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Analytical Landau-type model of polarization switching in ferroelectrics

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Abstract

The polarization switching properties of ferroelectric materials have been extensively studied, both experimentally and theoretically owing to their wide applications in industry and hence generating a need to gain a deeper understanding of factors affecting their switching behaviour. In this paper, an analytical Landau theory incorporating the Landau–Khalatnikov equation has been developed to describe the switching properties of second order ferroelectrics. Analytical expressions derived from exact results of Landau theory are used in modelling work carried out in this study for comparison with trends predicted by empirical laws used to describe polarization switching behaviour at high electric fields. As such this work has established the theoretical basis for empirical laws of polarization switching and developed simple numerical tools which can be quickly used to model trends in polarization switching behaviour of ferroelectrics.

Keywords: C. Ferroelectric properties; E. Functional applications; Polarization switching

1. Introduction

The properties of ferroelectric materials have been widely studied both experimentally and theoretically. In particular the polarization switching behaviour of ferroelectric material is often described by empirical formulae based on experimental studies of several ferroelectrics [1–3]. The focus of this paper is to provide a theoretical basis for the linear behaviour of the reciprocal switching time at high electric fields within the framework of the phenomenological Landau theory. Towards this end the Landau–Khalatnikov equation is solved exactly to produce an exact expression for polarization switching time that changes with temperature and electric field. Subsequently it is shown that the empirical formula [4] between the maximum switching current, time taken to reach the maximum switching current and the maximum polarization attained under the influence of high electric field is valid using the analytical Landau theory developed in this work. The second motivation for this work is to develop simple programs [5] where quick calculations can be performed to determine the general trends in the switching behaviour of ferroelectric materials in a straightforward fashion by varying the parameters affecting polarization switching behaviour directly.

2. Analytical expressions for polarization reversal time

In this section the universal dynamic behaviour of second order bulk ferroelectrics is described. From the scaled equation of the free energy f as shown below [6],

$$f = \frac{1}{2}(t-1) + \frac{p^4}{4} - \frac{2ep}{3\sqrt{3}} \tag{1}$$

where t denotes the scaled temperature, p denotes the scaled polarization and e denotes the scaled applied electric field. The dielectric equation of state is derived as follows:

$$e = \frac{3\sqrt{3}}{2}\left[p^3 - (1-t)p\right] \tag{2}$$

2.1. Maximum polarization

When the ferroelectric material at temperature t is subjected to an applied electric field e, complete polarization reversal only occurs if the applied electric field e

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exceeds the coercive electric field e_c as stated below,

$$e > e_c \text{ where } e_c = (1-t)^{3/2}. \tag{3}$$

During the switching process, the ferroelectric material undergoes a complete polarization reversal, starting from $-p_e$ until it reaches the maximum polarization p_e. The expression for the maximum polarization p_e given by

$$p_e = \sqrt{\tfrac{1}{3}}\left\{\left[e+\sqrt{e^2-(1-t)^3}\right]^{1/3}+\left[e-\sqrt{e^2-(1-t)^3}\right]^{1/3}\right\} \tag{4}$$

is obtained from the solution of Eq. (2) as a cubic equation [7].

2.2. Landau–Khalatnikov equation of motion

Then the factorized scaled Landau–Khalatnikov equation [5, 8] in the form

$$\frac{dp}{d\tau} = (p_e-p)\left(p^2+pp_e+\left(p_e^2-(1-t)\right)\right) \tag{5}$$

is integrated using the partial fractions method [9] to yield the polarization reversal time τ given by the following equation:

$$\tau = \frac{1}{3p_e^2-(1-t)}\left\{\tfrac{1}{2}\ln\left[p^2+p_e p+p_e^2-(1-t)\right] + \frac{3p_e}{\sqrt{3p_e^2-4(1-t)}}\tan^{-1}\frac{2p+p_e}{\sqrt{3p_e^2-4(1-t)}} - \ln(p_e-p)\right\}+c \tag{6}$$

since p_e is an explicit function of electric field e, the polarization switching time derived in Eq. (6) is an explicit function of both temperature t and applied electric field e.

