Theoretical and experimental investigations of polarization switching in ferroelectric materials

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(Received 4 April 2003; revised manuscript received 15 September 2003; published 27 February 2004)

The polarization switching process is certainly the most important feature of ferroelectric materials from fundamental as well as practical points of view. In this paper, a one-dimensional lattice model is presented in order to describe the polarization switching process in ferroelectric materials, incorporating the contribution of both dipolar defects and depolarizing fields to the domain reorientation. The influence of the interaction strength between switchable dipoles and dipolar defects, the medium viscosity, the depolarizing fields, and the frequency of the external electric field on the polarization switching were simulated. It was found that the degree of interaction between domains and dipolar defects has a strong influence on the coercive field, polarization, and backswitching behavior. Through an adequate analysis of the variables in the model it was also possible to describe the evolution of the polarization switching with the number of electric field cycles, which is commonly observed in the fatigue or depinning process. Comparison between simulated and experimental results revealed a remarkable concordance.

DOI: 10.1103/PhysRevB.69.064117 PACS number(s): 77.80.Fm, 77.80.Dj, 77.22.Ej, 77.22.Jp

I. INTRODUCTION

Undoubtedly, the most interesting feature of ferroelectric materials is that its spontaneous polarization can be reversed continuously under a high bipolar electric field.[1] Over the last years, significant experimental and theoretical advances have been reached in the ferroelectricity field, allowing us to understand and predict several ferroelectric properties. These advances are fundamental to understanding the mechanisms involved in the polarization switching process in order to produce high quality materials, mainly those related to memory devices.

According to Fatuzzo and co-workers,[1,2] the polarization switching mechanisms for $BaTiO_3$ single crystals involve the nucleation of antiparallel domains and their growth by domain wall motion. Nevertheless, obviously real crystals and ceramics are not perfect and infinite and, consequently, the polarization switching is strongly influenced by the presence of defects and surfaces.[3] Focusing specifically upon defects, they may be basically classified in two groups, i.e., space charges[4,5] and dipolar defects (also called complex defects),[6,7] which induce significant and, mainly, opposite influences on the switching properties.[8–10] For instance, it has been experimentally shown that dipolar defects act naturally as pinning points for the domain rotation, resulting in lower polarization and coercive field values compared to the defect-free case.[8,9,11] On the other hand, the progressive loss of the switchable polarization after continuous switching cycles is related to space charges, mainly oxygen vacancies. Indeed, for most ferroelectric samples in the virgin state these vacancies are distributed randomly into the bulk and can be considered as uncorrelated point defects.[12,13] Nevertheless, it has been proposed that continuous polarization switching induces their gradual ordering in two-dimensional planar arrays parallel to the electrodes, resulting in a pinning of the domain walls.[12,14,15] Additionally, lower values have also been found for the polarization as well as for the strain induced by electric field[16] in relation to those predicted theoretically.[17,18] However, theoretical predictions are strictly upper limits, because they do not consider some factors that can limit the domain reorientation as, for example, depolarizing fields.[16,19] Thus, these constraints must be taken into account in the theoretical analysis in order to obtain a more realistic ferroelectric model.

The conventional theory-experiment basis for scientific research has been expanded to include computer simulation, which is an increasingly important component of many research lines. In the last decades several models, based on a Landau-type transition, have been reported to explain the switching properties of ferroelectric materials. For instance, Ishibashi and co-workers[20–22] proposed a phenomenological one-dimensional model based on the free energy, assuming that all sites in the lattice have the same interaction coefficient between the nearest neighbor dipoles. This model has shown to be helpful in representing uniaxial ferroelectrics that contain only 180° domain and domain walls. In addition, in real experiments there are multiple nucleation events, thus the classical nucleation and unrestrictedly grow of domains would not be valid, as proposed recently by Tagantsev *et al.*[23] Although these models have furnished a good qualitative accordance with some experimental results, none of them is adequate to describe the characteristics of polarization switching and its evolution with the number of electric field cycles observed in polycrystalline ferroelectrics containing impurities. Therefore, a more general model, which takes into account the influence of several constraints such as defects and depolarizing fields, is necessary in order to represent properly the polarization switching process.

