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DYNAMICS OF DOMAIN STRUCTURE IN UNIAXIAL FERROELECTRICS

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The switching of polarization in ferroelectrics is considered as the first-order phase transition. By the analogy with the theory of crystal growth it is assumed that the switching process is determined by the oversaturation degree which correspond in ferroelectrics to the magnitude of electric field on the domain boundary. It is supposed that the mechanism of domain wall motion in strong field is due to the two-dimensional nucleation and in weak field is due to the one-dimensional nucleation. The criterion of strong field is defined. From this point of view it have been explained the peculiarities of domain structure dynamics in two uniaxial ferroelectrics: lead germanate and gadolinium molybdate.

INTRODUCTION

Domain structure of uniaxial ferroelectrics is chosen for the investigations for its simplicity: it consists of 180° domains only. But in reality, domain configuration arising during phase transition or polarization reversal in real crystal is rather complicated. The observed domain pattern depends on experimental conditions: electric field strength, sample thickness, type of electrodes, temperature and so on. In the present paper we shall deal only with the main features of the domain dynamics in uniaxial ferroelectrics under the action of electric field.

It is well known that the main steps of domain structure evolution during the switching are the arising of new domains, their forward growing and sidewise motion of domain walls.\cite{1,2} In order to explain the observed phenomena let us consider the switching of polarization by the analogy with the first-order phase transition.

THE KINETICS OF THE FIRST-ORDER PHASE TRANSITIONS

The kinetics of such transitions is well studied for the crystal growth from the melt.\cite{3,4} In last case the oversaturation of the melt leads to the formation of solid phase through the nucleation. One can distinguish three kinds of nuclei: three-dimensional, arising far from the phase boundary, two-dimensional, arising at the phase boundary (their thickness is of the order of lattice constant) and one-dimensional, arising at the steps of the phase boundary. It is clear that the probabilities of forming nuclei of different dimensions are quite different because surface energy input differs sufficiently for the nuclei with equal volume but of different dimensions.

At large oversaturation degrees the crystal is growing from the melt through two-dimensional nucleation at the phase boundary.\cite{3,4} Due to the disorder nature of this process the exponential dependence of growth velocity is observed and the obtained crystals become shapeless.
The decreasing of oversaturation degree leads to the suppression of the probability of two-dimensional nucleation. Nevertheless the growth of new phase is continued. It is common to explain this fact by the one-dimensional nucleation at the phase boundary steps and layer after layer growth of the crystal by the motion of these steps along the boundary. In this case phase boundary become regular shaped and the crystals with regular facets are obtained.
THE MECHANISMS OF SIDEWISE DOMAIN WALL MOTION IN LEAD GERMANATE AND GADOLINIUM MOLIBDATE

Let us try to apply the above mentioned considerations to the description of the domain pattern evolution of two uniaxial crystals with different properties: the ferroelectric-semiconductor lead germanate Pb$_2$Ge$_3$O$_{11}$ (LG) and improper ferroelectric-ferroelastic gadolinium molybdate Gd$_2$(MoO$_4$)$_3$ (GMO). Both of the crystals possess 180° domains optically distinguished by polarized microscope. So one can use optical methods for visualization of momentary domain pattern arising during the switching process. These methods possess high space and time resolutions. In LG the polar axis is 3-fold symmetry one and in GMO it is 2-fold one.

In LG in strong fields (more than $3 \times 10^5$ V/m) it has been observed exponential field dependence of domain wall velocity. In this field region the switching is accomplished through the arising of great number of new round section domains which become shapeless after coalescence (Figure 1A). Any preference in domain wall orientation is not observed in this case.

In GMO in strong fields a lot of domains with different orientations of boundaries are arising (Figure 1B). In this case only “switching velocity” (reciprocal switching time) can be measured and its value also depends exponentially on the applied electric field. So we can state that in both ferroelectrics in analogy with crystal growth the mechanism of domain wall motion in high field region is two-dimensional nucleation at the wall.

In weak fields (less than $2 \times 10^5$ V/m) in LG growing domains become the regular hexagons (Figure 2). The domain walls are parallel to the facets of the LG single crystal.
crystal pulled along the polar axis. The field dependence of sidewise motion velocity of these walls is approximately linear. In GMO such dependence is observed in wider field region. Polarization is reversed by the sidewise motion of plane domain walls which are parallel to the crystal facets (Figure 3).

Let's assume by the analogy with phase transition at small oversaturation (in ferroelectrics the oversaturation degree corresponds to the magnitude of applied electric field) that in weak field layer after layer growth of domains of preferable orientation takes place. In LG the trigonal anisotropy of the surface energy must lead to the preferable motion of the steps in three directions. It is easy to show that in this case six plane domain walls must be formed (Figure 2B). Thus the regular hexagonal domains are obtained. In GMO owing to the presence of 2-fold symmetry axis there are two preferable directions of steps motion. So, two plane parallel domain walls, moving in the opposite directions, must be formed, as it is observed in the experiment (Figure 3A).

From this point of view it is easy to explain the fact of domain walls orientation change, forming during the switching from different single domain states. In GMO it is known, that polarization reversal is accompanied with the replace of crystallography axis, so the preferable directions, which determine directions of steps motion and domain wall orientation, are replaced too (Figure 3C).

