Abstract of Invited Speech 1

Effects of Grain Orientations on the Stress Intensity Factor of a Crack in Ferroelectric Polycrystals Using the I-integral Method

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1. Introduction

Ferroelectric materials are widely used in modern technical fields due to their large ferroelectricity and related electromechanical properties. A drawback hindering their reliable application is their intrinsic brittleness so that ferroelectric materials are susceptible to cracking, resulting in critical failure and malfunction of ferroelectric devices. Ferroelectric materials possess spontaneous polarization that can be switched from one direction to another. Highly concentrated electro-mechanical fields near the crack tip often induce the changes of polarization orientations, i.e., domain switching. The domain switching in turn shields the crack-tip stress concentration from the external load via the electro-mechanical coupling. According to this fact, researchers proposed the switching-toughening model to determine the stress intensity factor (SIF). In the switching-toughening model, the crack-tip SIF can be obtained through superimposing the SIF induced by a remotely external load without any switching and the change of the SIF due to domain switching. A drawback of this model is that switching is limited to be small scale.

In the presence of external loads, domain switching usually occurs in most or even the entire micro-/nano-devices, that is to say large-scale switching happens. Large-scale switching arouses a great challenge for the determination of the SIFs of a crack in ferroelectric materials. We proposed the I-integral method to extract the crack-tip SIFs for large-scale switching problems [1, 2]. The I-integral overcomes the shortcoming of the traditional fracture mechanics methods, i.e., small-scale switching assumption is unnecessary, so that the I-integral are effective for large-scale switching analysis. Especially, the I-integral is proved to be independent of integration area size, regardless of the presence of grain boundaries and domain walls.

The phase field model developed from time-dependent Landau-Ginzburg theory is combined with the I-integral method to simulate domain switching process of the PbTiO3 ferroelectric polycrystals with an impermeable crack through increasing the tensile strain step by step. A sudden large-scale switching induces a sharp drop of the mode-I SIF. When grains orient evenly in circumferential direction or randomly, no critical load was observed. This study focuses on the effect of grain orientations on domain switching and variations of the SIFs.

2. Phase field model

In the phase field model, the total free energy of a ferroelectric block is expressed as an integral with respect to the electrical enthalpy density, which is the function of the spontaneous polarization, the strain and the electric field, i.e.,

$$h = f_{Lan}(P_i) + \frac{1}{2} g_{ijkl} P_{i,j} P_{k,l} + \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - q_{ijkl} \varepsilon_{ij} P_k P_l - \frac{1}{2} \kappa E_i E_i - E_i P_i \quad (1)$$

The first term is the Landau energy density

$$f_{Lan}(P_i) = a_i P_i^2 + b_{ij} P_i^2 P_j^2 + c_{ijk} P_i^2 P_j^2 P_k^2 \quad (2)$$

The parameters g_{ijkl}, C_{ijkl}, q_{ijkl} and k are respectively the gradient coefficients, elastic stiffness coefficients, electrostrictive coefficients and dielectric constant. And a_i, $b_{\mathbf{ij}}$ and c_{ijk} are Landau coefficients. The temporal evolution of the spontaneous polarization in a ferroelectric body under an applied electro-mechanical load is described by the time-dependent Ginzburg-Landau equation. The stress and electric displacement satisfy the equilibrium equation and Maxwell's equation, respectively. That is

$$\frac{\partial P_i}{\partial t} = -L \frac{\delta F}{\delta P_i}, \quad \sigma_{ij,j} = 0, \quad D_{i,i} = 0 \quad (3)$$

where L is the kinetic coefficient. Expressing the governing Eq. (3), the kinematic equations and the constitutive equations in weak forms, a nonlinear finite element method (FEM) can be used to solving the electro-elastic fields. The detailed discretization process can be referred to Wang and Kamlah [3].

