THE INFLUENCE OF FLEXOELECTRIC EFFECT ON THE DOMAIN STRUCTURE AND FRACTURE TOUGHNESS OF FERROELECTRIC MATERIALS

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Abstract

Due to the impressive electromechanical properties, ferroelectric materials have been widely used in actuators, memory devices and other electronic equipment. However, the instinct brittleness of ferroelectric materials makes it easy to failure under external force and electric field. Since giant strain gradient can be easily generated near the crack tip with the application of external force, the local domain structure and electromechanical behavior can be significantly influenced by the flexoelectric effect. In this work, the time-dependent Ginzburg-Landau (TDGL) theory and phase field model are used to determine the impact of flexoelectric effect on the domain structure and fracture toughness of $PbTiO_3$ in the vicinity of the crack tip. The simulation results show that the domain structure become asymmetric near the crack tip with the consideration of flexoelectric effect. In addition, the fracture toughness is increased or decreased depending on whether the crack tip is parallel or perpendicular to the original polarization direction. Furthermore, the fracture toughness parallel to the direction of polarization is much lower than that anti-parallel to the direction of polarization with flexoelectric effect. In conclusion, the flexoelectric can induce the asymmetry of electromechanical and fracture behavior near the crack tip. Thus, the flexoelectric effect must be considered in the reliability design of ferroelectric devices.

1. Introduction

As a smart material, ferroelectric materials have been broadly used in production and manufacture of many electronic equipment, such as transducers and memory devices. However, the instinct brittleness of ferroelectrics makes it easy to failure under external stimuli such as force and electric field. Duo to the size effect, giant strain gradient can be easily generated at nanoscale. Thus, the domain structure and the electromechanical behavior of ferroelectric materials can be significantly changed duo to the flexoelectric effect. Many works indicate that flexoelectric effect can be regarded as external electric, which can change the switching process of polarization domain and effect fracture toughness of ferroelectric materials. In this work, we employ phase filed method to explore the influence of flexoelectric effect on the domain structure and fracture toughness of ferroelectric materials around the crack tip.

2. Results

To show clearly the detailed polarization structure, we select the local region near the crack tip. Fig. 1 shows the steady state distribution of polarization component $P_1$with flexoelectric coefficients $f_{ij}^* = 0$, $f_{ij}^* = f_{ij}^0$, $f_{ij}^* = 3f_{ij}^0$ and $f_{ij}^* = 5f_{ij}^0$, respectively. The results show that domain configuration with $f_{ij}^* = 0$ is symmetric about both x_1 and x_2 directions. Whereas, the domain configuration become asymmetric about x_1 direction with the consideration of flexoelectric coefficients. As shown in Fig. 1(b)-(d) the average value of P_1 on the left side of the crack is larger than that on the right side. Besides, the domain structure is asymmetric with flexoelectric effect. Fig. 2 demonstrates local *J*-integral near the left and right side of crack

tips. According to Fig. 2, the flexoelectric effect can break the symmetry of fracture toughness, which makes the fracture toughness become larger along the direction anti-parallel to the original polarization.

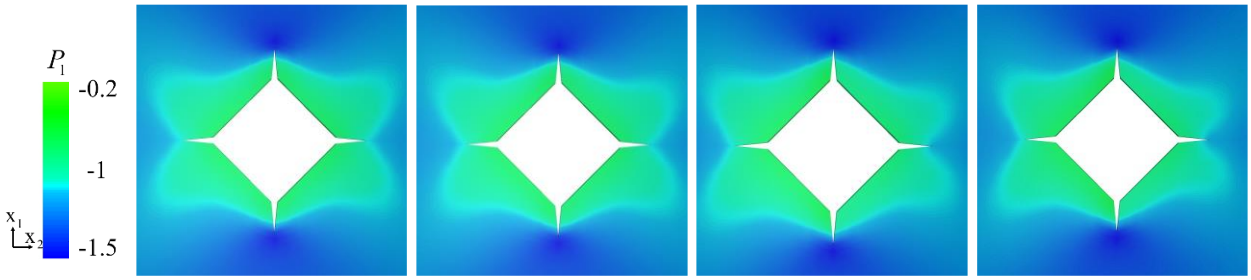

Fig.1. Steady state distribution of local polarization along x_1 direction under double tensile load: (a) $f_{ij}^* = 0$, (b) $f_{ij}^* = f_{ij}^0$, (c) $f_{ij}^* = 3f_{ij}^0$, (d) $f_{ij}^* = 5f_{ij}^0$.

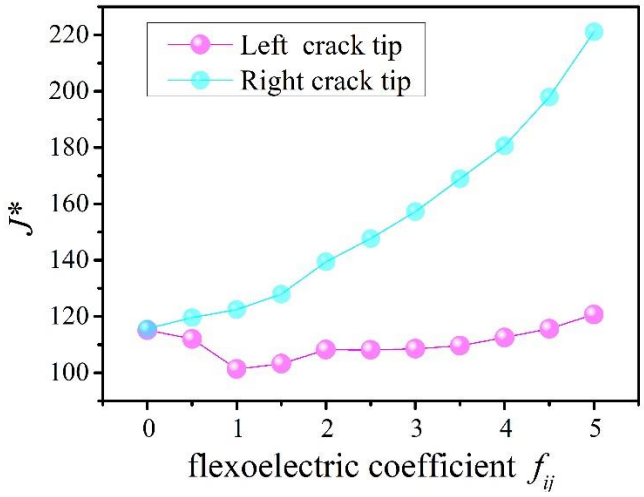

Fig.2. Local *J*-integral near left and right crack tips

3 Conclusions

In this study, we employ Ginzburg-Landau theory and the phase method to simulate electromechanical coupling behavior of ferroelectric materials with flexoelectric effect. The simulation results indicate that the flexoelectric effect can breck symmetry of domain configuration in the vicinity of crack tip. Furthermore, the J-integrals are calculated to determine the influence of flexoelectric effect on the fracture toughness. The result indicates that the fracture toughness for a crack parallel to original polarization direction is lower than that for a crack anti-parallel to original polarization with consideration of flexoelectric effect. Therefore, flexoelectric effect must be considered to design and manufacture of ferroelectric materials.