The coincidence of domain wall orientations with crystal facets is the additional confirmation of the unity of the processes governing the crystal growth at small oversaturation and domain growth in weak fields.

**LAYER AFTER LAYER DOMAIN GROWTH**

The main problem in the mechanism of layer after layer growth is the problem of step origin. In the theory of crystal growth it is commonly understood that the
steps are arising as a result of intersection of screw dislocation with the phase boundary. These steps provide spiral growth of crystal surface. On analogy of crystal growth Nakamura assumed that domain wall motion is due to the spiral step growth, produced by the screw dislocation, normal to the domain wall. But Miller and Weinreich showed, that this mechanism required unrealistic value of dislocations density for the explanation of experimental data.

We assume that residual nonthrough domains, which are always existing in ferroelectrics, can play the role of steps sources. In weak fields the probability of their growing is suppressed and they can not form through domains. When they are intersected by the moving domain wall they become two-dimensional nuclei, which then grow through the crystal and form steps on the wall (Figure 4). It must be stressed, that efficiency of residual domains is much higher than efficiency of dislocations, because the height of steps forming by these domains is about few microns. The estimations show that $10^3 - 10^4 \text{ mm}^{-2}$ of residual domains is sufficient for the mechanism of layer after layer growth. This value is correlated with the number of domains arising in LG during the switching in strong fields.

THE STRONG FIELD CRITERION

But up to the present moment the strong field criterion is not clear. First of all there exists the delay time between the moment of electric field switching and the beginning of nucleation process. The value of delay time is increasing with the increasing of nuclei dimensions $t_1 < t_2 < t_3$. If the time of field action, which is equal to the pulse duration or the switching time, is less than delay time, the dynamics of domain structure qualitatively changes.

When a train of short pulses of strong field (with duration, less than the time necessary for the arising of through domains) is applied to the sample of LG, the domain structure is changed by sidewise motion of domain walls, as in weak fields. During the growth domains acquire the form of scalene triangles, whose sides are parallel to the planes [100] (Figure 5). In order to explain these peculiarities we
must take into account that when a train of short strong field pulses are applied both mechanisms of domain wall motion take place. During the strong field action two-dimensional nuclei are formed on the wall. Their orientation is determined by the anisotropy of surface energy. These nuclei play the role of steps on domain walls. In the pause between pulses the walls are smoothed as a result of steps motion along the domain walls. In this case it is easy to see that the walls must move in three directions, orthogonal to the directions of motion of hexagonal domain walls. Thus triangular domains, whose sides are rotated with regard to the sides of hexagonal domains, are formed.

THE ADDITIONAL PECULIARITIES OF SIDEWISE DOMAIN WALL MOTION

The detail investigation of switching from the multidomain state shows that there are some additional peculiarities of sidewise domain wall motion. In this case the wall motion is rather nonuniform; in weak fields the wall shifts at some distance from initial position and stops; after the field is switched off spontaneous backward motion of the wall is observed. To explain this behaviour we must take into consideration that velocity of new phase growth is defined by the oversaturation degree at the phase boundary. Hence, the velocity of sidewise domain wall motion is defined by the field strength at the boundary of growing domain.

Let's consider in detail the fields distribution in ferroelectric capacitor (of thickness $d$) with effective dielectric layers (of thickness $L$) near the surfaces. The bound
charges produce depolarization field. Even after the finishing of external screening in the volume of crystal exists residual depolarization field\(^\text{14}\) \(E_{dr} = 2lp_e/e_0\varepsilon_s d\) due to the presence of surface layers (\(\varepsilon_s\)-dielectrical permittivity of surface layers). For \(d = 1\) mm \(E_{dr}\) is of order \(10^5\) V/m. The time of external screening is determined by the time constant of external circuit. The bulk screening of residual depolarization field is a result of redistribution of inner carriers and formation of bulk charges bound by traps. We must notice, that in our case the time constant of bulk screening is much longer than the time constant of external screening. Calculation shows that internal field at the domain boundary depends upon the value of wall shift from equilibrium position in the following way (Figure 6):

\[
E_{ib} = E_{ex} + kE_{dr} \times F(x/2L_s)
\]

where \(F(A) = 1/\pi[2\arctg A + A \ln(1 + A^{-2})]; L_s\) — effective screening length bulk charges and \(k\) — screening factor.

In both crystals experimental data of domain wall motion in external field and during the backward switching and theoretical results, obtained under these assumptions are in good agreement (Figure 7).

**CONCLUSION**

In conclusion, it must be noted that domain structure dynamics of ferroelectrics depends upon the relation between the time of field action and delay time; time constant of external screening and internal one; value of screening field and threshold field; sample thickness, surface layer thickness and screening length. These parameters depend also on many factors: value of spontaneous polarization, bulk and surface layer conductivity, dielectric permittivity and time constant of external circuit. On the one hand these facts require careful control of experimental conditions and make difficult the interpretation of experimental data obtained by anybody else. On the other hand the variation of these factors make it possible to control the ferroelectric domain structure and its behaviour in the electric field.
FIGURE 7 Time dependence of the domain wall shift from initial position (the dotted line—result of the calculation): a—in LG; b—in GMO.

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