Numerical investigation of polarization reversal characteristics in a ferroelectric thin film

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A small-sized symmetric thin ferroelectric (FE) film, assumed second order and in the FE phase, of thickness l is considered. The Landau-Devonshire free energy of the film is expressed using the Tilley-Zeks model. A special case, in which the polarization values at both film surfaces are zero, $p_\pm = 0$, is assumed. The initial spontaneous polarization profile of the film at equilibrium is approximated using a cosine function. The Landau-Khalatnikov equation of motion is then used to obtain numerically the initial stable polarization profile; and to describe the dynamics of polarization reversal in the film under the action of a step driving electric fields. A finite-difference time domain method is utilized to simulate the switching process. Changes in the average polarization and the average polarization current during the switching are calculated and studied. The influence of temperature and thickness on switching is investigated.

Keywords: polarization reversal, thin film, ferroelectric, finite system

INTRODUCTION

Ferroelectric thin film has increasingly drawn attention of physicists for many years and has recently become of greater urgency due to their application in memory device technology [1-3]. The need of integration and miniaturization of ferroelectric material especially in microelectronics devices, has made understanding film properties due to effect of thickness and surfaces becomes crucially important. This has stimulated fundamental studies on size effects in ferroelectric thin films. While extensive theoretical studies of polarization reversal [4-6] have been done for bulk and thick film geometries, very little work has been devoted to study reversal in nano-scaled geometries in which the surface conditions can dominate over the bulk. As the film thickness gets into a nano-sized dimension, investigation on its polarization behavior near the surface under the influence of an applied electric field becomes very important.

For this reason, we study a FE film by using a discrete model to unravel the effect on polarization and thus on switching due to the influence of interactions between adjacent layers in a discretized film under action of an applied electric field. The influence on switching due to film thickness and temperature under the action of step field is investigated.

THEORY AND MODELING

We consider a small-sized symmetric thin FE film, assumed second-order, of thickness l extending from $\zeta = -l/2$ to $\zeta = l/2$, and assumed approximately one correlation length thick. The theoretical formalism is adopted from Chew et al.[7], in which the model is one-dimensional with polarization and related physical quantities varying as a function of z. The discussion is restricted to in-plane geometries where the thickness is

much less than the lateral dimensions so that depolarization effects can be neglected. The Landau-Devonshire free energy [7,8] in dimensionless form for a small-sized thin film of thickness l under an action of an applied electric-field e is

$$F = \int_{-\frac{l}{2}}^{\frac{l}{2}} [\frac{1}{2}\alpha p^2 + \frac{1}{4}p^4 + \frac{1}{2}\left(\frac{dp}{d\zeta}\right)^2 - \frac{2}{3\sqrt{3}}ep] \, d\zeta + \frac{1}{2\delta_r}(p_-^2 + p_+^2) \tag{1}$$

where $p_\pm = p(\pm l/2)$ are the polarization values at the boundaries. Here, $\alpha = t - 1$ and t is scaled temperature. The surface and size effects of the film are studied by introducing the so-called extrapolation length δ_r leading to the boundary conditions $dp/dz = \pm p/\delta_r$ at $\zeta = \pm(l/2)$. However in this work, we are only interested in the special case where $p_\pm = 0$ at the film surfaces [10] because this case has physical meaning and can be realized experimentally.

The dynamic of polarization reversal in the film may be described by the Landau-Devonshire-Khalatnikov equation of motion, which is the scaled form, is

$$dp/d\tau_R = -\delta F/\delta p \tag{2}$$

where τ_R is the dimensionless time. We define polarization current as $i = dp/d\tau_R$ [11]. Using (1), (2) becomes

$$dp/d\tau_R = -\alpha p - p^3 + (2/3\sqrt{3})e + (d^2p/d\zeta^2) \tag{3}$$

This is solved numerically by using the finite difference method, where only the range inside the thin film is considered. The polarizations at both surfaces (at the film boundaries) are assumed zero since we assume polarizations at the surfaces experience a pinning effect in which their values do not change with the applied electric field. To simulate the switching process, an initial polarization profile based on a cosine function of the form

$$p(j) = \sqrt{-\alpha}\cos(\pi j/2N) \tag{4}$$

is used where $-N \leq j \leq N$, j is the running index to indicate position along the thickness of the film from $-N$ to N, and $\sqrt{-\alpha}$ is the bulk spontaneous polarization value at equilibrium. Using (4), a stable profile in zero field is generated and this is used as the starting profile.