In this paper, a phenomenological model that describes both the fundamental characteristics of domain switching and the influence of defects and depolarizing fields on the polarization switching behavior. Simulated and experimental results are compared and discussed based on the influence of defects, viscosity and restoring force on the domain dynamics. The paper is organized as follows. Sections II and III contain the theory and the experimental procedure, respectively, while the theoretical results as well as the discussions

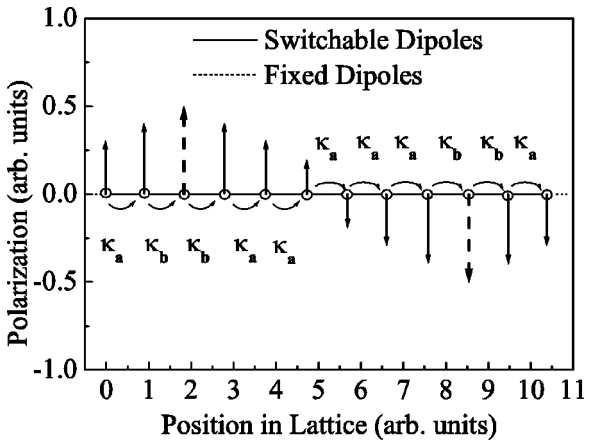

FIG. 1. Schematic representation of the ferroelectric system showing the interaction between the switchable dipole-switchable dipole (κ_a) and the switchable dipole-fixed dipole (κ_b).

are presented in Sec. IV. Finally, concluding remarks are given in Sec. V.

II. THEORY

The model consider an one-dimensional lattice with N sites where each site has a dipole moment p_n. In the case of a second order phase transition, the total free energy of the lattice is expressed as[20]

$$f=\sum_{n=1}^{N}\left\{\frac{\alpha}{2}p_n^2+\frac{\beta}{4}p_n^4+\frac{\kappa_n}{2}(p_n-p_{n-1})^2-p_n e\right\}, \quad (1)$$

where α and β are the Landau coefficients, which describe the second order ferroelectric-paraelectric phase transition, and κ_n is the interaction coefficient between the first neighbors. Among all dipoles in the lattice it is considered that there are N' fixed ones not switchable, called latent dipoles or simply latent nuclei that are randomly distributed in the lattice. It is possible to relate these fixed dipoles to nucleation seeds (dipolar defects) present in the material, as will be shown later. The amount of positive and negative latent nuclei in the lattice is the same, which can assume only values $p_n \geqslant 1$ and $p_n \leqslant -1$.

In this model we consider two different interaction coefficients. If the first neighbor of a switchable dipole is another switchable dipole it is assumed that the interaction coefficient between them is κ_a. However, if the first neighbor of a switchable dipole is a latent nucleus (positive or negative) the interaction coefficient is κ_b. In this way, it is possible to discriminate systematically the interaction between switchable dipole-switchable dipole and switchable dipole-latent nucleus. Figure 1 represents schematically the interaction between different dipoles. In a ferroelectric material the switchable dipole can hardly change its magnitude, but it can flip under the influence of an external electrical field. Thus, in the proposed model the variation of the dipole moment of the switchable dipole with time must be understood as the projection of a rotating dipole in a plan parallel to the latent dipoles. In this sense the model can be used to describe the behavior of a three-dimensional lattice.

It is assumed that each site in the lattice is influenced not only by the external electric field and the interaction between the first neighbors, but also by the instantaneous total polarization of the whole lattice, which cause a delay in the time dependence orientation of each dipole. In this way, the time dependence of the projection of each dipole in the lattice, under an external electrical field, is governed by the Landau-Khalatnikov equation[24]

$$\gamma\frac{dp_n}{dt}=-\frac{df}{dp_n}-\lambda\overline{P}, n=1,...,N, \quad (2)$$

where γ is the viscosity coefficient, λ is a constant and $\overline{P}$ is the average instantaneous total polarization (macroscopic polarization), given by

$$\overline{P}=\sum_{n=1}^{N}p_n(t). \quad (3)$$

The equation of motion for the dipoles [Eq. (2)] was integrated numerically using the predictor-corrector method of fifth order. Periodic boundary conditions were imposed. Simulations of systems consisting of $N=250$, 500, and 1000 dipoles with different amounts of latent nuclei (N') but always maintaining the same percentage of latent dipoles were done in order to analyze the size effects. It was verified that the results were independent of the system size. The maximum percentage of latent dipoles studied was $N'/N=6.5\%$. Therefore, the simulations reported here were performed for a system consisting of $N=250$ dipoles. The external electric field applied was given by $e=e_0\sin(\omega t)$, ω being the frequency of the applied electrical field. In the next section, we discuss the influence of the variables N', γ, κ_a, κ_b, and λ, and the frequency of the external electrical field in the ferroelectric properties as a whole.

III. EXPERIMENTAL PROCEDURE

$Pb(Zr_{0.53},Ti_{0.47})O_3$ bulk ceramics were prepared by conventional oxide mixing process and doped with either 1-wt.% Nb_2O_5 (softer or donors) or Fe_2O_3 (hardener or acceptors), hereafter labeled as PZTN and PZTF, respectively. Fe_2O_3 was added in the PZT to form dipolar defects (also called complex defects) due to the association of the acceptor atom (Fe^{3+}) with the oxygen vacancies (Vo^{2-}), which in the virgin state are aligned parallel to the polar direction of the domains.[6,7] The precursor oxides were mixed in ball mill, dried and calcined at 850 °C for 3.5 h. Discs shaped samples were sintered at 1250 °C in a saturated PbO atmosphere. Scanning electron micrographs showed that the average grain size is 3.0 μm. The sintered samples 17 mm in diameter were polished, and after that they were heat treated at 600 °C for 30 min to release stress induced during the polishing and to remove organic materials. Silver paint was used as electrode.