3. I-integral method

Noting the fact that the spontaneous polarization achieves a saturation state in ferroelectrics when the applied load is beyond a limit, we assumed that the spontaneous polarization is saturated in a small region around the tip. Correspondingly, we established the I-integral which is a line integral along a infinitesimal contour from the lower to the upper crack face [1]

$$I = \lim_{\Gamma_\varepsilon \to 0} \int_{\Gamma_\varepsilon} (\sigma_{ij} \varepsilon_{ij}^{\delta} \delta_{1i} - \sigma_{ij}^{\delta} u_{j,1} - \sigma_{ij} u_{j,1}^{\delta}) n_i d\Gamma \quad (4)$$

Here, the quantities marked by a superscript δ denote the auxiliary fields [1, 2]. After manipulation, we can obtain the equivalent domain for of the I-integral as

$$I = \int_A \begin{pmatrix} \sigma_{ij}^{\delta} u_{j,1} + \sigma_{ij} u_{j,1}^{\delta} - \varepsilon_{jk}^{\delta} \sigma_{jk} \delta_{1i} \\ + D_i^{\delta} \phi_{,1} + D_i \phi_{,1}^{\delta} + D_j E_j^{\delta} \delta_{1i} \end{pmatrix} w_{,i} dA + \int_A (2 \varepsilon_{ij}^{\delta} q_{ijkl} P_k P_{l,1} + E_l^{\delta} P_{l,1}) w dA - \int_A \left\{ \sigma_{ij,1}^{\delta} \sigma_{kl} \Delta C_{ijkl}^{-1} - D_{i,1}^{\delta} D_i \Delta \kappa^{-1} \right\} w dA \quad (5)$$

Here, $\Delta(*)$ denotes the difference between the quantity (*) at the integration point and that at the crack tip. The I-integral is independent of integration area containing arbitrary grain boundaries. With this feature, we refer to such an I-integral as the area-independent I-integral. Apart from this feature, the present I-integral has following advantages over the switching-toughening models: (1) Small-scale switching assumption is unnecessary. (2) It is independent of integration area, regardless of the existence of grain boundaries and domain walls. (3) It can directly solve the crack-tip SIFs. (4) The mixed-mode SIFs are decoupled. Therefore, the present I-integral is quite effective to solve the crack-tip

SIFs of ferroelectric polycrystals under large-scale switching.

4. Simulations of the tensile test of PbTiO3

As shown in Fig. 1, we consider a two-dimensional lead titanate (PbTiO3) ferroelectric plate of length 120 nm and width 103.9 nm with an impermeable crack of length 30 nm. Our previous studies found that when all grains orient in the same direction, domain switching occurs only as the applied tensile load is increased beyond a critical value. A sudden large-scale switching induces a sharp drop of the mode-I SIF. When grains orient evenly in circumferential direction or randomly, no critical load was observed. The reason is that multi-domains form even no applied load and as the tensile load increases, domain walls move smoothly. As a result, the mode-I SIF varies continuously during the loading process. This study focuses on the effect of grain orientations on domain switching and variations of the SIFs.

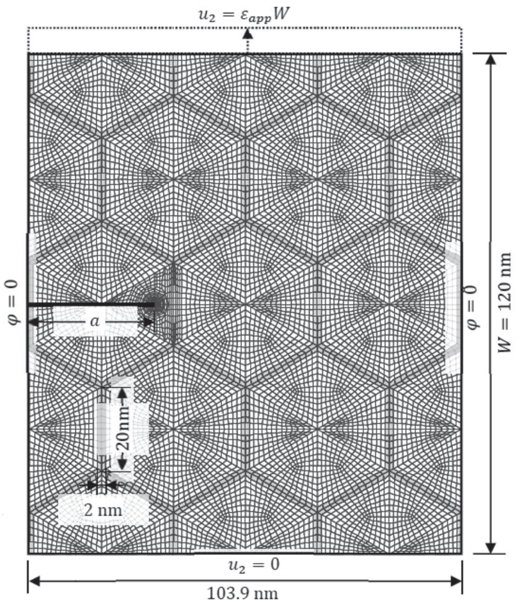

Fig.1 A nanoscale polycrystalline plate with an impermeable crack of length a=30nm.

5. Results and conclusions

The simulation showed that when a principle direction of grains exists, both the initial multi-domain structures will appear locally and a sudden large-scale switching will happen as the tensile load is increased. Correspondingly, the SIF drops suddenly at the critical load. The critical load is observed to be smaller than that for the polycrystal with uniform grain oritations.

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References

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