Simulation of the polarization switching in thin ferroelectric films

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Abstract. To study the polarization switching in thin ferroelectric films, we used a modified three-dimensional Ising model, which takes into account the depolarizing field. The hysteresis curves were calculated as functions of the temperature and the film thickness. The influence of the depolarizing field on the hysteresis curves for thin ferroelectric films was investigated. The dependence of the coercive field on the inverse film thickness was calculated.

1. Introduction
Currently, the main directions of theoretical and experimental studies of ferroelectric thin films are focused on such phenomena as the dynamic symmetry breaking [1-2], the hysteresis [3], the presence of an internal displacement field [4].
The polarization switching in most ferroelectric devices using ferroelectric thin films is related with the hysteresis and it occurs in the direction perpendicular to the film plane, that allows to control the film polarization with very small voltages for its small thicknesses. Many effects in thin films are more pronounced than in bulk ferroelectrics. In ferroelectric thin films, two factors such as surface energy and depolarization energy lead to a size effect, i.e. to the dependence of ferroelectric properties on film thickness [5]. The dependences of the long-range orientation order parameter on the thickness of the ferroelectric film were investigated in ref.[6], and it was shown that polarization in sufficiently thin films is not observed even at low temperatures. This is explained by the fact that the effect of the depolarizing field weakens with increasing thickness of the film. This effect has a negligible influence for the film thickness of greater than 10 unit cells. Therefore, the polarization decreases with decreasing thickness of the film, and it drastically changes to zero at a certain thickness.
The aim of the work is a theoretical study of the effect of film thickness and the mobility of the charge carriers on the polarization switching in thin ferroelectric films and the effect of the depolarizing field on the appearance of the hysteresis curve.

2. Model
We developed the model of a thin ferroelectric film (Fig. 1), in which it is taken into account that, there are charge carriers moving under the action of an electric field. In such case, the general electric field is determined by the following formula:

\[
\vec{E} = \vec{E}_{\text{ext}} + \vec{E}_{\text{int}},
\]  

(1)
where $\vec{E}_{\text{int}}$ is the strength of the internal electric field caused by spontaneous polarization and $\vec{E}_{\text{ext}}$ is the external alternative field with the frequency $\omega$ which is defined as follows:

$$\vec{E}_{\text{ext}} = \vec{E}_0 \cos \omega t$$  \hspace{1cm} (2)

The external electric field effects on the internal field, which is determined by the polarization in the ferroelectric. Under the general electric field $\vec{E}$, free particles move to the surface of the film and create a depolarizing field, which also effects on the polarization and the internal field (Fig. 2).

**Figure 1.** The model for study of the repolarization in a thin ferroelectric film.

**Figure 2.** Motion of charged particles in the electric field.

To study the polarization switching in thin ferroelectric films and to describe their properties, we used a three-dimensional lattice model with the depolarizing field, consisting of $N_1$, $N_2$ and $N_3$ nodes along the respective axes of the Cartesian coordinate system, where $N_i$ characterizes the layer number. The position of the lattice node is characterized by the set of three numbers $\vec{n} = (n_1, n_2, n_3)$.

In this paper, the potential energy of a single dipole located in the node $\vec{n}$ is described by the following formula:

$$V_n = -J \sum_m S_m S_n - pES_n - pS_n E_d,$$  \hspace{1cm} (3)

where the quantity $S_n$ takes two values +1 and -1, the quantity $J$ is the energy constant, $p$ is the dipole moment, $E_d$ is the strength of the depolarizing field.

The depolarizing field is defined by the following formula:

$$E_d = E_{d0} \beta \left( e^{-\delta(N-N_0)} + e^{-\delta(n-1)} \right),$$  \hspace{1cm} (4)

where the constants $E_{d0}$ and $\delta$ are determined by the number of free carriers in the film, and the factor $\beta$ characterizes the presence of a depolarizing field in the film, namely, $\beta = 1$ (at the presence of the depolarizing field) and $\beta = 0$ (when the depolarizing field is absent).

