Role of Domain Patterns in Ferroelectrics: From Basic Ideas to Phase-field Simulations

Pavel Mokrý[1,2,*]
[1]Regional Center for Special Optics and Optoelectronic Systems (TOPTEC), Institute of Plasma Physics of the Czech Academy of Sciences, Za Slovankou 1782/3, 182 00 Praha 8, Czech Republic
[2]Institute of Mechatronics and Computer Engineering, Faculty of Mechatronics, Informatics and Interdisciplinary Studies, Technical University of Liberec, Studentska 2, 46117 Liberec, Czech Republic
*Pavel Mokrý: mokry@ipp.cas.cz

The fundamental definition of ferroelectric materials, which says that the crystal lattice of a ferroelectric can exists in two or more configurations with different values of polarization, has an inevitable consequence. It allows the situation that the volume of a ferroelectric sample is split into domains, which differ in the value of polarization. Such a situation is called the polydomain state of the ferroelectric sample. Since the macroscopic properties of the ferroelectric sample are given by averaging the local properties over the whole volume of the sample, it is quite natural to expect that the presence of domains has tremendous effect on the effective material parameters. In some applications, the presence of domain patterns has a disastrous impact on their proper function as, for example, in pyroelectric sensors or nonvolatile ferroelectric memories. On the other hand, it was recognized by Kittel in 1951 that the motion of domain boundaries in ferroelectric samples may lead to an essential enhancement of macroscopic permittivity [1]. Methodology of experimental identification of the domain boundary motion (extrinsic) contribution to permittivity was established by Jan Fousek in 1965 [2]. Figure 1 shows the dependence of complex permittivity of $BaTiO_3$ single crystals on average polarization of sample, which indicates the difference in the dielectric response of the single domain ($P_a/P_s = -1$) and polydomain ($P_a/P_s = 0$) samples. This difference corresponds to the extrinsic contribution to permittivity. Since that time, the extrinsic contributions to macroscopic properties of ferroelectric have become the subject of intense experimental and theoretical research.

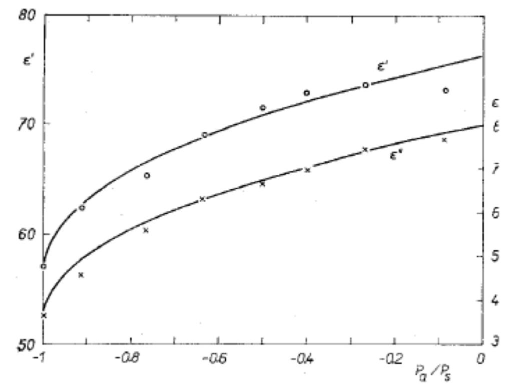

Fig. 1: Dependence of complex permittivity of $BaTiO_3$ single crystals on average polarization of sample (Adopted from [2]).

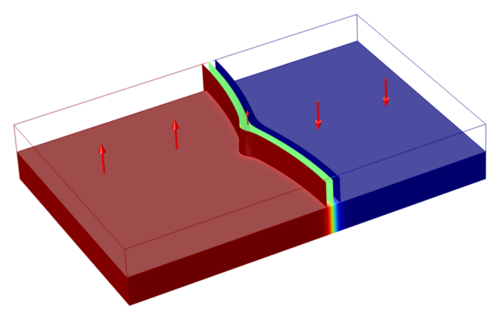
Fig. 2: Phase-field simulations of the interaction of the defect with the bent 180° domain wall (Adopted from [3]).

In this contribution, the review on the role of domain patterns in ferroelectrics will be given. The review will cover the thermodynamic principles of extrinsic contributions to permittivity, the role of restoring force acting on the disequilibrated domain wall (see Fig. 2). The consequences of group theory applied to the symmetry of crystal lattice and domain patterns will be discussed in the relation to domain engineering. Recent results on possibilities to use extrinsic contributions for the characterization of ferroelectric samples [3] will be discussed.

[1] C. Kittel, "Domain boundary motion in ferroelectric crystals and the dielectric constant at high frequency," Physical Review, vol. 83, no. 2, pp. 458–458, Jul. 1951.

[2] J. Fousek, "The contribution of domain walls to the small-signal complex permittivity of BaTiO3," Czechoslovak Journal of Physics, vol. 15, no. 6, pp. 412–417, Jun. 1965.

[3] P. Mokrý and T. Sluka, "Identification of defect distribution at ferroelectric domain walls from evolution of nonlinear dielectric response during the aging process," Phys. Rev. B, vol. 93, no. 6, p. 064114, Feb. 2016.