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# Domain shape in uniaxial ferroelectrics

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The variety of domains shapes appeared in uniaxial ferroelectrics will be presented, classified and described systematically. The obtained experimental results will be discussed using unified kinetic approach based on the analogy between domain structure evolution and growth of new phase during first-order phase transformations.

The classical theoretical approach predicted only the regular polygonal shape of isolated domains defined by crystal symmetry [1,2]. Nevertheless the unusual domain shapes, such as octagonal domains instead of squares in barium titanate $BaTiO_3$ [3,4] and triangular domains instead of hexagons in lead germanate $Pb_5Ge_3O_{11}$ (PGO) [5,6] have been obtained experimentally long ago. Recent systematic investigations of domain shapes with high spatial resolution allowed to reveal wide shapes variety, which can be divided into several groups: (i) circular shapes, (ii) regular polygons, (iii) irregular polygons, (iv) irregular shapes.

The kinetic approach to domain growth based on generation of steps (pair of kinks) and kink motion along the wall has been used for explanation of all obtained domain shapes [7,8]. According to this approach, the nucleation probabilities are determined by the local value of the sum of the external field produced by voltage applied to the electrodes, and partially screened (residual) depolarization field produced by bound charges. It is pointed out that the bulk screening allows stabilizing almost any metastable domain shape even with charged domain walls and complicated dendrite shapes.

The key role of the bulk screening retardation in formation of self-assembled nanodomain structures is demonstrated in various ferroelectrics [8]. The crucial role of screening ineffectiveness for domain shape complication was demonstrated both experimentally and by computer simulation [7]. It is shown how the highly non-equilibrium switching conditions has been realized. Two limiting variants of the step nucleation have been considered: (a) **stochastic** with equiprobable position of nucleation sites, and (b) **determined** with step generation at fixed points and anisotropic kink motion. For polygonal domains the nucleation sites are situated at the polygon vertexes [7,8].

**Stochastic nucleation** being the classical model of the domain wall motion leads to formation of the circular domain shapes [9]. **Determined nucleation** stimulated formation of the regular polygonal domain shapes depending on the crystal symmetry. The convex polygons with walls parallel to the main crystallographic axis appeared for effective screening: (a) *hexagons* for $C_{3v}$ symmetry, such as lithium niobate $LiNbO_3$, lithium tantalate $LiTaO_3$ and lead germanate $Pb_5Ge_3O_{11}$ (PGO) [6,10], (b) *squares* for $C_4$ symmetry, such as strontium-barium niobate $(Sr,Ba)NbO_3$, (c) *rectangles* for $C_2$ symmetry, such as potassium titanyl phosphate $KTiOPO_4$ (KTP) [11]. Screening retardation leads to changes of the domain shape caused by deceleration of the kink motion and formation of the irregular polygons and stars [12]. Creation of the artificial nucleation sites (scratches or electrode edges) allowed to decrease the number of polygon vertexes.

The fast restoration of the initial hexagon and rhombus shapes after domain merging (shape stability effect) demonstrated in KTP and LN crystals was attributed to formation of the short-lived superfast domain walls with high kink concentration [13]. The effect is obtained in LN and LT for switching at the temperature below $200^oC$.

The stochastic nucleation obtained at the elevated temperatures leads to lack of the domain shape stability effect and open the way to formation of the various complicated self-assembled (fractal) and dendrite domain shapes [14,15]. The dendrite domain structures (snowflakes) can be created by several mechanisms: (i) appearance of the isolated domains (discrete switching) with subsequent merging, (ii) lack of the domain shape stability, (iii) domain shrinkage under the action of the pyroelectric field or spontaneous backswitching, (iv) domain growth at the elevated temperature in the crystals covered by artificial dielectric layer.

The obtained fundamental results allowed formulating the physical basis for rapidly developing modern fields of technology named micro- and nano-domain engineering and domain wall engineering [16,17]. The recent achievements and future trends in creation of the short-pitch domain patterns are reviewed.

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1. V. Gopalan, V. Dierolf, D.A. Scrymgeour, *Annu. Rev. Mater. Res.* **37**, 449 (2007).
2. L. Tian, D.A. Scrymgeour, V. Gopalan, *J. Appl. Phys.* **97**, 114111 (2005).
3. R.C. Miller, A. Savage, *Phys. Rev. Lett.* **2**, 294 (1959).
4. R.C. Miller, A. Savage, *Phys. Rev.* **115**, 1176 (1959).
5. V.Ya. Shur, V.V. Letuchev, E.L. Rumyantsev, et. al., *Sov. Phys. Solid State* **27**, 959 (1985).
6. V.Ya. Shur, A.L. Gruverman, V. Letuchev, et. al., *Ferroelectrics* **98**, 29 (1989).
7. V.Ya. Shur. *J. Mater. Sci*. **41**, 199 (2006).
8. V.Ya. Shur In: Schmelzer, J.W.P. (ed.) *Nucleation Theory Applications*, pp. 178–214. WILEY-VCH, Weinheim (2005).
9. R.C. Miller, G. Weinreich, *Phys. Rev.* **117**, 1460 (1960).
10. V.Ya. Shur, E.V. Nikolaeva, E.I. Shishkin, et. al., *Ferroelectrics* **269**, 195 (2002).
11. V.Ya. Shur, E.M. Vaskina, E.V. Pelegova, et. al., *Appl. Phys. Lett*., **109**, 132901 (2016).
12. A.I. Lobov, V.Ya. Shur, I.S. Baturin, et. al., *Ferroelectrics*, **341**, 109 (2006).
13. V.Ya. Shur, A.I. Lobov, A.G. Shur, et. al., *Ferroelectrics*, **360**, 111 (2007).
14. V.Ya. Shur, D.S. Chezganov, M.S. Nebogatikov, et. al., *J. Appl. Phys*. **112**, 104113 (2012).
15. V.Ya. Shur, M.S. Kosobokov, E.A. Mingaliev, et. al., *J. Appl. Phys*. **119**, 144101 (2016).
16. V.Ya. Shur In: Ye, Z.-G. (ed.) *Handbook of Advanced Dielectric, Piezoelectric and Ferroelectric Materials. Synthesis, Properties and Applications*, Woodhead Publishing Ltd, Cambridge 622 (2008).
17. V.Ya. Shur, E.L. Rumyantsev, R.G. Batchko, et. al., *Ferroelectrics* **221**, 157 (1999).