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Analysis of Bulk Second-Order Ferroelectric Switching in Oscillatory Dynamical System

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ABSTRACT

A detailed analysis of polarization reversal in bulk for second-order ferroelectric (FE) *phase transition material in the framework of the Landau model is presented. We focus on the changes of polarization* P *and its switching current* j *with respect to time t in the presence of an external electric field* E*. By using the Landau-Khalatnikov (L-K) equation of motion, the dynamics of the* FE *material based on the oscillatory system is assumed. The changes in polarization and switching with respect to the different value of and temperature are* T_r *analyzed via numerical results.*

***Keyword (s)**: Ferroelectrics; Polarization Switching; Phase Transitions*

INTRODUCTION

In ferroelectric (FE), the spontaneous polarization P_S can be reversed in sense or reoriented by the application of an electric field larger than the coercive field. Reversal is also known as switching. The resulting states for each orientation are energetically and symmetrically equivalent in zero external electric field. P_S in most FE crystals is greatest at temperatures well below T_C and decreases to zero at T_C. In first-order ferroelectric-paraelectric phase transition, P_S may have a substantial value at temperatures very close to T_C, whereas in second-order phase transition, the decrease in P_S as temperature approaches T_C is more gradual.

The switching behavior in FE materials is very important because of its application in the FE memories. Ishibashi and Takagi[1] were the first to treat polarization reversal as an electrically induced phase transition, in the framework of the Kolmogorov-Avrami[2,3] theory. This theory is based on nucleation and growth of domains of opposite polarizations. Another approach is to use the Landau-Khalatnikov (L-K) equation of motion together with the Landau-Devonshire (L-D) expression for the free energy. Ishibashi[4] was the first to use the Landau theory of phase transitions to model the polarization reversal, obtaining dependencies of switching times according to experiments.

Switching behavior for the relaxational systems for both first and second order FE phase transition were given by Tan et al.[5] and Ricinschi et al.[6] in the bulk, semi-infinite and thin film. In reality, vibration of atoms in a FE material with the existence of electric field is

oscillatory in nature. Therefore, studying the switching phenomenon based on a damped oscillatory spring system is more realistic; that is what we have done and we present the results of the work here. The paper is organized as follows. The next section contains a detailed formalism of the switching dynamics beginning with the L-D free-energy expansion for the second-order phase transition. In Section 3, a brief outline of a numerical method using the Central Finite-Difference Approximation (CFDA) is described. The results obtained and some discussions are presented in Section 4.

METHODLOGY

Landau Model for Switching

The Landau-Devonshire (L-D) free-energy expansion for second-order phase transition in a non-equilibrium state is

$$F = (A/2\varepsilon_0)P^2 + (B/4\varepsilon_0^2)P^4 - EP \quad (1)$$

A and B are positive, and EP describes the coupling to the electric field and $A = a(T - T_0)$, where a is the inverse Curie constant. T_0 is temperature and P is the order parameter, polarization and ε_0 is a constant permittivity in vacuum. For an oscillatory damped system, the Landau-Khalatnikov (L-K) equation of motion may be written as

$$m(d^2P/dt^2) + \gamma(dP/dt) + \beta P = -(\delta F/\delta P) \quad (2)$$

where γ is the damping parameter. For ferroelectric (FE) materials, the restoring force constant β may be omitted. To have a universal result in the calculation that follows, we use standard dimensionless variables[5]. These are free-energy $f = F/F_0$ with $F_0 = (a^2T_0^2/B)$, polarization $p = P/P_0$ with $P_0 = (aT_0\varepsilon_0/B)^{1/2}$, electric field $e = E/E_0$ with $E_0 = (a^3T_0^3/\varepsilon_0 B)^{1/2}$, and temperature $T_r = T/T_0$. In terms of these, (1) becomes

$$f = [(T_r - 1)/2]p^2 + (1/4)p^4 - ep \quad (3)$$

and applying the Euler-Lagrange (E-L) equation to (3), (2) becomes

$$(d^2p/d\tau^2) + g(dp/d\tau) = (1 - T_r)p - p^3 + e \quad (4)$$

where damping parameter $g = \gamma / \gamma_0$ with $\gamma_0 = (m\varepsilon_0^3 / a^3 T_0^3)^{1/2}$ and time $\tau = t / t_0$ with $t_0 = (m\varepsilon_0 / aT_0)^{1/2}$. The LHS in (4) describes the soft-mode dynamic in damped oscillatory systems observed in many displacive FE. For a relaxational system, the second derivative of (4) vanishes and the problem can be solved analytically but for oscillatory system a numerical method is needed.