In conjunction with Eq. (6), the root solving procedure given by,

$$\tau(p_i) = k_i \tag{7}$$

is carried out such that for each particular instant of time k_i, the corresponding value of polarization p_i is determined. Following this procedure, the temporal variation of the polarization current is evaluated using the equation,

$$j(\tau) = (1-t)p(\tau)-p^3(\tau)+\frac{2e}{3\sqrt{3}}. \tag{8}$$

By applying standard analytical methods to Eq. (8), the maximum polarization current j_M at temperature t and electric field e is obtained as shown below,

$$j_M = \tfrac{2}{3\sqrt{3}}(e+e_c). \tag{9}$$

when the polarization current reaches its maximum value j_M, the polarization of the ferroelectric material is

$$p_M = \sqrt{\tfrac{1-t}{3}} \tag{10}$$

Then by substituting the value of p_M from Eq. (10) into Eq. (6) the time τ_M required by the ferroelectric material to reach a maximum polarization current j_M can be determined.

3. Relationship between the empirical laws of polarization switching behaviour and analytical Landau theory

3.1. Reciprocal polarization switching time

Empirically, it has been shown the reciprocal switching time of several ferroelectric material such as Lead Zirconate Titanate [1], Barium Titanate [4,11] and Tryglycine Sulphate [10] obey a linear law at high electric field E is given by,

$$\tfrac{1}{\tau_s} = kE \tag{11}$$

with k as a constant.

In this work, the theoretical basis of this empirical law is re-examined using the analytical Landau theory. This aspect of the study begins by modelling the linear trend in reciprocal switching time, as predicted by the empirical Eq. (11). The exact expression for switching time given by Eq. (6) is used to generate graphs of reciprocal switching time at three selected temperatures $t=-1$, 0 and 0.5 with the graph for each selected temperature shown from low ($e=1.01e_c$) to high ($e=10$) electrics fields.

Fig. 1 shows the trend of reciprocal polarization switching time at high electric fields. It is seen that the reciprocal switching time curves generated from Eq. (6) at all the three selected temperatures produce an apparent linear trend similar to the linear behaviour reported in previous experimental studies [10,11] at high electric fields. The origin of this linear trend is investigated further using the analytical Landau theory, i.e. by deriving from Eq. (6) an expression for reciprocal switching time valid at the high electric field region given below as,

$$\frac{1}{\tau_{pe}} = \frac{(2e)^{2/3}}{\ln 2\sqrt{3}+\sqrt{3}\pi/2-\ln(1-\delta)} \tag{12}$$

Eq. (12) shows that at a high electric field e, the reciprocal switching time is predominantly an $e^{2/3}$ phenomenon. The graph of reciprocal switching time at high electric fields given by Eq. (12) is also shown in Fig. 1 beside the three graphs generated from Eq. (6).

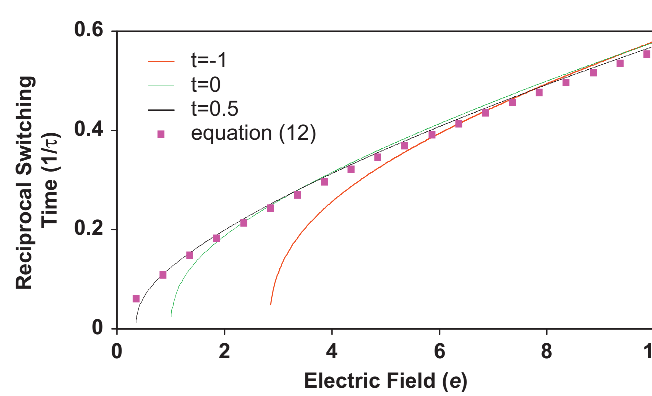

Fig. 1. Reciprocal switching time for temperatures $t=-1$,0 and 0.5. Dotted lines represent Eq. 12.

The results of Fig. 1 show that the reciprocal switching time $1/\tau_{pe}$ at all the three selected temperatures satisfy Eq. (12) in regions of high electric fields. In regions where the electric field is low (nearer to the coercive electric field) the curves for $1/\tau_{pe}$ do not overlap with the curve produced from Eq. (12) except in the case for temperature $t=0.5$. In this case due to the weak coercive electric field the curve for $1/\tau_{pe}$ overlaps with the curve generated from Eq. (12) almost from the beginning of its graph. Based on Eq. (12) it has been established that the apparent linear change of $1/\tau_{pe}$ at high electric field is actually due to a dependence on $e^{2/3}$ and not e.