The bulk free energy is described by $F = (1/2)\alpha p^2 + (1/4)p^4 - pe$. At equilibrium, $\partial F / \partial p = 0$ and $\partial^2 F / \partial p^2 = 0$, and this gives the bulk coercive field, which is $e_C = \pm(-\alpha)^{3/2}$. It is temperature dependent.

RESULTS AND DISCUSSION

We examine the polarization reversal process by applying an external field in a form of a simple step field, $e(\tau) = \phi(\tau)e_o$ (where $\phi(\tau)$ is a step function of time, τ). Sequence of changes in the polarization profile during the switching process is shown in Fig. 1 which are plotted at different times for film of size, $2N = 20$ (Fig. 1(a)), and $2N = 50$ (Fig. 1(b)). Assume that the initial polarization at temperature $\alpha = -1.0$ is in the positive state at time $\tau = 0$ and the electric field, with magnitude $e_o = 1.01e_c$, is switched on at time $\tau = 0$. Comparison of these two figures shows that a thicker film takes a longer time to complete the switching process and that it occurs at the film surfaces first then gradually gets to the interior. The effect is obvious for thicker films, $2N = 50$, as illustrated by Fig. 1(b) and 1(c) at two different temperatures, $\alpha = -1.0$ and $\alpha = -2.0$, respectively. We also find that films at a lower temperature require shorter time to switch.

Fig. 2 shows the average polarization, p_{ave}, and $i_{ave} = dp_{ave} / d\tau$ for various strengths of step fields. For each field, we simulate the switching process starting at $\tau = 0$ and stop when the film reaches a new equilibrium state. As shown in Fig. 2(a) for

$2N = 20$ and at $\alpha = -1.0$, the initial average polarization is $p_{ave} \sim 0.8785$. We find that as the electric field strength increases it takes shorter time to switch to the opposite state. Observation of Fig. 2(b) shows that there is a peak in i_{ave} whenever there is complete switching. This suggests that a peak in the average polarization current indicates occurrence of switching.

Fig. 3 shows graphs of switching time versus electric field for four different sample of sizes $2N = 10$, 20, 50 and 100 at temperature $\alpha = -1.0$. Here, we define a switching time as the time taken for an initial value p_{ave} to reach $-p_{ave}$ under an action of external field. At the vicinity of coercive field ($e \approx 0.4$ in this case), the switching time is infinite. As the size decreases, the switching time gets shorter with an increase in the amplitude of the electric field. The inset shows the graphs for large applied electric field values. Notice that as the electric field increases the switching times for different thickness approach a certain limiting value close to zero.

CONCLUSION

We have found that for the step driving field the strength of the electric field needed to achieve complete switching can be much lower in a small-sized ferroelectric film, i.e. $e_o = 0.9e_c$, than the bulk coercive field value. However, it takes a much longer time to complete the switching process. And we also discover that as the field strength increases, the time taken to relax the thin film system decreases; and that thicker films take longer time to achieve polarization reversal. However, as the driving field strength increases, there seems to be an approach to a limiting switching time value, for any film thickness. It is also observed that the effect of temperature tends to have an influence in increasing the switching time. The results presented here are just preliminary. The

studies can be extended further to include other types of driving fields. Further studies

on the effects of $\delta < 0$ and cases involving $P_{\pm} \neq 0$ could be investigated.

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FIGURE CAPTIONS

Fig.1. Polarization profiles at selected times under the influence of a step field for $e_0 = 1.01 e_C$: (a) $2N = 20$, $\alpha = -1.0$, (b) $2N = 50$, $\alpha = -1.0$, and (c), $2N = 50$, $\alpha = -2.0$.

Fig. 2. Graphs of (a) average polarization, and (b) average polarization current versus time. Both for $2N = 20$, and $\alpha = -1.0$.

