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ABSTRACT

Previous Landau-type models of two-phase state formation in clamped systems whose material exhibits first-order phase transitions in free state neglects the existence of interphase boundaries. Here, we take them into account in the framework of a Ginzburg–Landau one-dimensional model to study the dependence of characteristics of the two-phase state on system size. Unlike earlier works, we find that the transition to the two-phase state from both the symmetrical and nonsymmetrical phases is not continuous but abrupt. For a one-dimensional system with length L studied in this work, we show that the formation of two-phase state begins with a region whose size is proportional to $\sqrt{L}$. The latent heat of the transition is also proportional to $\sqrt{L}$ so that the specific latent heat goes to zero as $L \to \infty$, recovering the earlier result for infinite systems. The temperature width of the two-phase region decreases with decreasing of L, but we are unable to answer the question about the critical length for two-phase state formation because the approximation used in analytical calculations is valid for sufficiently large L. A region of small values of L was studied partially to reveal the limits of validity of the analytical calculations. The main physical results are also obtainable within a simple approximation that considers the energy of interphase boundary as a fixed value, neglecting its temperature dependence and the thickness of the boundary. A more involved but consistent treatment provides the same results within the accepted approximation and sheds light on the reason of validity of the simplified approach.

I. INTRODUCTION

Theory of first-order phase transitions in clamped solid systems which was mostly of conceptual interest several decades ago is now of experimental relevance. This is due to the advent of systems such as films on substrates or structures like nanobeams that can be partially clamped by the substrate or fixed at their ends. If the material exhibits first-order phase transition in the bulk free crystal, a natural question arises: what occurs for such transitions in the above systems? The most well-known effect is the formation of domain structures due to several elastic variants of the new phase(s) that was studied many years ago, see Roitburd (1978). There are, however, effects of clamping even when only one elastic variant of the new phase is present and the only strain effect of transition is dilatation, i.e., a change in the system density. This is the most general feature of any transition, but we are discussing here only those that occur without material transfer between different parts of the system, ferroelectric and ferroelastic phase transitions exemplify this type of transitions, where change in density here is solely due to a change in the unit cell volume or, more generally, due to the change of space occupied by the same structural unit in the two phases. A general feature of clamping is that it puts some external limits on the system either by fixing its volume or

some sizes or by hampering displacements of the material at some boundaries such as at the interfaces between the film and the substrate, but it cannot prevent displacements of the material at every point of the system which occur if such displacements result in a decrease in the system's energy. In other words, if the system "wants" to change its density at every point but is prevented from doing so by external conditions, it does it to an extent that is possible: it might do this locally and inhomogeneously given that the global homogeneous option is excluded. If a first-order phase transition occurs in the system, the abrupt change in the system density naturally exhibited in a free system cannot take place in all of the system homogeneously because of fixing of the volume or the sizes, but it will occur inhomogeneously if it decreases the system energy. If it occurs, it strongly influences the phase transition in the clamped system. One can, for example, speculate that the smearing of ferroelectric phase transitions, which is more pronounced experimentally in thin films than in the bulk material, is connected, at least to some extent, with this phenomenon whose theoretical understanding is still insufficient to provide even rough estimations relevant to experiments. The aim of the paper is to contribute to the development of the corresponding theory. The naturally expected form of the inhomogeneity is some form of coexistence of the two phases in a temperature interval close to the temperature of what would be the first-order phase transition without clamping. This is what the term "two-phase state" in the title refers to. They were directly observed in nanobeams (Wu *et al.*, 2006; Wei *et al.*, 2009), and there is little doubt that this tendency may reveal itself in some form in other clamped or partially clamped systems such as perovskite films on substrates given that, in bulk perovskite crystals, ferroelectric and other phase transitions are mainly of the first order. The coexisting phases are, naturally, not the only possible form of the inhomogeneities, see Levanyuk *et al.* (2018), but we believe that a consistent development of the theory implies an exhaustive study of the simplest cases first and that is the approach followed in this paper.