Numerical Approach

Here we used the Finite-Difference Method (FDM) to solve (4). Using the central finite-difference approximation (CFDA) in particular, (4) may be expressed as

$$p_{N+1} = \frac{\left((g\Delta\tau/2)-1\right)p_{N-1} + \left[2+(1-T_r)(\Delta\tau)^2\right]p_N - (p_N{}^3 - e)(\Delta\tau)^2}{\left[1+(g\Delta\tau/2)\right]} \qquad (5)$$

where p_{N+1} is the polarization to be computed, p_{N-1} is the previous calculated value and p_N the current value. The increment of time is given by $\Delta\tau$. Since the switching occurs in bulk FE, we take the initial polarization as $p_{N-1} = p_N = 1$. This is possible because the polarization in bulk medium is constant. Note that the switching current j is defined as *dp/dτ* and can be easily calculated from the numerical scheme. From Chew et al.[7], where $\beta = (1/aT_o) = 5.0$, $m = 6.4\times10^{-21} kgm^3 s^{-2} A^{-2}$ and $\varepsilon_o = 10^7/(4\pi c^2)$ for $BaTiO_3$, we can estimate the damping term viz, $g = 0.05$. Here, we assume that switching is completed if it changes the polarization from negative state to positive state or vice versa. We assume the initial polarization begins from the negative state, $p_{initial} = -1$.

RESULTS AND DISCUSSIONS

Figures 1 – 4 illustrate the behavior of polarization reversal or switching, , and the corresponding switching current, , versus time, , for various values of dependent parameters.

Figure. 1 shows the effect of temperature, , on switching for an applied electric field, . The oscillation behaves like a transient response[7]. The system reaches a steady state after all transients have died out and the time taken to reach this state is called the settling time[8]. For FE, it is called switching time in which it is the time taken for complete switching. Switching is defined as complete when the final polarization attains its absolute initial value and its direction is reversed. Fig. 1 shows that temperature has an influence on the switching state. Fig. 1(a) shows complete switching for = 0.2 but this is not attainable for the case = 0.99, that is as approaches 1 (the scaled critical temperature). This is as expected since as '! 1, the spontaneous polarization goes to zero.

