracture energy
K_{IC}	critical stress intensity factor
E	Young's modulus of isotropic materials
υ	Poisson's ratio
κ	interfacial thickness
χ	tuning parameter to relate the mobility parameter $M$to the interfacial thickness
c_{ijkl}	the elastic modulus of the broken phase
F_{tot}	free energy of in the coupled phase field model
C^M, C^T	elastic constants of the monoclinic and tetragonal phase respectively
$\mathbf{n}$	outward normal to the boundary

effect of the phase transformation. The first approach, originally adopted by McMeeking and Evans [2], uses linear elastic fracture mechanics to compute the stress-shielding effect resulting from the transformation-induced strains near the crack tip. The second approach involves estimates of the energy changes, or work of fracture, that result from the transformation associated with a growing crack [3]. These theoretical models have managed to capture the essence of transformation toughening and to provide a firm foundation for the topic. In most of these studies, the microstructural details such as the phase boundary, grain boundary and crystal orientations of the grains are ignored. Thus the microstructures of the transformed crystals are homogenized with transformation strains distributed in the transformed zone. The microstructural evolution process, for example, the initiation and propagation of the monoclinic phase inside or across tetragonal grains under the stress field around a stationary crack tip or during the crack propagation cannot be captured from these models. Such microstructure information is important to develop a more robust transformation toughening model.

In the past few years, the phase-field (PF) model has become a powerful tool for modeling the evolution of microstructures [15]. Khachaturyan [16] developed the phase-field microslasticity theory based on the time dependent Ginzburg–Landau (TDGL) kinetic equations. This theory has been successfully applied to study the phase transformations, static and propagating crack problems in single phase or multiphase materials [17–22]. It has been shown that the PF model can capture most of the important features of the martensitic transformations. Fan and Chen [23] adopted the PF model to study the cubic to tetragonal phase transformation in Yttria stabilized zirconia. More recently, Mamivand et al. [24–28] applied the PF model to study the tetragonal to monoclinic phase transformation in zirconia in both 2D and 3D cases. Mamivand et al. [25] studied the stress-induced phase transformation and its toughening effect on a static elliptic crack. She et al. [29] used the very similar model to simulate the heterogeneous cubic to tetragonal martensitic transformation. On the other hand, great progresses have also been made to study the crack propagation problems in materials within the framework of PF method [30–40]. Ambati et al. [41] provide a thorough review on this topic recently. The convergences of these models have been carefully checked and compared with the Griffith's theory. Some models have been validated with experimental results. As the diffusive crack model can simulate the crack initiation, propagation and branching behaviors, it a robust tool to simulate the fracture behavior of cracks with complex patterns. What's more, in the framework of PF method, the crack propagation behavior can be naturally coupled with other physical processes such as phase transformation, and diffusion. For example, Abdollahi and Arias [42–44] investigated the crack propagation problems in ferroelectric crystals. Zuo and Zhao [45] adopted Hakim and Karma's model [33] to study the coupling effects on the lithiation diffusion and crack nucleation.