The natural starting point to present the state of the arts is a paper by Devonshire (1951) who claimed to show that the first-order paraelectric-ferroelectric phase transition in $BaTiO_3$ would convert into a second-order one if the crystal volume were fixed. The reason was the change of sign of a coefficient of the Landau-like thermodynamic potential due to clamping. A weak point of this claim was a tacit assumption that the constrained system remained homogeneous. This became clear much later, but in a widely cited paper (Pertsev *et al.*, 1998), a similar conclusion was made about partially clamped $BaTiO_3$ and $PbTiO_3$ in the form of thin films on thick substrates once again because of a similar reason and due to the same assumption. Later this assumption was abandoned in Pertsev *et al.* (2000) and Koukhar *et al.* (2001) where, with the help of a numerical procedure, multidomain and heterophase states were revealed but no two-phase states (TPSs) consisting of the paraelectric and ferroelectric phases so that the above-mentioned conclusion about paraelectric-ferroelectric transition in $BaTiO_3$ and $PbTiO_3$ remained unquestioned. However, several years later, Onuki and Minami (2007), considering the compressible Ising system within the Ginzburg–Landau model, explicitly showed that the clamping of an elastically isotropic system with first-order phase transition leads to the formation of TPS instead of second-order transition as it was claimed in the above papers for real, i.e. anisotropic, systems. The situation with the two-phase formation is, indeed, trickier for anisotropic systems (Onuki *et al.*, 2007), but it is legitimate to be surprised by the numerical results of Pertsev *et al.* (2000) and Koukhar *et al.* (2001) about the paraelectric-ferroelectric transitions in $BaTiO_3$ and $PbTiO_3$. If the results published in Pertsev *et al.* (2000) and Koukhar *et al.* (2001) for the paraelectric-ferroelectric transition with no two-phase existence are a consequence of the phenomenological constants they used, it may well be not the case for other reported material constants (see Hlinka *et al.*, 2006) or other compositions undergoing first-order phase transitions. This question certainly deserves attention, but it is beyond the scope of this paper. We think that, before studying the effects of crystal anisotropy, the simplest elastically isotropic case should be carefully studied.

We build upon the work of Onuki *et al.* (2007) and another work by Tselev *et al.* (2010) that provided a simplified derivation of some of the results given by Onuki *et al.* (2007). The matter is that when defining the parameters of the TPS, interphase boundaries (IBs) have been neglected in both works. This may seem reasonable for large samples since the relative contribution of the IB energy (IBE) goes to zero when the sample size tends to infinity. However, the observable values are not necessarily relative. Our initial intention was to study dependence of characteristics of the TPS on the system size expecting the most interesting results for small sizes where an explicit consideration of the IBs is obligatory. To our surprise, the results proved to be of relevance not only for small systems but also for arbitrary large ones. Indeed, our 1D analysis reveals that, at the formation of TPS both from symmetrical and from homogeneous nonsymmetrical phases, the length of the region of the new phase depends on the system length L as $L^{1/2}$, i.e., the transitions into TPS are discontinuous. The total latent heat of the sample at both transitions depends on L in the same way. Evidently, the specific latent heats tend to zero when the system size goes to infinity. The L dependence of boundaries of the temperature region of TPS is also power-like, i.e., it is essential even at large L unlike our initial expectation that it will start to be visible at L comparable with the order parameter correlation radius which is the only material characteristic length of the theory. The emphasis of this paper is on the lengths larger than the correlation radius despite some preliminary results on the smaller lengths have been already reported (Levanyuk *et al.*, 2020). The profiles of the order parameter are different from what is conventionally understood as TPS, this case clearly deserves a separate discussion and we left it beyond this paper not to overload it.