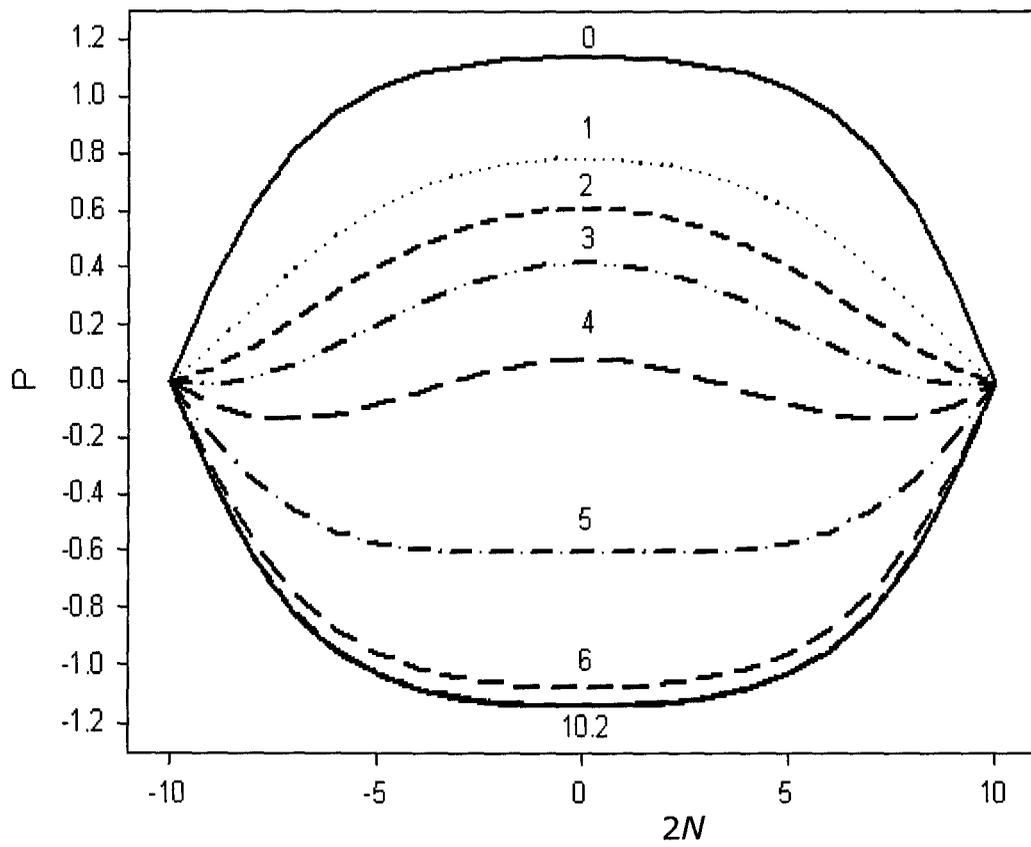Fig. 3. Graphs of switching time versus electric field of four different film thickness $2N = 10$, 20, 50 and 100 at $\alpha = -1.0$.
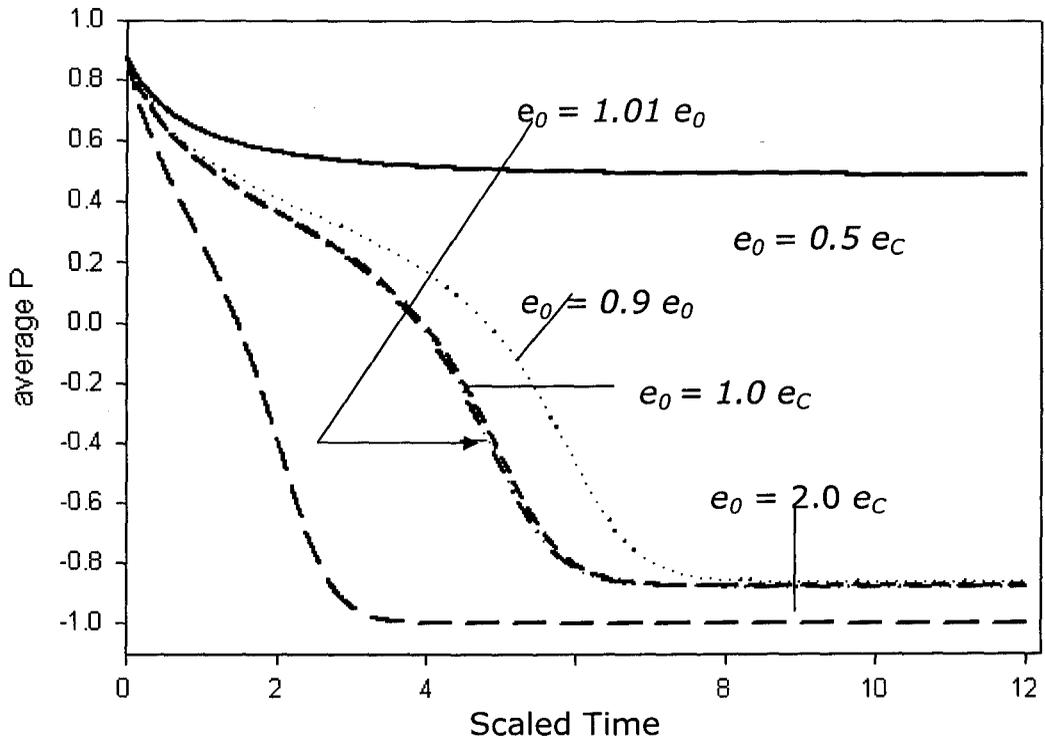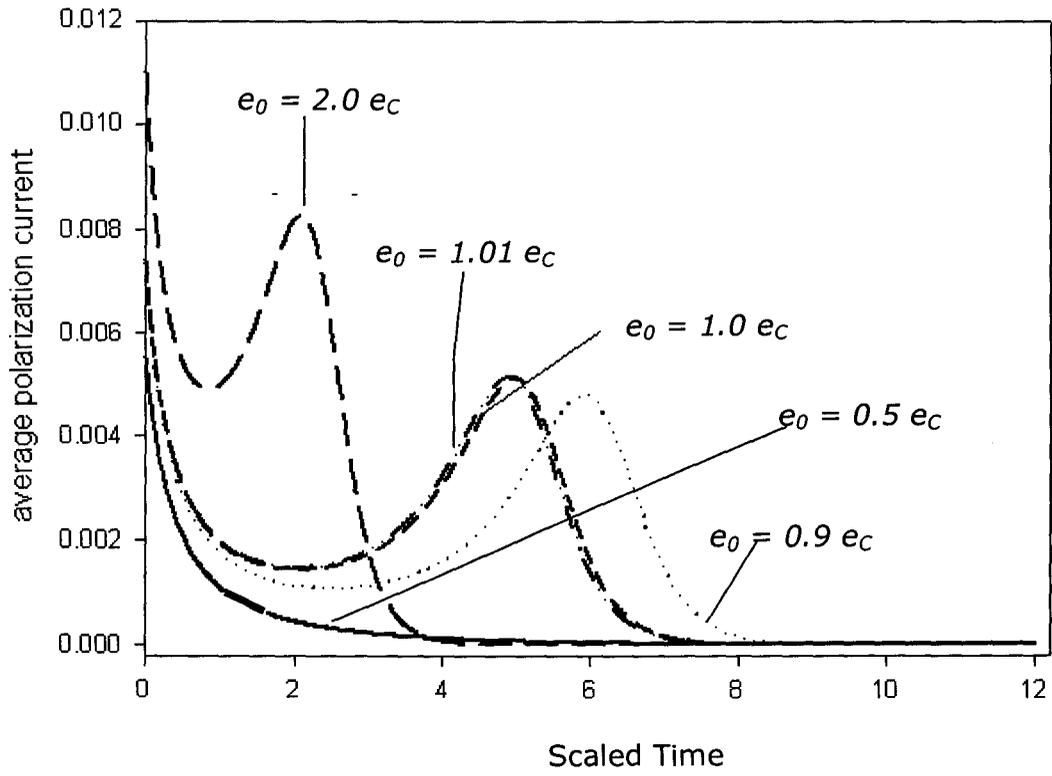