For the characterization of the transient current, a set up constituted by a symmetrical dc source (+1500 and 1500 V)

and a resistor ($R=20\ \mathrm{k}\Omega$) in series with the sample was constructed. In parallel with the resistor were connected an oscilloscope (Tektronix-model 2232) and a voltmeter (GB8050A). Both were interfaced with a microcomputer where the data could be stored. The oscilloscope measure shorter times ($300\ \mu\mathrm{s}<t<80$ ms), while the voltmeter measure longer times ($t>80$ ms) for the transient current. The external electric field was previously applied on the samples for 30 min, after that it was inverted with the aid of a manual switch. Thus, the transient current was measured as a function of the time until a steady state current to be detected. In order to estimate the *RC* charging (*C*-sample capacitance) or nonswitching current contribution to the total current, two consecutive pulses of the same polarity were applied on the samples. The pure current related to the ferroelectric polarization reorientation was computed subtracting the no-ferroelectric switching current (*RC*) in all measurements. A Sawyer-Tower circuit was used for the ferroelectric hysteresis characterization. The resistive branch of the circuit is composed by two resistors of $R=22\ \mathrm{M}\Omega$ and $r=30\ \mathrm{k}\Omega$. In serie with the sample is found a capacitor of $C=10\ \mu\mathrm{F}$. A triangular electric field of 25 kV/cm was applied on the samples in a frequency range from 10 mHz to 1 Hz, and both samples were immersed in silicone oil. Comparison between results from both techniques revealed a remarkable accordance. As the results from the transient current are free from parasitic components, it is clear that the hysteresis loop measurements really represents the true ferroelectric information. All measurements were made at room temperature. More details about the experimental procedures to produce and to characterize the samples were described in details in previous works.[9,11,28]

IV. RESULTS AND DISCUSSIONS

A. Theoretical results

Let us first analyze the response of the system to a pulse of an external electrical field. Starting with the system negatively polarized, two pulses of 50 *n* arbitrary units in width and 250 *n* arbitrary units separated from each other were applied. Figure 2(a) shows the applied electric pulse, the response current (shifted from each other by 7×10^{10} arbitrary units) and the polarization as function of the time for a system with $N'=10$ latent dipoles, $\gamma=1.0\times10^{-8}$, $\kappa_a=5$, $\lambda=0.018$, $\alpha=-1$, and $\beta=1$ and several values of the interaction coefficient κ_b. It is verified that for higher κ_b the saturation polarization is smaller, being reached slowing. After the removal of the electrical field a gradual decrease of the polarization with time is observed, however, having different ratios depending on κ_b. It is noticed that smaller κ_b result in a smaller and faster polarization decay. An opposite behavior is noticed for higher values of κ_b. In addition, Fig. 2(b) shows the results obtained for several concentrations of latent dipoles, N' and for $\gamma=1.0\times10^{-8}$, $\kappa_a=5$, $\kappa_b=2.5$, $\lambda=0.018$, $\alpha=-1$, and $\beta=1$. These data reveal similar changes in comparison to those obtained considering different values for the interaction coefficient κ_b, as presented in Fig. 2(a).