The paper is organized as follows. In Sec. II, we reproduce, for the reader's convenience and for further use of the formulas, the method to define the temperature width of the two-phase region neglecting the boundaries. Here, we follow Tselev *et al.* (2010) while providing more details than can be found in the original work. In Sec. III, we present a simple though temporarily unsubstantiated method to obtain the main physical results of the paper. It consists of adding to the free energy of TPS of Sec. II the energy of IB at the phase equilibrium in the free system which is known from literature (Larkin *et al.*, 1969; Lajzerowicz, 1981). The results of Sec. III are also obtained in Sec. IV by consistent analytical calculations, thus justifying (for large L) the method presented in

Sec. III to obtain the results. In Sec. V, we present numerical results to demonstrate the expected deviations of the analytical results from the numerical ones at low values of L. In Sec. VI, we summarize the results of the paper. To avoid excessively complicated formulas, we consider explicitly only the case where the virtual homogeneous transition in the clamped system coincides with the tricritical point. More general results are presented in the supplementary material without derivation but only providing formulas.

II. SIMPLIFIED LANDAU-TYPE ONE-DIMENSIONAL MODEL OF TWO-PHASE STATE FORMATION

In the paper as well as in Tselev *et al.* (2010), which we follow in this section, only the simplest case of one-component order parameter is considered, which has the symmetry transformation properties neither of a component of a polar vector nor a component of a symmetrical tensor of second rank, i.e., the phase transition is neither ferroelectric nor ferroelastic. This is to avoid complications associated with the effects of long-range electric fields, in the case of ferroelectrics, or elastic fields associated with symmetry-breaking strains, in the case of ferroelastics, and concentrate, at this stage, on the long-range elastic effects of clamping which are common for any type of phase transition and are associated with fixing the volume, area, or length of the system. As well in Tselev *et al.*, only 1D system is considered so that the linear density of the Ginzburg–Landau free energy can be written as

$$f = \frac{\alpha}{2}\eta^2 + \frac{\beta}{4}\eta^4 + \frac{\gamma}{6}\eta^6 + q\eta^2 u + \frac{Q}{2}u^2 + \frac{\delta}{2}\left(\frac{d\eta}{dx}\right)^2, \tag{1}$$

where η is the order parameter, u is the strain tensor component along the only direction (x), and Q is the longitudinal elastic modulus. As usual $\alpha = \alpha'(T - T_c)$, and all other coefficients are supposed to be independent of temperature. The condition of lateral clamping is that the average strain $\langle u\rangle = 0$. Since we explicitly consider only the case of tricritical transition in the clamped homogeneous system, we put $\beta = 0$. In this section, only piecewise constant distributions of η and u are considered (homogeneous symmetrical and nonsymmetrical phases) and the contributions of discontinuities (interphase boundaries) are neglected. Therefore, we can omit the gradient term in Eq. (1) and call the theory Landau-type one-dimensional model. The total free energy F of the system is then

$$F = \int_0^L \left(\frac{\alpha}{2}\eta^2 + \frac{\gamma}{6}\eta^6 + q\eta^2 u + \frac{Q}{2}u^2\right)dx. \tag{2}$$

The equilibrium piecewise distributions of η and u are to be found from the condition of minimum of F given that for the distribution of u the condition $\langle u\rangle = 0$ is fulfilled. In the case of a system that is nonclamped but is subjected to an external stress σ, the full energy includes that of the stress source that is equal to $-L\sigma_{ext}\langle u\rangle$, where $\langle u\rangle$ is no more fixed. For a free ($\sigma_{ext} = 0$) and homogeneous ($\langle u\rangle = u$) case, the integration in Eq. (2) is reduced to multiplication of the integrand by L. To consider the behavior of the unclamped system (which is known to be homogeneous), it is convenient first to minimize over u to obtain

$$F = L\left(\frac{\alpha}{2}\eta^2 - \frac{q^2}{2Q}\eta^4 + \frac{\gamma}{6}\eta^6\right). \tag{3}$$

