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Toughening effect of ferroelectric ceramics induced by domain switching and dislocations

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ABSTRACT

The multi-scale analysis of fracture toughness of ferroelectric ceramics under complicate mechanical–electrical coupling effect is carried out in this paper. The generalized stress intensity factor (SIF) arising from spontaneous strains and polarization transformation in switching domain zones is accurately obtained by using an extended Eshelby theory. Taking $BaTiO_3$ ferroelectric ceramic for example, it is discovered that the crack propagation can be induced by domain switching arising from negative electrical field when the crack surface is parallel to the isotropic plane, and the obtained critical electric displacement intensity factor (EDIF) approximates closely to that obtained by the Green's function method. Additionally, as pinning dislocations and slip dislocations can strongly influence properties of ferroelectric devices and induce the property degradation, it is necessary to investigate the dislocation toughening effects on fatigue and fracture mechanisms. The results show that the dislocation shielding and anti-shielding effects on mode II SIF, mode I SIF and EDIF are obviously different when a dislocation locates at a position near the crack tip. Through the calculation of the critical applied EDIF for crack propagation by using mechanical energy release rate (MERR) theory, it is discovered that the slip angles obviously influence fracture toughness, and the mode II SIF arising from dislocation has little influence on fracture toughness, however, the mode I SIF and EDIF arising from dislocation have great influences on fracture toughness.

1. Introduction

The mesoscopic and microscopic information structure mechanics of function materials under multi-field coupling effect have been proposed. When the interaction effects between stress, strain, heat and electromagnetic behavior are very strong, the meso and micro structural mechanics become important for properties and designs of intelligent devices. For example, domain wall motions, dislocations pinning effect, dislocation thermally activated slip, nucleation and propagation of micro cracks, etc., often induce invalidation and damage of the intelligent devices and structures subjected to electrical, mechanical or electromechanical loads. Fatigue, fracture, depolarization, plasticity, etc., are the main property degradation patterns.

The earliest experimental investigations on fracture mechanisms of ferroelectric ceramics should go back to the eighties of 20th century. Winzer et al. [1] reported the fracture phenomenon of cofired multiplayer electrostrictive actuators at the earliest. Chung et al. [2] observed the intergranular cracking and damage of barium titanate and lead zirconate titanate

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induced by electric field. McHenry and Koepke [3] observed phenomena were explained qualitatively by certain microstructural features, in particular internal stresses [4] and energy dissipation [5] by domain switching processes. At the beginning of nineties of 20th century, Furuta and Uchino [6] observed the process of crack nucleation and propagation in internal electrode of ferroelectric detent. Pak [7,8] and Park and Sun [9] obtained the crack extension force and fracture criterions of piezoelectric materials, discussed the suitability in using the stress intensity factor, the total energy release rate, or the mechanical strain energy release rate as the fracture criterion, and also analyzed the effect of electric field on fracture of piezoelectric ceramics. However, the effect of local stresses arising from domain switching on crack extension was not considered.