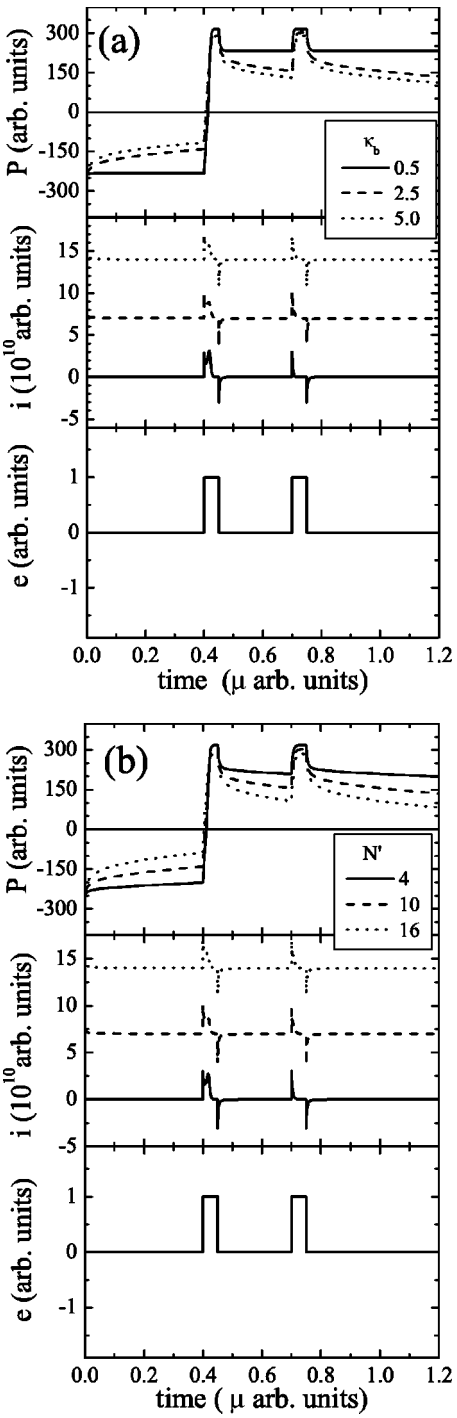

FIG. 2. (a) Response current, polarization, and applied electric pulse dependence with time for several values of the interaction coefficient κ_b. (b) Response current, polarization, and applied electric pulse dependence with time for several values of the fixed dipoles, N'.

The effect of the parameter λ, the inclusion of an internal electric field that comes from the total polarization of the material [Eq. (2)], is illustrated in Fig. 3. The effect of the internal field is to cause a decrease in the polarization of the system,[25] so the saturation polarization, remanent polarization, and coercive field decrease when $\lambda\neq0$. Another impor-

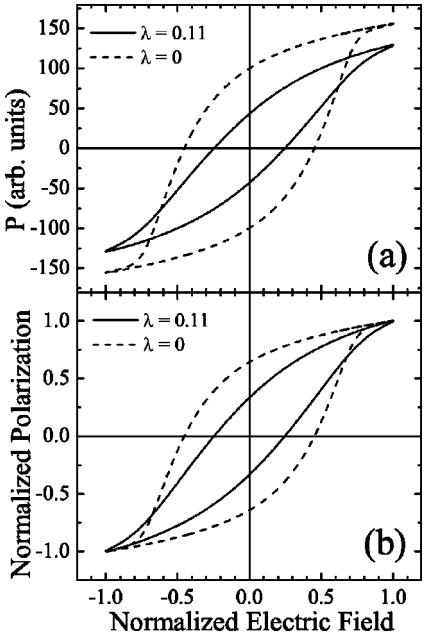

FIG. 3. (a) Dependence of the parameter λ in the hysteresis loop. (b) Same as (a) but for normalized polarization.

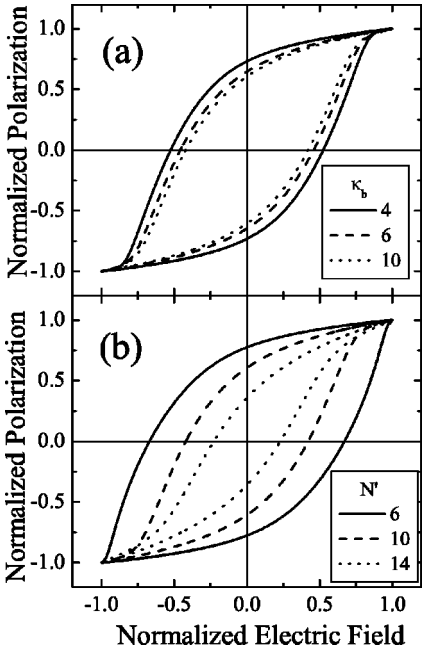

FIG. 4. Simulated hysteresis loop dependence on (a) several values of the interaction coefficient κ_b, and (b) the number of fixed dipoles (N').

tant effect due to the inclusion of this term in the equation of motion is that the saturation polarization is reached more smoothly and the most dramatic change in the susceptibility (dP/de) is observed. Thus, with the inclusion of the parameter λ the hysteresis loop is no longer square shaped, as observed in the PZTF in its virgin state. As we will see later this result is very important in order to reproduce experimental hysteresis loops, result that we could not fit only with the other parameters.

The influence of the interaction coefficient κ_b and the number of latent dipoles (N') on the ferroelectric hysteresis loop is shown in Figs. 4(a) and 4(b), respectively. The hysteresis loops were normalized to the maximum polarization (P/P_S) and maximum electric field (e/e_{Max}). It is clear that the ferroelectric characteristics are strongly dependent on both parameters (κ_b and N'). The data reveal that increasing the fraction of N' or increasing κ_b leads to a remarkable decrease in the remanent polarization as well as in the coercive field. Therefore, as observed in Fig. 2, the number of latent dipoles and the κ_b values produce similar effects on the ferroelectric properties. From the experimental point of view, the amount of latent dipoles (N') can be associated with the amount of dipolar defects introduced by doping in a ferroelectric material. On the other hand, the absolute values of the interaction coefficient κ_b can be related to the relative orientation between the dipolar defects and the domains in the material.[11] This will be discussed in detail in the next section, where theoretical and experimental results will be compared.