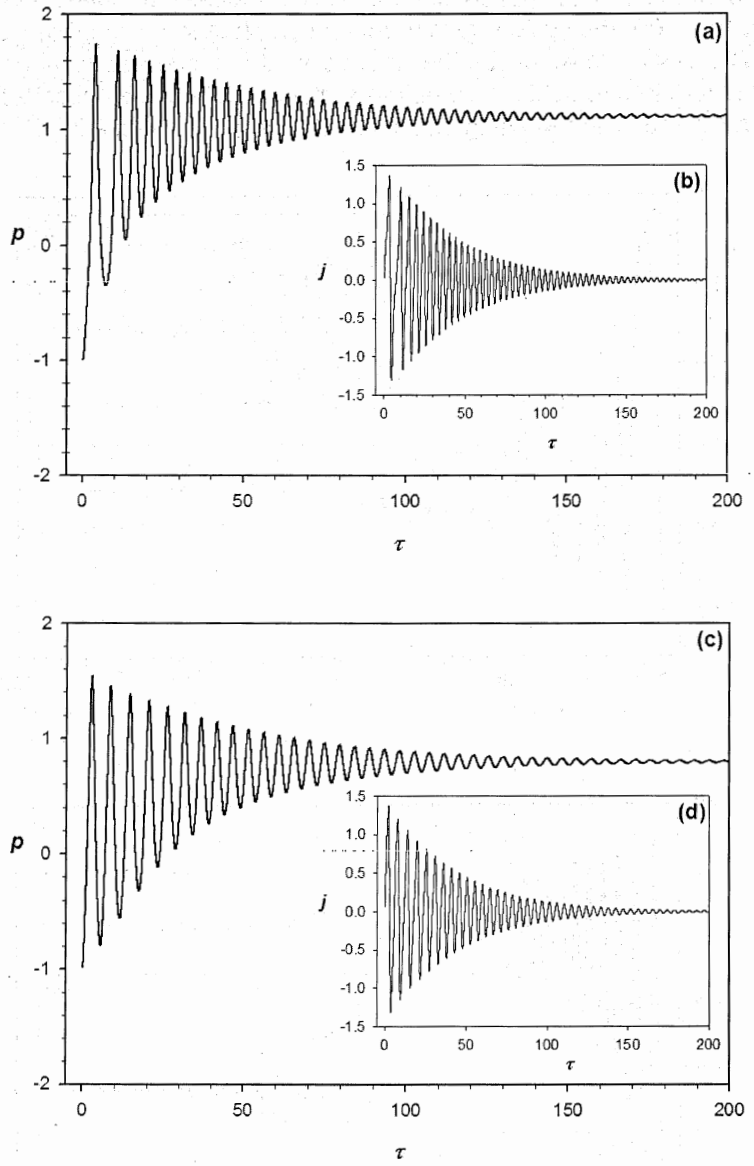

Figure 1 Temperature, T_r, effect in the ferroelectric phase with changing of polarization, p, versus time, τ, for (a) $T_r = 0.2$ and (c) $T_r = 0.99$. (b) and (d) are the switching current, j, for both temperatures respectively. Here, damping parameter, $g = 0.05$, and electric field, $e = 0.5$.

Figure. 2 shows the effect of applied electric field on switching or polarization reversal. As illustrated by Fig. 2(a), the system fails to reach complete switching if the applied field is small (e=0.01), e<<1. However, as the applied filed is increased towards 1 which is a minimum field required to achieve complete switching, it becomes possible as displayed by Fig. 2(b) for e=0.8. The switching current is also larger here (see inset).