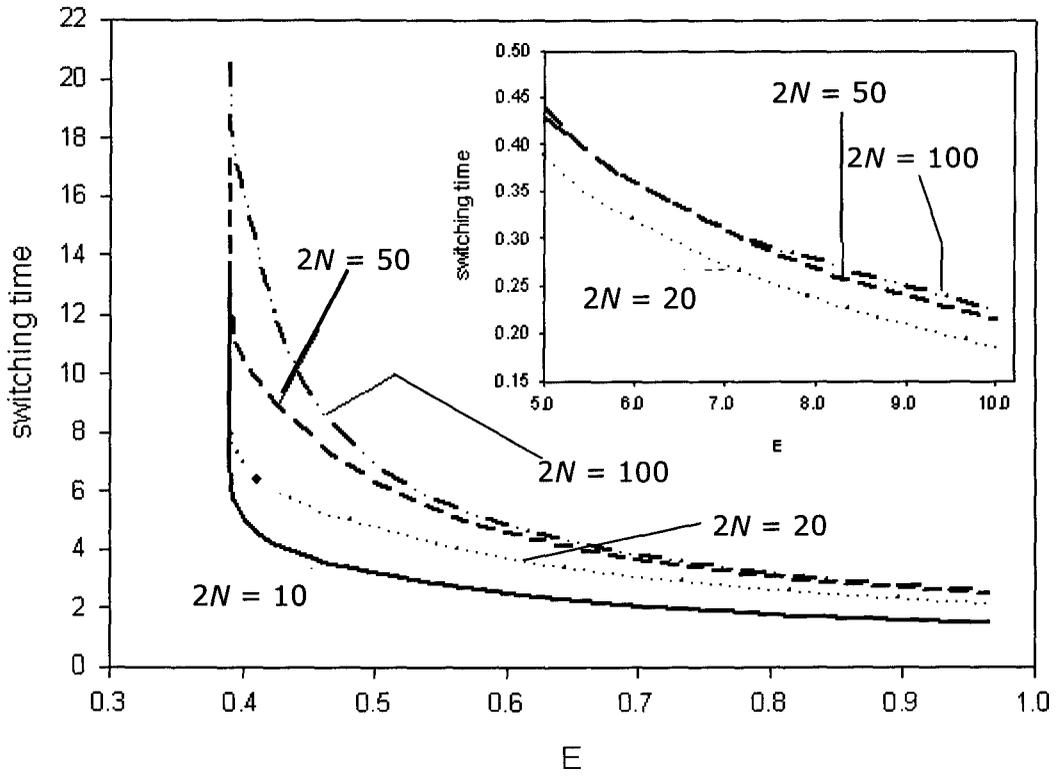
Fig. 1(a)
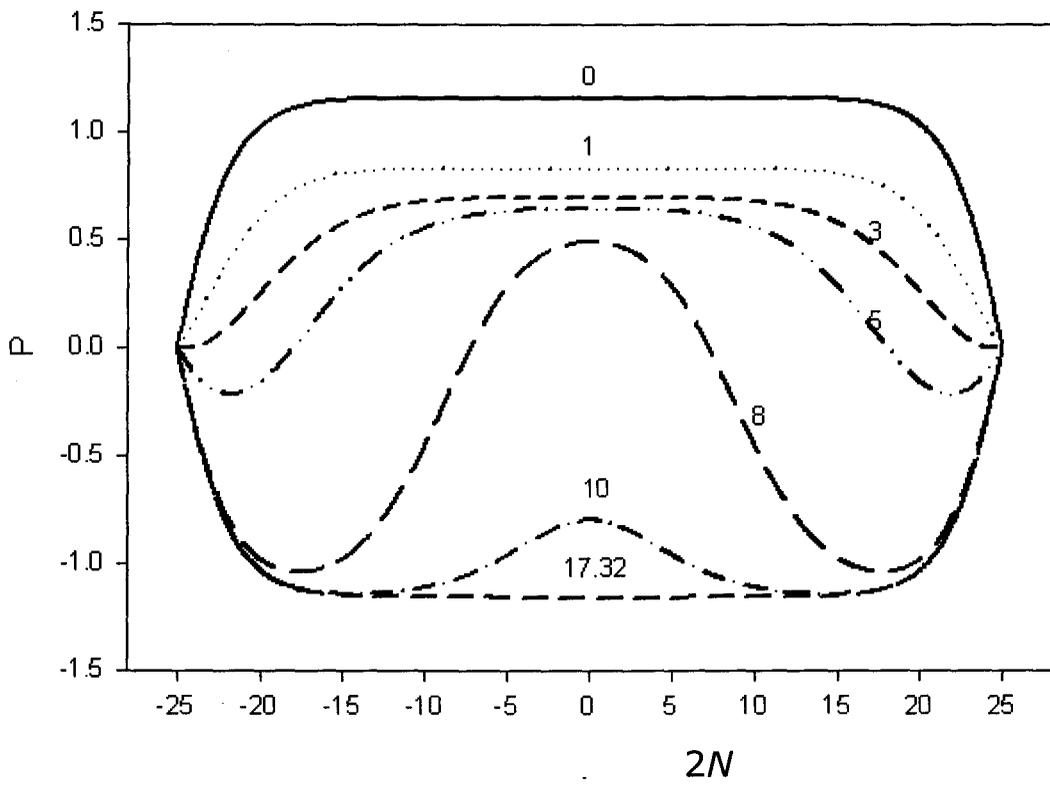
Fig. 1(b)

Fig. 1(c)

Fig. 2(a)

Fig. 2(b)

Fig. 3