It is also found that the viscosity coefficient (γ) and the frequency of the electric field (ω) have a significant influence on the ferroelectric characteristics. The simulations of the frequency dependence of the ferroelectric properties were performed in a frequency range from 1 to 3 Hz. The adopted parameters were $\kappa_a=4$, $\kappa_b=4$, $N'=10$, $\gamma=1.47\times10^{-3}$, and $e_0=0.12$. The results are displayed in Fig. 5(a). The data show that both the normalized coercive field and the normalized remanent polarization increase with the increase of the frequency. The effect of the viscosity coefficient on the hysteresis loops is shown in Fig. 5(b). The importance of the viscosity of the medium has been already considered theoretically and experimentally to explain some polarization switching properties such as switching time[20,22] and self-heating.[8] Comparing Figs. 5(a) and 5(b) it is curiously

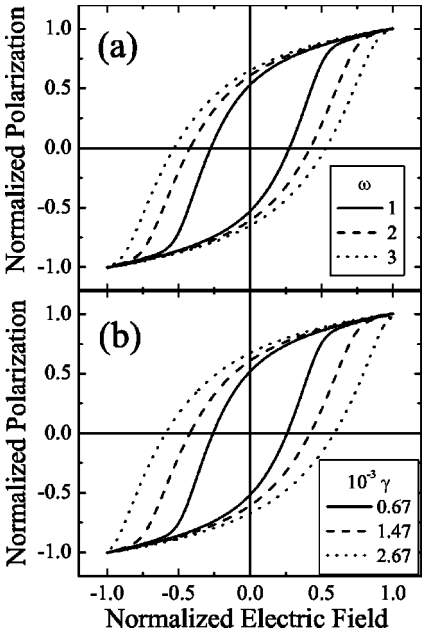

FIG. 5. (a) Frequency dependence of the ferroelectric hysteresis loop. (b) Hysteresis loop dependence on the viscosity coefficient, γ.

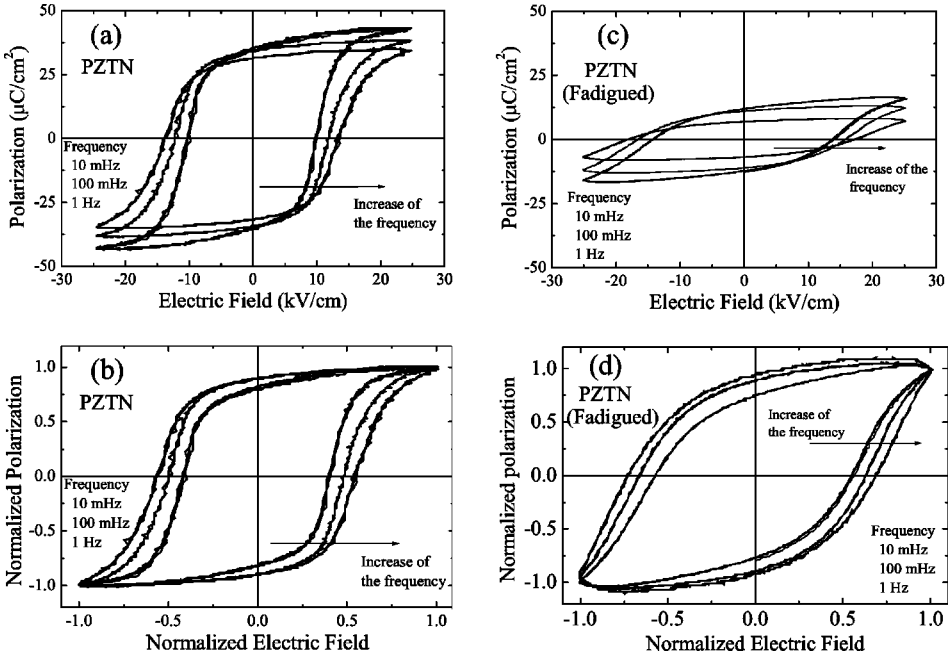

FIG. 6. (a) Hysteresis loop for the PZTN in the virgin state. (b) Respective normalized curves (P/P_S vs e/e_{Max}). (c) Frequency dependence of the hysteresis loop for PZTN in the fatigued state. (d) Respective normalized curves (P/P_S vs e/e_{Max}).

verified that an increase in the viscous coefficient (or viscous force) is analogous to an increase in the frequency of the electrical field. Thus, under an applied external electric field, it is reasonable to consider a viscous force (VF), which is proportional to domain speed, acting contrarily to the domain motion. Additionally, a restoring force (RF) acts on the domains forcing the non-180° domains to return to their equilibrium position.[26] Therefore, the coercive field may be interpreted as an effective field necessary to overcome the resistance forces (VF+RF) during the polarization switching. Consequently, at higher speeds, which means higher frequencies, the viscous force increases the coercive field significantly. However, at lower frequencies, when the velocity of the domains is low, the viscous force may be neglected and, therefore, the coercive field is reduced. On the other hand, during the removal of the electric field, domains tend to return partially to their minimum energy configuration due to the restoring force (the backswitching effect). Then, at higher frequencies (faster electric field removal) the viscous force makes the return of the domains to their equilibrium position difficult, because the viscous force and the restoring force have opposite directions, thus decreasing the percentage of backswitching. Nevertheless, at lower electric field frequencies (slower electric field removal) the domains move slowly to their equilibrium position. As a result, the viscous force may be neglected and, consequently, only the restoring and electric forces act on them. Therefore, at lower frequencies, when the viscous force may be neglected, the domains relax by longer time increasing considerably the percentage of backswitching.