This form of free energy is well known in the Landau theory of first-order phase transitions, see Strukov *et al.* (1998). According to this theory, the transition occurs at

$$\alpha = \alpha_t = 3q^4/(4\gamma Q^2) \tag{4}$$

and with two possible discontinuities of η: from zero to $\pm\eta_t$, where

$$\eta_t^2 = 3q^2/(2\gamma Q). \tag{5}$$

Going back to a clamped system we suppose that it consists of two-phases: one part with $\eta \neq 0$, $u = u_1$, and length l_1, and the other part with $\eta = 0$, $u = u_2$, and length l_2. Then,

$$F = \left(\frac{\alpha}{2}\eta^2 + \frac{\gamma}{6}\eta^6 + q\eta^2 u_1 + \frac{Q}{2}u_1^2\right)l_1 + \frac{Q}{2}u_2^2 l_2. \tag{6}$$

The condition of clamping of the system reads

$$u_1 l_1 + u_2 l_2 = 0 \quad \text{or} \quad u_2 = -u_1 l_1/l_2. \tag{7}$$

Introducing a new variable $\xi = l_1/L$ and noting that $l_2 = (1 - \xi)L$, we obtain

$$\frac{F}{L}(\eta, u_1, \xi) = \left(\frac{\alpha}{2}\eta^2 + \frac{\gamma}{6}\eta^6 + q\eta^2 u_1 + \frac{Q}{2(1-\xi)}u_1^2\right)\xi. \tag{8}$$

To determine the equilibrium state of the system, one must minimize F/L over all the three variables. One obtains (for $\xi \neq 0$ and $\eta_e \neq 0$)

$$u_{1e} = -\frac{q\eta_e^2}{Q}(1 - \xi_e), \tag{9}$$

$$\alpha = -\gamma\eta_e^4 + 2\frac{q^2\eta_e^2}{Q}(1 - \xi_e), \tag{10}$$

$$\alpha\eta_e^2 + \frac{\gamma}{3}\eta_e^6 + 2q\eta_e^2 u_{1e} + \frac{Q}{(1-\xi_e)^2}u_{1e}^2 = 0. \tag{11}$$

From these three equations, the dependence of η_e, u_{1e}, and ξ_e on α, i.e., on temperature can be found. One obtains

$$\eta_e^2 = \frac{3q^2}{2Q\gamma} = \eta_t^2, \tag{12}$$

i.e., in all temperature range of existence of the two-phase state, the value of η does not change with temperature and is equal to discontinuity in η at phase transition in free sample. The relation

between ξ_e and α is given by

$$\xi_e = \frac{\alpha_t - \alpha}{4\alpha_t}. \tag{13}$$

High temperature limit (HTL) ($\xi_e = 0$) is at $\alpha = \alpha_1 = \alpha_t$, i.e., at the same temperature as the first-order transition in free crystal, and low temperature limit (LTL) ($\xi_e = 1$) takes place at $\alpha = \alpha_2 = -3\alpha_t$. To find equilibrium free energy of TPS, we use Eqs. (8), (9), (12), and (13) to get

$$F_{etp} = -L\alpha_t \eta_t^2 \xi_e^2. \tag{14}$$

The lower limit of the two-phase state coincides with equality of equilibrium free energies of TPS given by Eq. (14) and of the homogeneous, clamped state of the nonsymmetrical phase at the same temperature. From Eq. (2) with $u = 0$, it follows that this energy is

$$F_{enhc} = -L(-\alpha)^{3/2}/3\gamma^{1/2}. \tag{15}$$

Substituting $\alpha = -3\alpha_t$ into Eqs. (14) and (15) and having in mind Eqs. (4) and (5), one can check that these two energies are equal.

