PHASE FIELD MODELING OF COUPLING EVOLUTION OF POLARIZATION, FRACTURE, AND DIELECTRIC BREAKDOWN IN FERROELECTRIC MATERIALS

Yong Zhang[1]*, Jie Wang[2,3]

[1]Tongji University, Shanghai, China, [2]Zhejiang University, Hangzhou, China
[3]Zhejiang Laboratory, Hangzhou, China
** Presenting Author email: yong_zhang@tongji.edu.cn*

Abstract

Ferroelectric materials have attracted increasing attention due to their distinguished electromechanical performance. As two main failure behaviors, fracture and dielectric breakdown may occur simultaneously in ferroelectric materials. Understanding the coupling evolution of polarization, fracture, and dielectric breakdown is crucial for the application of ferroelectric materials under complex electromechanical environments. A phase field model was developed to investigate the coupling evolution behavior of polarization, fracture and dielectric breakdown in ferroelectric materials subjected to both mechanical and electrical loadings. Driving forces for fracture and dielectric breakdown were analysed based on the generalized configurational forces. The phase field simulations showed that dielectric breakdown can be induced by the concentrated electric field at impermeable crack tips. At the same time, the dielectric breakdown can influence the stress distribution around the crack tip as well as the driving force for crack propagation. The attraction of fracture to breakdown path and the deflection of breakdown to fracture path were observed during the coupling evolution of fracture and breakdown. The developed model framework can be employed to investigate more complex coupling failure behaviours of ferroelectric and dielectric materials.

1. Introduction

Ferroelectric materials have been widely used in various electromechanical devices such as sensors, actuators, transducers and energy storage devices due to their distinguished electromechanical coupling properties. Ferroelectric materials usually bear large mechanical loads and high electric fields in order to give full play to their potential. The interaction between fracture and dielectric breakdown is able to occur since the filler inside a crack will change the dielectric behaviors around it and dielectric breakdown can change the local mechanical properties of dielectric materials because of its weakening of chemical bonds. Therefore, a comprehensive and in-depth understanding of the fracture and dielectric breakdown behavior of ferroelectric materials and their interaction is very important for the advanced and reliable application of ferroelectric materials.

A phase field model was developed to investigate the coupling evolution behaviours of polarization, fracture and dielectric breakdown in ferroelectric materials subjected to mechanical and electrical loadings. Generalized configurational forces of fracture and breakdown were derived from the phase field model to analysis the driving forces for their evolution. Interactions among polarization, fracture and breakdown in ferroelectric materials can be captured effectively and detailedly by the proposed model.

2. Results

Utilizing finite element method, the model was numerically implemented to predict the coupling evolution of fracture and breakdown. Under a set of interface boundary conditions, systematic simulations were carried out. The main results are outlined as follows:

a. The highly concentrated electric field at the impermeable crack tips can lead to the initiation of breakdown. The crack-tip breakdown will change the overall breakdown patterns within the materials. The influence of cracks on breakdown depends heavily on their relative directions to the electric field and polarization vectors.
b. If the breakdown can cause mechanical degradation of the material, the breakdown will relieve the stress concentration at the tip of the crack propagating through the breakdown defect. The stress relief effect

of the breakdown defect at the crack tip may decrease the crack driving force and slow down the crack propagation under fixed tensile displacement loadings.

c. If the mechanical degradation caused by the breakdown is negligible, the influence of breakdown on the crack propagation mainly comes from the change in the electric field, polarization and spontaneous eigenstrain. In this situation, the influence of breakdown on crack is more sensitive to the overall loading conditions and shows stronger nonlocality because of the participation of the polarization domain structures.
d. Simultaneous evolution of fracture and breakdown in the ferroelectric material exhibits more complex interactions. When the impermeable crack and the conductive breakdown channel meet each other, the crack attracts the electric tree because of the redistribution of the electric field. On the contrary, the deviation of the crack path occurs when the crack approaches to and leaves from the breakdown region.

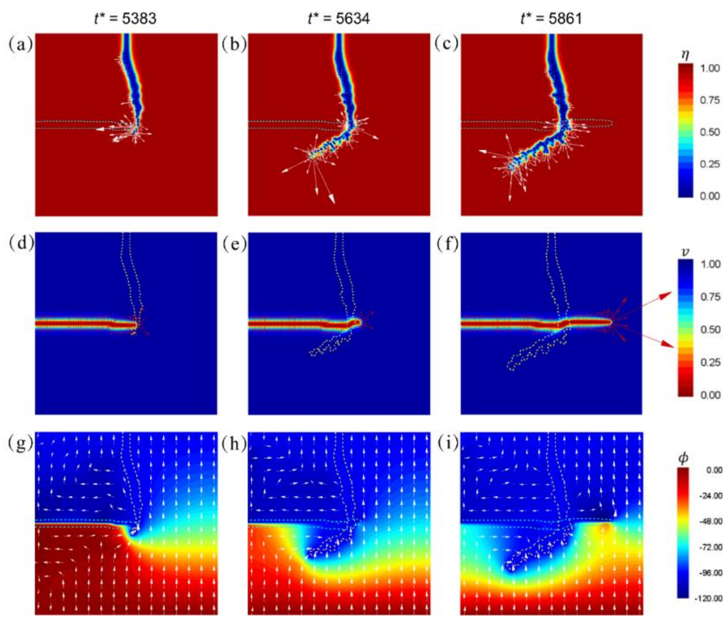

Fig.1 – Phase field simulation of coupling evolution of polarization, fracture, and dielectric breakdown in ferroelectrics.

3. Conclusions

The above results show that the phase field model is able to model the coupling behavior of simultaneous evolution of polarization, fracture and dielectric breakdown in ferroelectric materials. A set of interface boundary conditions were selected in the current demonstration, and more various interface boundary conditions can be easily implemented in current model framework by properly defining the detailed forms of the degradation functions. Furthermore, more complex electromechanical coupling failure in dielectric, piezoelectric and ferroelectric polycrystals, thin films and superlattices can be investigated by using the phase field model.

Acknowledgements

The financial support of the National Natural Science Foundation of China (Grant No. 12102387, Grant No. 11972320, Grant No. 12192214) and the Key Research Project of Zhejiang Laboratory (Grant No. 2021PE0AC02) is gratefully acknowledged.