TOUGHENING OF FERROELECTRICS BY THE OUT-OF-PLANE POLING*

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ABSTRACT: Subjected to the prior out-of-plane poling, the ferroelectrics can be toughened considerably. The present paper describes the variation of the stress intensity factor (SIF) by 90° switching in ferroelectrics. The analysis is carried out for the combined mechanical and electrical loading, with simple relations obtained for the case of the purely electrical loading. The out-of-plane poling is found to raise the SIF for the crack initiation, but appreciably reduces the SIF for the crack growth in a steady state. More stable fracture resistance curves can be achieved by the out-of-plane poling. This prediction is supported quantitatively by the testing data of SENB specimens of PZT-5 samples, when the toughening effects of polings in three orthogonal directions are compared.

KEY WORDS: ferroelectrics, domain switching, out-of-plane poling, fracture toughness, stress intensity factors

1 INTRODUCTION

Ferroelectric ceramics feature with the large switching strain and the low fracture toughness. The incompatible strain during domain switch may cause an internal stress as high as hundreds of mega-Pascals, while the fracture toughness assumes a typical value of 1 MPa·m$^{1/2}$. Therefore, fracture may occur from a flaw of a few microns. In fact, the actuators made by ferroelectrics are often found to crack around the edges of their internal electrodes when subjected to a high electric field. Fracture toughness anisotropy for poled ferroelectrics was extensively reported in the literature through the Vickers indentation[1~3] and the single edge notch beam[4]. Yang and Suo[5] modeled the relaxor ferroelectrics and derived the stress intensity factor (SIF) of a flaw around an electrode edge under the electric load. Lynch et al.[6] provided an explanation for the cracking in the relaxor ferroelectrics, either originated from an electrode or an impermeable flaw. Gao et al.[7~8] proposed a strip saturation model for electric yielding to investigate the variation of fracture toughness by the electric loading.

The stress and electric fields around a flaw assist the domain to reorient. Constrained by the unswitched material outside, the stress distribution near the flaw is altered. The variation of SIF at the crack tip dictates the fracture of ferroelectrics, whether under the electrical or the mechanical loading. Based on the approach[9] for the case of the mechanical loading, the present paper explores the case of the combined mechanical and electrical loading when the ferroelectrics are subjected to the prior out-of-plane poling. The analysis indicates that the out-of-plane poling raises the SIF for the crack initiation, but appreciably reduces the SIF for the crack growth in a steady state. The prediction is supported quantitatively by the tests of SENB specimens of PZT-5 samples[4], when the toughening effects of the polings in three orthogonal directions are examined.

2 SMALL SCALE 90° DOMAIN SWITCHING

In the presence of the electric and mechanical fields, the switch of 90° is activated by the combined mechanical and electrical work[10]

\[
\sigma_{ij}\Delta \varepsilon_{ij} + E_i \Delta P_i \geq 2P_s E_c
\]  

In Eq.(1), $\sigma_{ij}$ and $\Delta \varepsilon_{ij}$ are the stress and the switching strain tensor, $E_i$ and $\Delta P_i$ the electric field and the polarization switch vectors, $P_s$ the spontaneous polarization, and $E_c$ the coercive field. The right hand side of Eq.(1) describes an energy threshold for the polari-
ization switch. It is the domain switch of 90° that causes the variation of the fracture toughness of ferroelectrics.

The recent experiment by Zhu et al. \cite{11} supported the case of small scale switching for the crack growth in PZT-5 below the coercive field. Under an electric loading below the coercive field, the zone of domain switching is either focused at the crack tip or along the crack wake. If the applied field exceeds the coercive field, a 90° switching zone in the vicinity of the flaw is formed as a contrast to the 180° strain-free switching in the bulk. For the case of a mechanical loading, the presence of a flaw necessarily causes the stress concentration. As the result, the zone of domain switch activated by the crack tip stress is confined near the crack tip\cite{12',13'}.

For the case of small scale switching, the geometry can be regarded as a semi-infinite crack in an otherwise infinite medium. The stress field near the crack tip is characterized by $K_{app}$, the applied SIF, and is given by

$$
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix} = \frac{K_{app}}{\sqrt{2\pi r}} \begin{bmatrix}
1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \\
\sin \frac{\theta}{2} \sin \frac{3\theta}{2} \\
\frac{\theta}{2} \sin \frac{3\theta}{2}
\end{bmatrix}
$$

(2)

where $r$ and $\theta$ are polar co-ordinates centered at the crack tip.

The electric field concentration near the crack tip is also square-root singular. It is characterized by $K_E$, the electric intensity factor, and given by

$$
\begin{bmatrix}
E_1 \\
E_2
\end{bmatrix} \approx \frac{K_E}{\sqrt{2\pi r}} \begin{bmatrix}
-\sin(\theta/2) \\
\cos(\theta/2)
\end{bmatrix}
$$

(3)

The presence of a 90° switching zone alters the apparent fracture toughness. The toughness variation $\Delta K$ can be evaluated in the spirit of McMeeking and Evans\cite{14} for the case of transformation toughening. For a uniform switching zone bounded by an anti-clockwise contour $\Gamma_s$, $\Delta K$ is given by

$$
\Delta K = \oint_{\Gamma_s} T_i h_i d\Gamma
$$

(4)

For an instantaneous elastic isotropic response, the amount of the body force layer $T_i$ is given by

$$
T_i = 2\mu \Delta \varepsilon_{ij} n_j
$$

(5)

In Eq.(5), $\mu$ denotes the shear modulus, and $n_j$ the outward normal of $\Gamma_s$. Volume conservation during the domain switch is used in deriving Eq.(5). The weight function $h_i$ denotes the SIF caused by a unit point force along the $i$-th direction. The expressions of $h_1$ and $h_2$ are given as

$$
\begin{cases}
\hat{h}_1 = \frac{\hat{h}_1}{(\kappa + 1)\sqrt{2\pi r}} \\
\hat{h}_2 = \begin{bmatrix}
(1 - \kappa) \cos \frac{\theta}{2} + \sin \theta \sin \frac{3\theta}{2} \\
(1 + \kappa) \sin \frac{\theta}{2} - \sin \theta \cos \frac{3\theta}{2}
\end{bmatrix}
\end{cases}
$$

(6)

For the case of plane strain, $\kappa = 3 - 4\nu$; and for the case of plane stress, $\kappa = (3 - \nu)/(1 + \nu)$, where $\nu$ denotes the Poisson’s ratio.

3 DOMAIN SWITCH FOR FERROELECTRICS POLED OUT-OF-PLANE

3.1 Out-of-Plane Poling

Consider a specimen poled in the out-of-plane direction. With the presence of a crack, the in-plane singular stress field (2) and the electric field (3) may cause various domain switches of 90° near the crack tip. With a domain switch of 90°, the out-of-plane poling axis rotates to an in-plane polarization of an angle $\omega$ with the crack, see Fig.1. The angle $\omega$ can be arbitrary in the $x_1 \sim x_2$ plane, and will be determined by the methodology illustrated in subsection 3.2. The induced domain switching strain is

$$
\Delta \varepsilon_{ij} = \gamma_{s} \begin{bmatrix}
\cos^2 \omega & \sin \omega \cos \omega & \sin^2 \omega
\end{bmatrix}
$$

(7)

Fig.1 The crack tip domain switching for a specimen poled out-of-plane.