B. Comparison between simulated and experimental results

In order to validate the proposed model, we will compare our theoretical results with some typical experimental ferroelectric properties of hard and soft ferroelectric materials. Typical example of materials belonging to these classes are $Pb(Zr_{0.53},Ti_{0.47})O_3$ bulk ceramics doped with 1-wt.% Nb_2O_5 (softer-PZTN) and Fe_2O_3 (hardener-PZTF),[27] which have been prepared and characterized in our laboratory.

Figure 6(a) shows the hysteresis loop dependence with frequency for PZTN in the virgin state, while Fig. 6(b) shows the respective normalized curves (P/PS vs e/e_{Max}). We can see a well-saturated loop, which is strongly frequency dependent. At lower frequencies the PZTN reaches higher polarization values and lower coercive field. Analogously, Figs. 6(c) and 6(d) show the hysteresis loop results and the normalized curves, respectively, for the PZTN in the same frequency range but in the fatigued state, which was induced by a continuous polarization switching ($\sim 10^5$ cycles). As proposed in some works, it is possible to suppose that the repeated switching of the polarization induces a continuous motion of the oxygen vacancies in the PZTN, thus resulting in their clustering and, consequently, inducing a fatigue process.[12,13] The data reveal that at lower frequencies the PZTN always reaches both higher polarization and lower coercive field values independently of the fatigued state. However, in relation to the virgin state, the fatigued one shows a large increase in the coercive field as well as a remarkable reduction in the polarization values. Figure 7(a) shows the hysteresis loop behavior for the PZTF measured in the virgin state (annealed state) and during a continuous polarization switching, while Fig. 7(b) shows the respective normalized curves. The frequency dependence of the normalized hysteresis loop for depinned PZTF (after 10^7 cycles) is shown in Fig. 7(c). It is observed that, remarkably, all features observed experimentally in the hysteresis loop measurements can be fully reproduced by the proposed model. These parallels are now discussed.

It is verified that the PZTF in the virgin state presents an unsaturated and constricted hysteresis loop, which is related to the presence of the complex defects (Fe^{3+}-VO^{2-}).[8,10,11] In the virgin state these defects are aligned along the polar

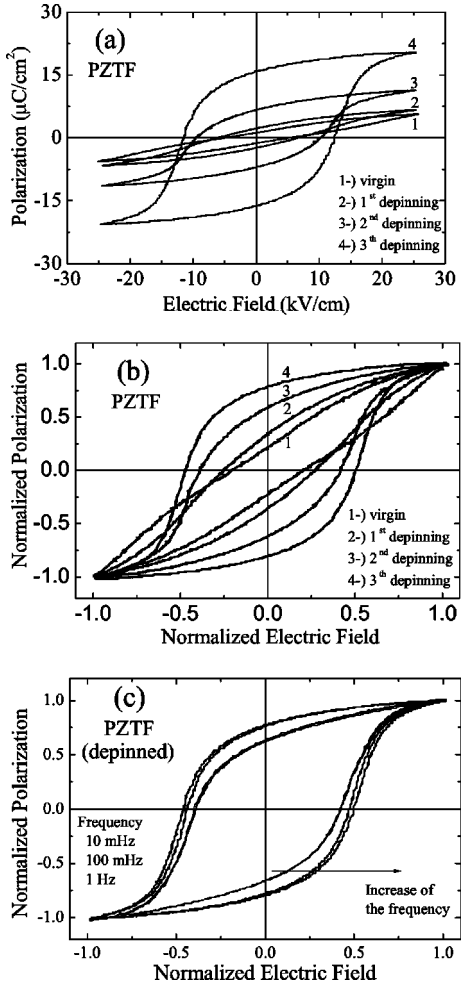

FIG. 7. (a) Hysteresis loop behavior for PZTF measured in the virgin state and during continuous polarization switching. (b) The respective normalized curves (P/P_S vs e/e_{Max}). (c) The frequency dependence of the hysteresis loop for PZTF.