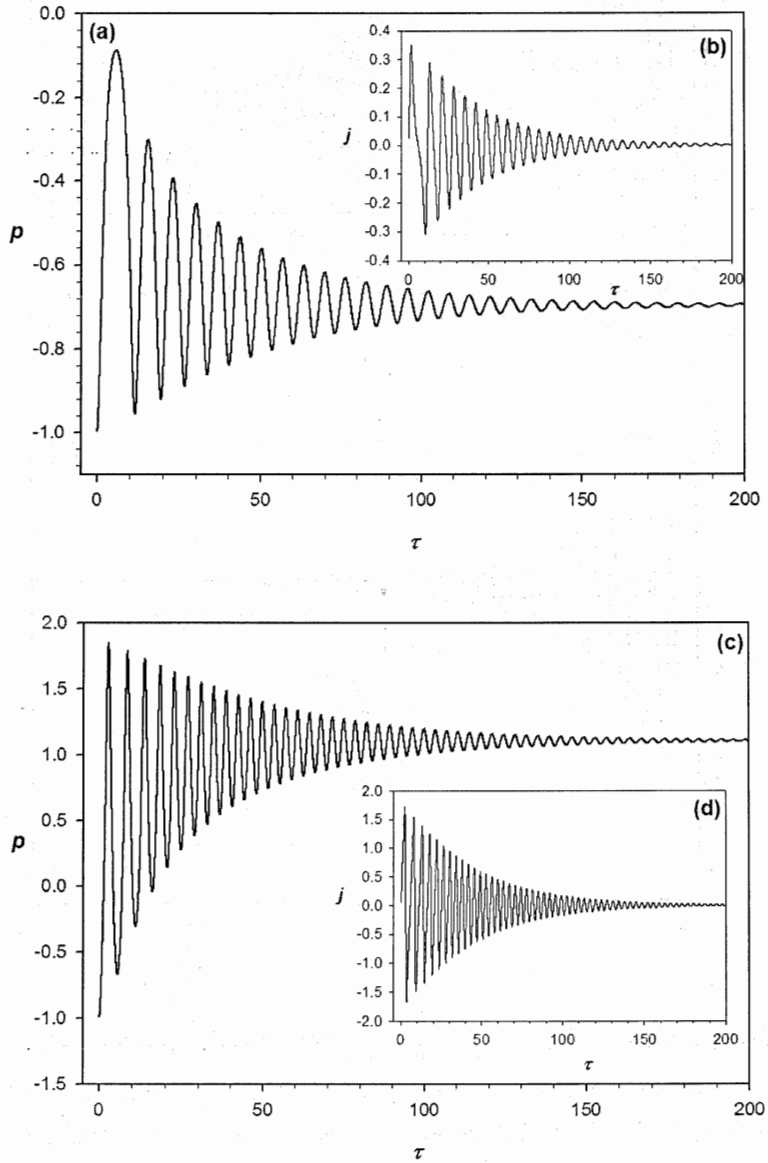

Figure 2 Switching behaviors for different electric field with (a) $e = 0.01$ and (c) $e = 0.8$ for $T_r = 0.5$. Fig. 2(b) and 2(d) refers to the current switching. Damping parameter, $g = 0.05$.

In an oscillatory damped system, the damping value *g* plays an important role in switching. This is illustrated with two values of damping parameter, $g = 0.001$ and $g = 0.5$ in Fig. 3. As expected, the graph in Fig. 3(b) shows that a high damping parameter results in a fast switching process.

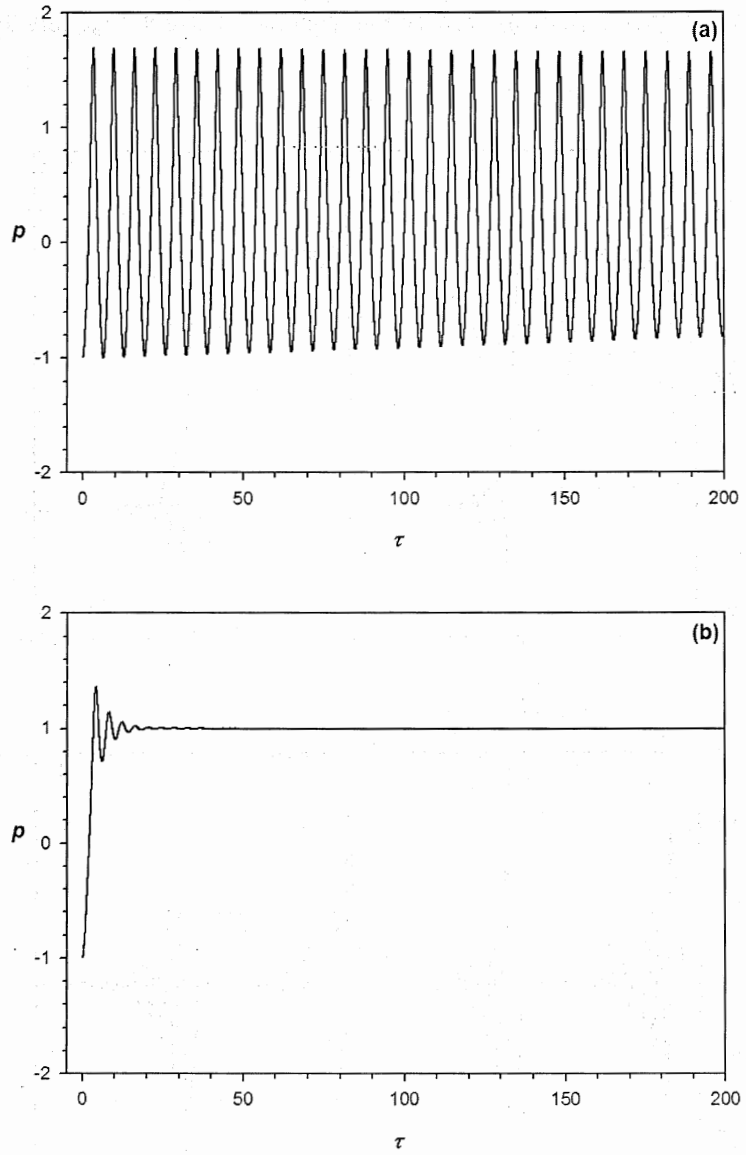

Figure 3 Polarization switching behavior for different damping values with (a) $g = 0.001$ and (b) $g = 0.5$ for $T_r = 0.5$ and $e = 0.5$.

