Field-induced vortices in weakly anisotropic ferroelectrics

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Abstract

In the micro- and nanoscale ferroelectric samples, the formation and the growth of domains are the usual stages of the polarization switching mechanism. By assuming the weak polarization anisotropy and by solving the Ginzburg-Landau-Khalatnikov equation we have explored an alternative mechanism which consists in ferroelectric switching induced by vortex formation. We have studied the polarization dynamics inside a ferroelectric circular capacitor where switching leads to formation of a metastable vortex state with a rotational motion of polarization. Our results are consistent with recent first-principa simulations [I. I. Naumov and H. X. Fu, Phys. Rev. Lett. 98, 077603 (2007)] and with experiments in PbZr$_{0.2}$Ti$_{0.8}$O$_3$ [A.Gruverman et al, J. Phys. Condens. Matter 20 342201(2008)] and demonstrate that vortex induced polarization switching can be the effective mechanism for circular nano-capacitors.
Key words: ferroelectric domains, polarization switching, vortex.

For a long time, lot of attention has been given to study of finite size surface and interface effects in ferroelectric materials because of their fundamental interest and potential applications in electronic devices. As an example the up- and down- polarized domains can serve as the binary information units in Ferroelectric Random Access Memories (FRAM) \[1\]. In micro- and nanoscopic thin films the domains can form the periodic thermodynamically stable structures, provided by interplay of ferroelectric condensation energy and electrostatic energy \[2\]. Stability of ferroelectric domains and switching conditions are therefore the crucial aspects from the viewpoint of the reliability of ferroelectric devices.

When an electric field is applied the polarization changes its direction. Two mechanisms of polarization reversal are possible: the discontinuous overturn from “up” to “down” of the polarization and the Bloch one when the direction of polarization continuously changes conserving the modulus of amplitude.

The objective of the present communication is to study the Bloch polarization dynamics in ferroelectric capacitor and to discuss the results, relevant for their application in ferroelectric devices. Our static and dynamic results are consistent with first-principia simulations of stable vortex states by Naumov et al \[3\] and can explain the existence of metastable vortex state experimentally observed by Gruverman et al \[4\].

The problem set up having the geometry of the ferroelectric circular capacitor of radius $R$ shown in Fig\[\infty\]. The uniform external field $E= - E_n$ is applied perpendicular to capacitor plats. In addition no depolarizing charge is induced in the bulk i.e. condition

$$\text{div } P = 0 \quad \text{ (1)}$$

is satisfied. The surface depolarization field is screened by electrodes.

The general form of the texture of polarization satisfying the condition \[1\] can be present in cylindrical coordinate $P (P_\rho, P_\phi, P_z)$ as:

$$P_\rho = 0, \quad P = P_\phi(\rho)n_\phi + P_z(\rho)n_z \quad \text{ (2)}$$

We also assume that the polarization at the boundary of the capacitor is fixed.

$$P(\rho = 0) = P(\rho > R) = P_zn_z \quad \text{ (3)}$$
The Bloch switching mechanism implies that the only Goldstone mode is involved into polarization reverse and the amplitude of polarization remains constant.

The key feature of the Bloch switching process is the weak interaction of polarization with the crystal axes that we believe takes place in PbZr$_x$Ti$_{1-x}$O$_3$ close to morphotropic point.

Neglecting for beginning the polarization anisotropy at all we present the free energy $F$ of the system as

$$F = K' \nabla_i P_i \nabla_j P_j + K'' \nabla_i P_j \nabla_i P_j - \kappa \frac{\varepsilon}{4\pi} P_i E_i$$  \hspace{1cm} (4)$$

(tensor summation is used).

The first two terms are the gradient energy and the last one is interaction between the polarization and the applied field. Coefficients $K'$, $K''$ corresponds to the Ginzburg coefficients and $\kappa$ to the permittivity.

Numerical minimization of the free energy (4) should give the polarization distribution in the presence of an applied field. Fig. 2 presents the polarization profiles for different values of applied field. Below some critical electrical field $E_{z}^{*}$ the equilibrium state corresponds to a uniform “up” polarization state ( $P_\phi$ =0, $P_z$ =1) that means that uniform polarization
FIG. 2: Evolution of profile of polarization P (P_φ, P_z) as function of dimensionless radius for different values of applied field.

distribution is stable at $E < E_{cr}^z$. The calculation of the numerical value of $E_{cr}^z$ will be given elsewhere.

Above the critical electrical field the polarization starts to deviate from the uniform state and exhibits both non zero $P_\phi$ component, which form the vortex structure [5].

We observe that above the critical field, the equilibrium polarization distribution is asymmetric. Moreover this asymmetry is enhanced by the increase of the electrical field.

To better understand the formation of the vortex structure, we have studied the evolution of the polarization from the initial homogeneous up state to the final vortex structure as a function of time. The dynamic of the system can be described by the Ginzburg-Landau-Khalatnikov equation [6]

$$\frac{\partial P_i}{\partial t} = -\gamma_i \frac{\delta F}{\delta P_i}$$ (5)
where $\gamma_i$ are kinetic coefficients and $i = \{\phi, z\}$.

Dynamical behavior of polarization pattern is presented in Fig. 3. We observe the time evolution of the polarization vector from an initial polarized state “up”. It progressively rotates and in the intermediate state the polarization component $P_z$ changes in sign. The final state exhibits a doughnut shape i.e. with “up” polarization state at the center and at the electrode perimeter limit, and with “down” polarization state in the interior region.

Up to now we considered the particular case of the uniform gradient energy functional [1]. We believe however that square-like anisotropy terms can be considered as perturbation that will quadratically deform the vortex shape but not change the principal conclusions about the switching dynamics.

In conclusion, using thermodynamical approach and assuming the weak polarization anisotropy and the absence of depolarizing field we have determined the equilibrium state in the presence of an applied field for ferroelectric system with circular electrodes. We obtained the unusual domain pattern which looks like a doughnut and that were previously observed experimentally [4]. Time dependent simulation allowed us to describe the vortex formation.

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FIG. 3: Time evolution of polarization pattern between initial up polarized state and final doughnut-shape state