direction of domains,[10,11,29] reducing sensibly the polarization switching and the coercive field compared to the complex defect-free case, as observed for the PZTN. Nevertheless, it has been proposed that under high bipolar electric fields the complex defects are forced to realign perpendicularly to the polar direction of domains, thus starting a depinning process.[8,11,30] Consequently, a remarkable increase in the polarization as well as in the coercive field is observed, which is characteristic of a depinning process,[11] as observed in Fig. 7(b). Therefore, comparing the similarity between the data contained in Figs. 4 and 7(b) it is possible to associate the experimental and theoretical data, associating dipolar defects with the latent nuclei (fixed dipoles). Obviously the switchable dipoles in the model must necessarily be related to the ferroelectric domains. Consequently, we can give a clear physical meaning to the coefficients κ_b and κ_a proposed in the model, as follows. It is reasonable to expect that the interaction between switchable dipole-switchable dipoles is different from the interaction between dipolar defect-switchable dipoles. Therefore, the coefficient κ_b proposed in the model can be related experimentally to the interaction strength between dipolar defects and switchable dipoles,

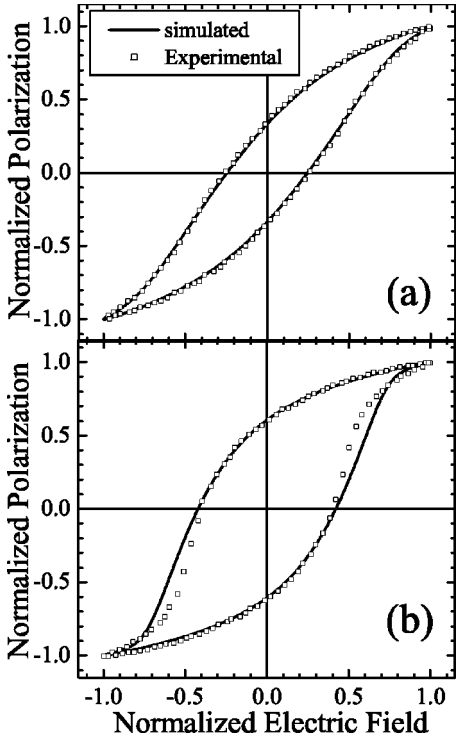

FIG. 8. Comparison of the simulated results with experimental hysteresis loop shown in Fig. 7(b) for (a) second depinning and (b) third depinning processes.

while κ_a can be assigned to the interaction between switchable dipoles and switchable dipoles. Then, very small values for κ_b furnish a well-saturated loop with low backswitching and a high coercive field, being similar to those observed for the PZTN, where complex defects are supposed to be absent. On the other hand, larger κ_b values give a nonsaturated hysteresis loop with high backswitching and low coercive field, which is completely similar to the experimental data observed for the virgin PZTF. Nevertheless, we can see that the gradual domain depinning process in the PZTF [Fig. 7(b)], where the relative orientation between domains and complex defects goes from parallel to perpendicular,[11,30] is totally equivalent to a gradual decrease in the interaction coefficient κ_b in the model [Fig. 4(b)]. The theoretical limit case is when κ_b tends to zero, which experimentally may be related to either a sample without complex defects (e.g., PZTN) or to one whose defects are oriented perpendicularly to the domains [e.g., the depinned PZTF in Fig. 7(c)].

A direct comparison of our model with the experimental results can be done. Fixing $\gamma = 1.47 \times 10^{-3}$, $\kappa_a = 12$, $e_0 = 0.10$, $\omega = 2$, $\alpha = -1$, and $\beta = 1$, the parameters κ_b and λ were fitted to experimental curves for PZTF and an excellent agreement is achieved as seen in Fig. 8. For virgin samples we have $\kappa_b = 12$ and $\lambda = 0.11$, and after the sample has been depinned (after 10^7 cycles), we obtain $\kappa_b = 10$ and $\lambda = 0.018$. Curiously enough, comparing the results in Figs. 6(b) and 7(c), it is noticed that the hysteresis loop for the PZTF after the depinning process is similar to the hysteresis observed for the PZTN.

Focusing on the coercive field, the theoretical results show that higher κ_b reduces the energy barrier of the system, thus reducing the coercive field as a whole, as observed experimentally in Fig. 7(a) or 7(b) for the virgin PZTF. It is also noticed that for lower κ_b the rate of polarization reorientation, dP/de at e_c (coercive field), is much higher than that observed for higher κ_b. In other words, near e_c the slope of the hysteresis curve is higher. It means that for lower κ_b it is possible to visualize the polarization switching as a collective motion of domains (homogeneous), whereas for larger κ_b it occurs gradually (inhomogeneous). This fact is theoretically explained in the model considering that the hindering of switchable dipoles in the neighborhood of positive/negative fixed dipoles (latent nuclei) is higher, thus being reoriented only at much higher fields. On the other hand, the dipoles situated far away from the fixed dipoles are practically not affected by them, thus switching firstly at lower fields (see the scheme in Fig. 1). This means that higher κ_b furnishes a wide distribution function for the coercive field, which is centered in an effective value.[31] Therefore, according to the model, the depinning process may be also visualized as a change from an inhomogeneous to a homogeneous reorientation of the switchable domains, resulting in a gradual reduction in the width of the distribution function for the coercive field.