In Figure 4, we show the switching behavior and the polarization current respectively for a step function electric field, where here the applied electric field is a function of time, . We assume = 0.2, g = 0.3, and the amplitude of the step field is e = 2 (from -1.0 to 1.0). As expected, complete switching is achieved with the values of the parameters chosen. The choice of damping is strong enough to stop the oscillation before the electric field changes its value again. The switching current surges to a high value whenever the applied electric field changes its sign (see Fig. 4(b)). A surge in switching current suggests the onset of polarization reversal.

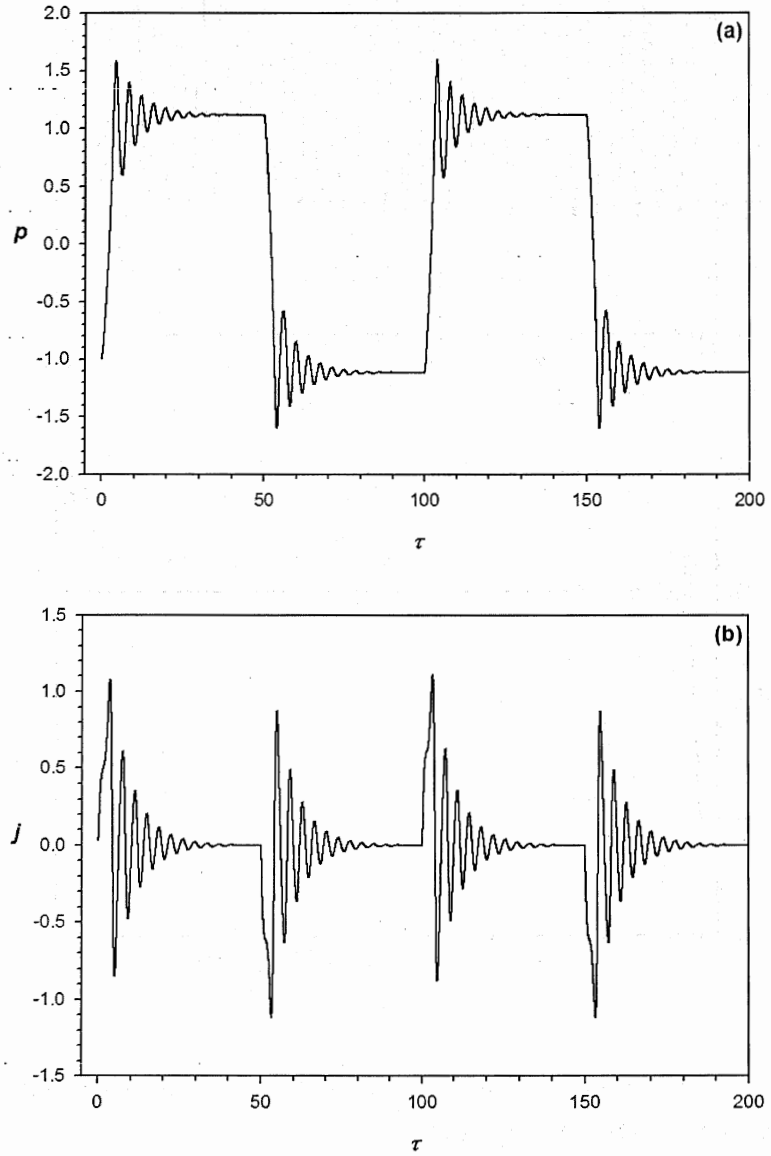

Figure 4 (a) Polarization switching behavior for step function electric field for $T_r = 0.2$ with damping parameter, $g = 0.3$. (b) The corresponding switching current, j, versus time, τ.

We can estimate real switching time predicted using our model. Based on the experimental value of $BaTiO_3$ parameters, we find that . Based on the switching behavior displayed by Fig. 1(a) for and e=0.5 where we find is the time taken for complete switching, hence . In reality, the switching behavior for a FE material is in the nanosecond (s) range. Nevertheless, our theoretical estimation is valid since we have neglected other effects like domain wall movement, surface effect which exists in FE films and etc. As an extension of this work, it will be interesting to investigate the behavior of polarization reversal in a thin FE film. We are currently investigating it and hope to publish the results in the near future.

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