Account for mutual influence of electrical, elastic and thermal phenomena for ferroelectric domain wall modeling

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It is well known that for the description of the ferroelectric behavior is necessary to consider the electric and elastic fields simultaneously [1,2]. However, the influence of thermal phenomena has not been discussed in the literature before. In this work we have shown that the account of latter ones is essential in the context of proper modeling of ferroelectric materials.

At domain wall motion the changing of polarization take place fast enough. This fact due to the electrocaloric effect results in the release or absorption of heat at the domain interface. The temperature gradient corresponding to this process excites a strong change in the elastic field (because of the small heat emission area). Moreover, it is necessary to consider the elastic field gradient at the domain wall. As a consequence, flexoelectric and flexothermal effects must be taken into account. For this purpose the following generalization of the free energy is suggested

$$F = F_0(T) + F_{\text{Landau}} + F_{\text{elast}} + F_{\text{grad}} + F_{\text{coup}} + F_{\text{coup grad}}, \qquad (1)$$

where $F_0(T)$ is the independent on field part of the free energy. The second and third summands in (1) are Landau potential and the elastic part of the free energy containing the thermal stress tensor, respectively. Temperature and electrical displacement gradients are included in F_{grad}, while the fifth summand in (1) describes the interaction between elastic and electric phenomena (piezoelectric and electrostrictive effects). Finally, $F_{\text{coup grad}}$ contains six terms describing the influence of the gradient of one variable on the rest two variables. The condition of the minimization of (1) results in a differential equation system. The analytical solution of this system is possible to find in the case of some simplifications. Obtained findings confirm the significance of the developed theoretical approach.

1. S.V. Kalinin, E. Karapetian, M. Kachanov, *Physical Review B* **70**, 184101 (2004).
2. A.K. Tagantsev, L.E. Cross , J. Fousek, *Domains in Ferroic Crystals and Thin Film (*Springer New York*),* 123 (2010).

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