3.2. Relation between the maximum switching current and the maximum polarization

Empirically, the three parameters involved in the polarization switching phenomena: (i) maximum polarization current j_M, (ii) switching time for maximum polarization current τ_M and (iii) the maximum polarization p_e are related according to the following equation:

$$\tau_M \times J_M \propto p_e \tag{13}$$

This empirical law was originally proposed by Fatuzzo and Merz [10] and re-derived recently by Tura and Mitoseriu [4] who based their work on domain growth caused by a nucleation process dependent upon the applied electric field.

In the following section, it is shown that Eq. (13) is obtained analytically from the exact solution of the Landau–Khalatnikov equation. Under the condition of high electric field, with the initial polarization of the material at $-p_e$, an electric field e acting in the positive polarity is suddenly applied to switch the material until it reaches the maximum polarization current j_M.

The switching time τ_M taken to reach the maximum polarization current j_M is obtained by simplifying Eq. (6) to become,

$$\tau_M = \frac{\left[\pi/\sqrt{3}+\ln 2+3(1-t)^{1/2}/(2e)^{1/3}+(1-t)/2(2e)^{2/3}\right]}{(2e)^{2/3}-(1-t)} \tag{14}$$

and the corresponding maximum polarization current is already given in Eq. (9). Therefore, the product of j_M and τ_M given by Eqs. (9) and (14), respectively, reduces to Eq. (13) after performing algebraic reductions based on the assumption of high electric fields. In the derivation of Eq. (13) the maximum polarization p_e given by

$$p_e = \frac{(2e)^{1/3}}{3^{1/2}}\left[1+\frac{1-t}{(2e)^{2/3}}\right] \tag{15}$$

is used. Eq. (15) is derived from Eq. (4) under the condition of high electric field. The work in this section establishes the empirical law stated in Eq. (13) as part of the Landau–Khalatnikov description of polarization reversal of second order bulk ferroelectrics.

In order to model the relationship represented by Eq. (13), Fig. 2 has been produced. The graph of the product

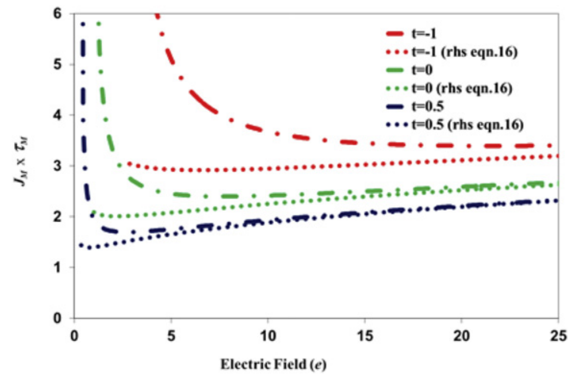

Fig. 2. Product rule of maximum polarization current with its switching time. Squares represent expression on the right-hand side of Eq. (16).

$\tau_M \times J_M$ is shown by dashes whereas the graph of the expression on the right-hand side of Eq. (16) below

$$\tau_M \times J_M = \frac{p_e}{3}\left(\frac{\pi}{\sqrt{3}}+\ln 2+\frac{3(1-t)^{1/2}}{(2e)^{1/3}}+\frac{(1-t)}{2(2e)^{2/3}}\right) \tag{16}$$

is shown in the same figure represented by circles. Both sets of graphs are produced at the three selected temperatures $t=-1.0$, 0 and 0.5.

The overlap of the two sets of curves when the electric field is high establishes the validity of the empirical formula represented by Eq. (13) within the analytical Landau theory of ferroelectric phase transitions. However the value of the constant term is not fixed as derived in previous empirical studies. Instead, it has been shown to depend on both temperature and electric field in this paper. From Fig. 2, it is deduced that at each selected temperature, Eq. (13) is not satisfied at electric field with magnitude around the coercive electric field e_c but close agreement with Eq. (13) occurs at higher electric fields.

4. Conclusion

The analytical Landau theory developed in this work has produced an exact expression for the polarization switching time of ferroelectrics. Using this result in the regime of high electric field, the linear behaviour of the reciprocal switching time described empirically as due to the linear effect of e is attributed instead to the $e^{2/3}$ effect. Another important result obtained is to derive theoretically the empirical formula relating the product of the maximum switching current and the time taken to reach the maximum switching current to the maximum polarization reached under conditions of high electric field. As such this work provides the theoretical basis for the empirical formulae used in the description of polarization switching behaviour of ferroelectrics. Due to their analytical nature, the results obtained in this work are suitable for modelling polarization switching behaviour of ferroelectrics in a straightforward procedure.

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