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THREE-DIMENSIONAL PHASE-FIELD SIMULATION OF CRACK PROPAGATION IN FERROELECTRIC POLYCRYSTALS

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The design and implementation of electromechanical systems demand multifunctional materials with strong electromechanical coupling and reasonable reliability. Ferroelectric ceramics are the main candidates also exhibiting short response times. However, due to their inherent brittleness, a deep understanding of the fracture behavior of these materials is key to assure optimum reliability of the systems. Interactions between the microstructure, grain boundaries, localized stress and electric fields near the crack tips lead to the complexity of fracture phenomena in ferroelectric polycrystals. The main objective of this work is to study the fracture processes of ferroelectric polycrystals in three dimensions, and to produce more realistic simulations in 3-D, explaining the toughening mechanisms in these materials. For this purpose, we propose a phase-field model of fracture in ferroelectric polycrystals. Previous results with this model in 2-D prove its potential to capture complex interactions between the crack and the material microstructure [1].

A representative simulation is shown in Fig. 1. Figure 1(a) presents a snapshot of the polycrystalline microstructure evolution obtained from computer simulations of 3-D grain growth [2]. The final computed crack path (when the sample is splitted into two parts) is presented by plotting the isosurface of the fracture parameter in Fig. 1(b). It is obvious that the crack propagates both along the grain boundaries (intergranular mode) and through the grains (transgranular mode), creating a deflected and complex fracture surface. In the intergranular mode, the crack is forced to move around the grain since the fracture toughness of the grain interior is higher than the grain boundary, leading to crack deflection along the grain boundary. On the other hand, the transgranular mode of fracture allows the crack to interact with the ferroelectric domain microstructure inside the grains. The inter- and trans-granular modes lead to different toughening mechanisms in ferroelectric polycrystals.

In addition to crack deflection, the simulations show that crack bridging, crack branching and ferroelastic domain switching act as the main fracture toughening mechanisms. These mechanisms are intrinsically three-dimensional and our fully 3-D simulations illustrate how the combination of all of them enhances the macroscopic fracture toughness of the material [2]. All of these toughening mechanisms have been observed in experiments of ferroelectric ceramics [3].

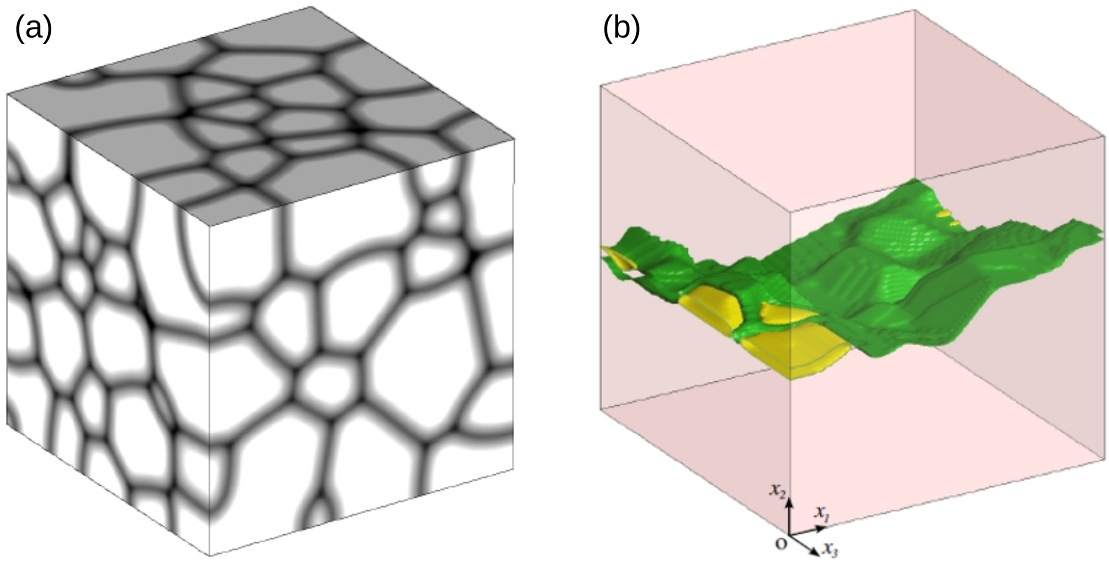

Figure 1: (a) Snapshot of the 3-D polycrystalline microstructure. Grain boundaries correspond to darker regions. (b) Isosurface of the fracture parameter indicating the inter- and trans-granular crack surfaces highlighted with green and yellow, respectively.

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