Let us discuss more about the obtained results. From Eq. (1), we find that the local longitudinal stress (σ) is given by $\sigma = \frac{\partial f}{\partial u}$, i.e.,

$$\sigma = Qu + q\eta^2. \tag{16}$$

The equilibrium stresses in the symmetrical and nonsymmetrical regions are as follows:

$$\sigma_{sym} = Qu_{2e} = q\eta_t^2 \xi_e, \tag{17}$$

$$\sigma_{nsym} = Qu_{1e} + q\eta_e^2 = q\eta_t^2 \xi_e, \tag{18}$$

where Eqs. (7), (9), and (12) were used. We see that $\sigma_{sym} = \sigma_{nsym}$, i.e., the condition of the mechanical equilibrium

$$\frac{d\sigma}{dx} = 0 \tag{19}$$

is satisfied.

Let us now ask ourselves why the value of η remains equal to η_t through all the temperature region of TPS despite the changes in temperature? To answer this question, consider the region of the nonsymmetrical phase at a given temperature as the system of our interest and the region of the symmetrical phase as a source of stress that is exerted on our system. We fix this stress as given by Eq. (17) and find equilibrium η and u in our region by minimizing the free energy

$$F = \left(\frac{\alpha}{2}\eta^2 + \frac{\gamma}{6}\eta^6 + q\eta^2 u_1 + \frac{Q}{2}u_1^2 - \sigma_{ext}u_1\right) l_1. \tag{20}$$

Minimizing first with respect to u_1, we find

$$u_1 = \frac{\sigma_{ext}}{Q} - \frac{q}{Q}\eta^2. \tag{21}$$

Substituting Eq. (21) into Eq. (20), we obtain

$$F = \left(\frac{\alpha^*}{2}\eta^2 - \frac{q^2}{2Q}\eta^4 + \frac{\gamma}{6}\eta^6 - \frac{\sigma_{ext}^2}{2Q}\right) l_1, \tag{22}$$

where

$$\alpha^* = \alpha + \frac{2q}{Q}\sigma_{ext}. \tag{23}$$

Comparing Eqs. (22) and (3), we see that the η-dependent terms in both parentheses are the same with the only difference that instead of α in Eq. (3) we have α^* in Eq. (22), which, according to Eq. (23), reflects the difference between a free and a stressed system. Using Eq. (17) or (18) and Eq. (13), we find that

$$\alpha^* = \alpha_t, \tag{24}$$

i.e., is independent of temperature. That is why the value of η_e is constant within the TPS: the stress from the region of the symmetrical phase keeps the region of the nonsymmetrical phase in the conditions of the first-order phase transition in free system.

III. IMPROVED LANDAU-TYPE ONE-DIMENSIONAL MODEL: ADDING ENERGY OF INTERPHASE BOUNDARY

Trying to amend the complete neglection of interphase boundaries in Sec. II, we note that the simplest amendment is to consider the energy of the boundary and not its width. This may be called as the approximation of infinitely thin boundaries. In Sec. IV, it will be shown that, for not very small L, it gives the same results as the consistent analytical theory so that for large L the finiteness of IBE is more important than finiteness of the boundary width. When a TPS system is in equilibrium, it has as few interphase boundaries as possible. Depending on the boundary conditions, there will be just one or two boundaries in the whole system. In Sec. IV, we consider the case of a single boundary as the equilibrium case, and here, we will consider the same. From the discussion in the final part of Sec. II, it is clear that of our interest is the IBE at the first-order transition in free sample. As far as we know, within the Ginzburg–Landau model, this energy was calculated for the first time in Larkin *et al.* (1969); see also Lajzerowicz (1981). We add it to the energy of TPS (in our notions and correcting a misprint and a calculational error) first to Eq. (8) to mention that, being a number, it disappears after minimization so that Eqs. (9)–(13) remain valid for this section also. Then, we go to Eq. (14), and the full equilibrium free energy of the system is now

$$F_{etp} = -L\alpha_t \eta_t^2 \xi_e^2 + \frac{\alpha_t \eta_t^2}{4} r_{ct}, \tag{25}$$