It has been proposed that successive domain reorientation in ferroelectric ceramics can induce a fatigue process through motion of either space charges or oxygen vacancies, which are mainly trapped at domain boundaries.[8,11,32,33] Consequently, the domain rotation is hindered reducing gradually the domain degree reorientation and increasing simultaneously the coercive field, as verified in Figs. 6(c) and 6(d). These results reveal a strong similarity to those obtained from the effect of the viscosity coefficient in the hysteresis loops represented in Fig. 5(b). It is believed that the increase in the concentration of defects in the domain walls due to the fatigue process may be related to an increase the viscosity of the medium.[34] In other words, the increase in the fatigued state corresponds, in our model, to an increase in the values of the variable γ. It is shown in dislocation theory that an increase in the concentration of pinning points corresponds theoretically to an increase in the dragging force. Analogies between ferroelectric domain wall movement and dislocation models have already been pointed out.[35,36]

The time dependence of the polarization process for the PZTN and PZTF obtained for an electric field of 3.0 kV/mm is presented in Fig. 9, as recently reported.[9] This polarization behavior is typical for a poling process of piezoelectric ceramics. It is verified that PZTN reaches the saturation polarization faster than PZTF. After the electrical field removal it is also observed that PZTN presents a nearly instantaneous and a small decrease of the polarization. The opposite behavior is noticed for the PZTF. These results are identical to those obtained theoretically with the model, taking into account the latent dipoles as shown in Fig. 2. Therefore, as discussed for the hysteresis loop measurements, these experimental results seem to corroborate with the proposed correlation between the coefficient κ_b (fixed dipoles) and the dipolar defects. The lower polarization values as well as the higher backswitching found for PZTF in Fig. 9 may again be related in the model to a strong interaction between the fixed dipoles and the switchable dipoles. This interaction makes difficult the reorientation of the switchable dipoles that are near to the fixed ones, reducing the polarization values and demanding more time to complete the poling process. On the other hand, this interaction is also responsible for the tendency of dipoles to return to their original orientation after the removal of the field, inducing a high and long time backswitching, as observed in Figs. 2 and 9.

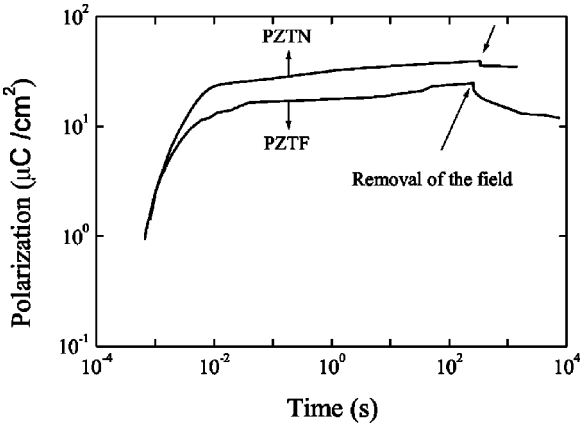

FIG. 9. Time dependence of polarization for PZTN and PZTF during and after the removal of the electric field.

It was found that the coercive field for PZTN and PZTF increases when the frequency of the electric field is increased (Figs. 6 and 7). This behavior has also been observed in single crystals,[37,38] bulk ceramics,[26,35] and thin films.[39] In addition, the results in Figs. 5(a) and 5(b) showed that an increase in the viscosity coefficient (γ) or an increase in the frequency of the electrical field have analogous effects. Therefore, these data corroborate the hypothesis that the domain reorientation occurs in a viscous medium being an inherent feature of ferroelectric materials, which can be successfully represented by the viscosity coefficient in the model.

V. CONCLUSIONS

In this work, a one-dimensional lattice phenomenological model, which includes the contribution of dipolar defects and depolarizing fields, was proposed in order to describe the polarization switching process in ferroelectric materials. A comparison between simulated and experimental results revealed that dipolar defects (latent dipoles in the model) can be associated with the presence of impurities or dopant elements commonly incorporated in ferroelectric materials for technological applications. Through an adequate analysis of the variables of the model it was possible to describe the evolution of the polarization switching with the number of cycles, which is observed for fatigue or depinning processes in these materials. So, the authors believe that the proposed model, when used to fit experimental data, can be helpful to describe fundamental properties of ferroelectrics, suck as coercive fields, saturation and remanent polarizations.

ACKNOWLEDGMENTS

This work was parcially supported by Fundação de Amparo à Pesquisa do Estado de São Paulo-FAPESP, Conselho Nacional de Desenvolvimento Científico e Tecnológico-CNPq and Coordenação de Aperfeiçoamento de Pessoal de Nivel Superior-CAPES.

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