Recently, many experimental, theoretical and numerical investigations on fracture toughness, initiation and propagation of cracks in ferroelectric ceramics subjected to mechanical or electrical or electromechanical loads were shown. Electric-field-induced fatigue crack propagation in pre-cracked PZT ferroelectric ceramics is investigated experimentally by Fang et al. [10], the experimental results showed that the frequency, waveform, as well as the amplitude ratio, of the electric loading, play important roles in electric-field-induced fatigue cracking. Domain switching criterion which can differentiate 90° switching and 180° switching was proposed [11]. Using a general energy balance for crack propagation under the action of a dissipative crack tip zone, the fracture toughness of ferroelectric ceramics subjected to electromechanical loads was analyzed by Kreher [12]. Beom and Atluri [13] investigated the disciplines of style, size and shape of domain switching zones around crack tip in ferroelectric ceramics subjected to electrical load by using the theory of electrical nonlinearity and criterion of domain switching. The domain switching toughening of crack tip in ferroelectric ceramics subjected to mechanical load was studied [14]. The corresponding domain switching and the criterion in ferroelectric crystal subjected to increasing electric field were observed and discussed through combining experimental observations and theoretical analysis without considering the electrical nonlinearity by Jiang and Fang [15,16] and Engert et al. [17]. However, Miehe and Rosato [18] indicated its importance, and presented a variational-based modeling and computational implementation of the non-linear, rate-dependent response of piezoceramics under electro-mechanical loads. Besides, Linder and Miehe [19] made a computational investigation of a proposed simplified account for electric displacement saturation on the initiation and propagation of cracks in poled ferroelectric ceramics within the linear regime of piezoelectricity by finite element method, and the performed numerical simulations of a compact tension test and an off-centered three point bending test showed excellent agreements with experimental results given in the literature. Contrary to earlier accounts of electric displacement saturation, the exponential saturation of the electric displacement versus electric field relation was also applied in the problems like propagating cracks in fracturing piezoelectric ceramics [20]. Additionally, a new finite elements method to account for strong discontinuities in the mechanical displacement field and the electric potential was presented in the works [21,22] to model failure in electromechanical coupled materials, which is very useful to model the electromechanical responses for a class of materials with even more general ferroelectric effects, brittle/ductile failure mode transitions and crack branching. A continuum phase field modeling of dynamic failure mechanisms in brittle solids governed by complex fracture phenomena like crack initiation, multiple crack branching or crack arrest was also proposed by Hofacker and Miehe [23].

These previous investigations also indicated that ferroelectric materials contain fracture toughness anisotropy. As the driving force of crack extension, the combination of applied loads and local stresses arising from domain switching can be used to reasonably explain some phenomena like toughening and toughness anisotropy of ferroelectric ceramics.

In addition, the property degradation arising from pinning dislocations and slip dislocations in ferroelectric devices was also studied by many researchers. The investigations [24–26] indicated that dislocation effect has significant influences on the ferroelectric properties in succession. By electron microscopic observation, Liu et al. [27] proposed that domain switching is a process with strong influence of dislocation activities which probably arises from the existence of dislocation stress fields. Kontsos and Landis [28] proposed a theoretical and numerical framework of interaction between domain switching and dislocation. Zheng et al. [29] studied the interaction between dislocations and ferroelectric film and indicated that interfacial dislocations play an important role in suppressing the remnant polarization and the coercive field of the polarization. As is know to all, the coexistence of pinning dislocations and domain walls can also strongly influence the toughness of ferroelectric ceramics and induce the depolarization and plasticity. Moreover, as the brittle-ductile transition exists objectively under thermal activation [30,31], it is unreasonable to neglect the important dislocation slip in studies of fracture mechanism of high temperature ferroelectric ceramics. The competition and interaction mechanisms between dislocation emission and crack cleavage are the cores of brittle-ductile transition and fracture physics, and determine the strength, toughness and fatigue life of high temperature ferroelectric ceramics. Many previous investigations indicated that the dislocation shielding effect is exactly the most significant interaction behavior. However, the investigations on meso-micro fracture mechanism of ferroelectric materials, especially the researches about interaction effect between dislocations, domain switching and cracks are few, and the influences of that effect on the fatigue, fracture and plasticity in piezoelectric coupling field are still unclear.

In this paper, the highlights are focused on the calculation methods of multi-scale fracture toughness of ferroelectric ceramics based on a complicate mechanical–electrical coupling constitutive model which describes realistically appearing physical phenomena like anisotropy. The multi-scale effects on fracture are composed of the linear part arising from applied electric field, and the nonlinear part arising from domain switching and dislocations. In the nonlinear part, the domain switching toughening effect is evaluated by an extended Eshelby technique, and the dislocation toughening effect is analyzed by using mechanical energy release ratio.