NONUNIFORM FERROELECTRIC DOMAIN SWITCHING CRITERION AND RELATED TOUGHENING DRIVEN BY TWO-PARAMETER CRACK-TIP STRESS FIELD

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Summary This paper issues a simple criterion to characterize nonuniform domain switching. The criterion is obtained by minimizing switch-induced system energy change computationally. Combining the numerical result and experimental observations, we propose a quasi-analytic criterion defined by a piecewise function. As examples, we apply the criterion to portray a nonhomogeneous switching zone near a stationary crack tip and to quantify the switch zone size. Then using the criterion we address a nonuniform ferroelastic domain switching model driven by two-parameter crack tip stress field. The model is applied to analyze the effect of transverse stress (T-stress) on switching zone geometry and switch induced toughening. The tensile T-stress decreases the switch toughening, while the compressive T-stress increases the toughening. As an example, the analytical result of the switch toughening is used to interpret the test dependency of the R-curve.

NONUNIFORM DOMAIN SWITCHING CRITERION

Minimum Energy

Consider a ferroelectric grain embedded within a homogenized ferroelectric matrix subjected to remote stress and electric field. The electromechanical load may drive domain to switch from one variant to another. Domain switching would cause a change of the system free energy. Using a composite Eshelby model, Yang et al. [1] quantified the system energy change of a switched grain with banded domain configuration. For convenience of analysis, the energy change is rewritten to be [2]

$$\triangle U = b_2 V_{90}^2 - b_1 V_{90} + b_0 \sqrt{f(V_{90})}\ , \tag{1}$$

where V_{90} is the volume fraction of the switched portion that undergoes 90° reorientation, b_2 and b_0 are constants only dependent on material properties, b_1 is a variable signifying the external work of complete switching. The energy change is composed of three terms, which all bear the meaning of energy densities per unit volume. The first term signifies the long-range elastic mismatch energy. The second denotes the external work. The third is the sum of three contributions : the short-range elastic mismatch energy, the electric depolarization energy, and the domain wall energy.

For any given load, the true V_{90} should minimize $\triangle U$ and vice versa :

$$\min_{0 \leqslant V_{90} \leqslant 1} \triangle U \Longleftrightarrow V_{90}\ , \tag{2}$$

where V_{90} is constrained on the interval $[\,0,1\,]$. To obtain the load dependency of V_{90}, we need to solve the minimum of the energy functional. Regretfully, it is impossible to find an analytical solution to V_{90} to exactly satisfy Eq. (2) because of nonlinearity. Thus far, seeking the nonuniform switching criterion is transformed into minimization of the energy functional, formulated in Eq. (2). Because of the nonlinear character, one has to resort to a computational technique to solve the minimum problem. Algorithms of golden section search and successive parabolic interpolation are combined to find the minimum computationally.

Combining the numerical result and the switch saturation effect observed experimentally, we put forward the following piecewise function to simulate the fraction versus energy density curve :

$$V_{90} = \begin{cases} 0 & \triangle W < \triangle W_{\text{th}} \\ V_{90}^{\text{th}} + k(\triangle W - \triangle W_{\text{th}}) & \triangle W_{\text{th}} \leqslant \triangle W \leqslant \triangle W_{\text{sat}} \\ V_{90}^{\text{sat}} & \triangle W > \triangle W_{\text{sat}} \end{cases}, \tag{3}$$

applicable to either mechanical or electrical loading. In above equation,

$$k = \frac{V_{90}^{\text{sat}} - V_{90}^{\text{th}}}{\triangle W_{\text{sat}} - \triangle W_{\text{th}}} \tag{4}$$

is the gradient of linear portion of the criterion, $\triangle W_{\text{th}}$ denotes a threshold work to trigger domain reorientation, $\triangle W_{\text{sat}}$ an ultimate work to saturate switching, and V_{90}^{sat} the corresponding fraction.

Applications of the criterion

After suggesting the criterion, this section devotes itself to depicting stress-induced nonuniform switching zone around the tip of a stationary crack, and to quantifying the switching zone size, in which PIC 151 is taken an example. According to our criterion, the switching zone near the crack tip is naturally divided into a saturated inner core and a transitional outer annulus. Based on the criterion, the contours of V_{90} can be simulated. The outmost contour line corresponds to the boundary of the switching zone. On the other hand, one applies the criterion to compute the switching zone size. The computed results are summarized in Table 1.

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Table 1. The comparison of the switching zone sizes between theoretical predictions and experimental data for PIC 151

$K^{\mathrm{I}}_{\mathrm{app}}$ (MPa$\sqrt{\mathrm{m}}$)	σ_{th} (MPa)	Prediction (μm)	Measurement (μm)
1.32[a]	11.5	408	420[a]
0.88[b]	11.5	181	290[b]
	9[b]	296	

[a] [3]
[b] [4]

Table 2. Testing data and $K^{\mathrm{T}}_{\mathrm{app}}$ for the bending and roller tests

			$K^{\mathrm{T}}_{\mathrm{app}}$ (MPa$\sqrt{\mathrm{m}}$)		
	σ_{T} (MPa) [7]	λ	Spherical	Cylindrical	Mean
TPB	2	0.087	0.97	2.13	1.65
Roller	20	0.87	0.93	1.44	1.18

NONUNIFORM SWITCH-TOUGHENING DRIVEN BY TWO-PARAMETER CRACK-TIP STRESS FIELD

With the presence of the domain switching, generally, the crack tip SIF K_{tip} is not equal to the remote SIF K_{app} any more. A toughness variation $\triangle K$ appears, by which K_{tip} is related to K_{app} as

$$K_{\mathrm{tip}} = K_{\mathrm{app}} + \triangle K\,. \tag{5}$$

If $\triangle K < 0$, the toughening effect functions and the external load is partially shielded.Here, we employ the two-dimensional weight function that characterizes the interaction between the crack and transformation strain [5]. Based on the above weight function, one arrives at

$$\frac{K^{\mathrm{T}}_{\mathrm{app}}}{K_{\mathrm{intrinsic}}} = \frac{1}{1 - \eta\, N(\alpha, \beta)\, F(\phi)}\,, \tag{6}$$

where

$$\eta = \frac{1}{32\,\pi}\frac{Y\,\epsilon_{\mathrm{sp}}}{1-\nu^2}\,,\; N(\alpha,\beta) = \alpha + k\,\ln(1+\beta)\,. \tag{7}$$

In above equation, η is a combination of material constants, $N(\alpha,\beta)$ is a toughness control factor that we will discuss later, $K_{\mathrm{intrinsic}}$ denotes the intrinsic fracture toughness, α and β are expressed as

$$\alpha = \frac{V^{\mathrm{th}}_{90}}{\sigma^{\mathrm{T}}_{\mathrm{th}}}\,,\; \beta = \frac{\sigma^{\mathrm{T}}_{\mathrm{sat}} - \sigma^{\mathrm{T}}_{\mathrm{th}}}{\sigma^{\mathrm{T}}_{\mathrm{th}}}\,, \tag{8}$$

and $F(\phi)$ is an analytic toughening function of the poling angle ϕ. [2, 6]

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