To analyze the movement of charged particles in the electric field (Fig. 2), we use Ohm’s law in differential form:

$$\vec{j} = \sigma \vec{E},$$  \hspace{1cm} (5)

where the coefficient of conductivity $\sigma$ is determined by the following expression:

$$\sigma = \eta e \lambda,$$  \hspace{1cm} (6)

and the quantity $\eta$ is the concentration of the charged particle, $e$ is the magnitude of their charge, $\lambda$ is the charge carrier mobility.
Then, the differential equation of motion of a charged particle along the axis $x$ has the form:

$$\dot{x} = \lambda E(t),$$  

(7)

where $x$ is the coordinate of the region center in which the concentration of positive charged particles is maximal.

Preliminary calculations allowed to analyze the maximum concentration of the free carrier. It was assumed that the internal field is lagging in phase from the external field. The dependence of the coordinate $x$ on the external field was studied. The results of the calculations are shown in Figure 3. The motion of charged particles in the film is an oscillatory motion with the frequency $\omega$ and the amplitude depending on the mobility. At the film thickness $L=10a$ ($a$ is the size of the unit cell) and low mobility of particles ($\lambda \leq \lambda_0$), most of the particles do not reach the surface of the film, so there is no depolarization field and we have $\beta = 0$ (Fig.3a,b). The value of the mobility $\lambda_0$ of the charged particles is chosen in such a way that most of the particles reach the surface of the film, but their duration of their presence on the surface is equal to zero. As the mobility increases ($\lambda > \lambda_0$) (Fig.3c) or the film thickness decreases ($L=3a$) (Fig.3d) a depolarizing field appears ($\beta=1$) in the boundaries of the ferroelectric film at certain time intervals. The direction of the depolarizing field is changed depending on which surface the particle is located. As we see from Figure 3, the time during which the depolarizing field exists depends on the mobility of charge carriers ($\lambda$) and on the film thickness ($L$).

![Figure 3](image-url)

**Figure 3.** The charge particle motion in the electric field at different values of their mobility: $\lambda = \lambda_0(a), \lambda < \lambda_0(b), \lambda > \lambda_0(c,d)$, and thickness of the ferroelectric film $L = 10a(a,b,c), 3a(d)$. 
3. Results of the simulation
The hysteresis curves, i.e. the dependences of the long-range orientation order parameter $\mu$ on the strength of the general electric field were calculated for the model (Figure 1). In contrast to the preliminary results shown in Figure 3, the internal field was calculated taking into account the depolarizing field in the Ising model. The hysteresis curves for different values of the ferroelectric film thickness are shown in Figure 4. It can be seen that the curves are displaced relative to the center along the horizontal axis, that is the evidence of the presence of an internal displacement field, which increases with decreasing the film thickness.

![Figure 4](image)

**Figure 4.** The hysteresis curves for different values of ferroelectric film thickness $L = 7a, 10a, 15a, 20a$ at different reduced temperatures $k_B T / J = 5(a), 7(b)$.

Figure 5 shows the dependence of the coercive field on the inverse thickness of the film $(1/L)$.

![Figure 5](image)

**Figure 5.** The coercive field $E_c / J$ vs. the reverse thickness of a thin ferroelectric film $1/L$ at different reduced temperatures $k_B T / J = 2(1), 5(2)$.

4. Discussion
This model allows to calculate the dependence of the coercive field on the film thickness. The coercive field is determined by the magnitude of the depolarizing field that occurs in thin...
ferroelectric films due to the migration of charged particles in alternating electric fields. At low temperatures below the phase transition point in the bulk ferroelectric, the dependence is linear (curve 1 in Fig. 5), which is consistent with many experiments, for example in ref. [7]. With increasing film thickness at a certain value, there is a sharp drop of the value of the coercive field (curve 2 in Fig. 5).

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