where $r_{ct} = \sqrt{\delta/\alpha_t}$, i.e., is the order parameter correlation radius at temperature of the first-order phase transition. We see that the full

energy becomes zero, i.e., it is equal to energy of the symmetrical phase not at $\xi = 0$ (see also Fig. 1) but at

$$\xi_{ein} = \sqrt{\frac{r_{ct}}{4L}} \tag{26}$$

or at

$$l_{1ein} = \frac{\sqrt{r_{ct}L}}{2}. \tag{27}$$

This means that the initial size of region of the non-symmetrical phase is large and increases with increasing size of the system. Using Eq. (13), we find for HTL as

$$\alpha_1 = \alpha_t\left(1 - 2\sqrt{\frac{r_{ct}}{L}}\right). \tag{28}$$

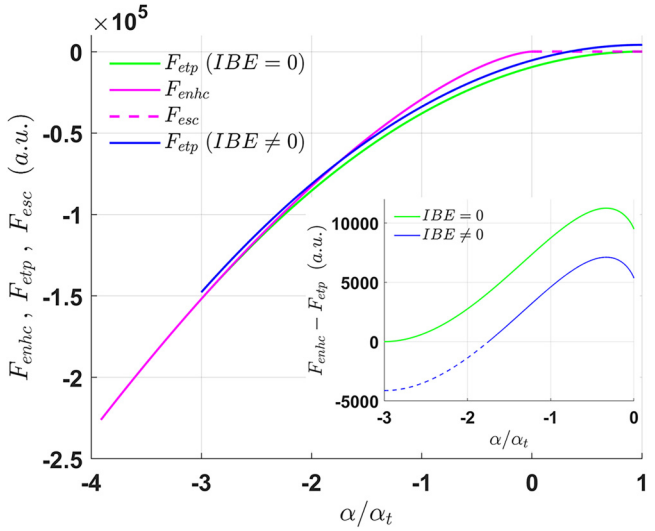

FIG. 1. Plot of equilibrium energies of two-phase state (with and without a finite value for IBE), F_{etp}, along with nonsymmetrical homogeneous clamped, F_{enhc}, and symmetrical clamped, F_{esc}, states as a function of α/α_t. The value of α/α_t at which F_{etp} curves intersect $F = 0$, i.e., the energy of the symmetric clamped phase, marks the transition temperature between the symmetric clamped phase and TPS. For the case of $IBE = 0$, this transition takes place at $\alpha/\alpha_t = 1$, i.e., at the same temperature as in unclamped system. The nonsymmetric homogeneous phase becomes possible, though metastable, in clamped system at $\alpha/\alpha_t = 0$. The difference between F_{enhc} and $F_{etp}(IBE = 0)$ is given in the inset (green solid line), and it is seen that two energies become equal to each other at $\alpha/\alpha_t = -3$. Although for the case of $IBE \neq 0$, the phase transition between the symmetric clamped phase and TPS occurs at $\alpha < \alpha_t$. The nonsymmetrical homogeneous phase in the clamped system remains metastable until its curve (magenta) crosses the curve of F_{etp} ($IBE \neq 0$, blue). This happens at $\alpha > -3\alpha_t$, i.e., a finite value of IBE shrinks the temperature interval in which TPS is the equilibrium phase. The difference between energies of nonsymmetrical homogeneous clamped and TPS ($IBE \neq 0$) phases is shown in the inset (blue line), and the blue solid line indicates the temperature interval in which TPS ($IBE \neq 0$) is the equilibrium state for $\alpha/\alpha_t < 0$.

Expectably, due to IBE, $\alpha_1 < \alpha_t$, i.e., account for IBE leads to a decreasing HTL. Note that α_1 cannot be negative because at $\alpha = 0$ the symmetrical phase loses its stability with respect to the formation of a *homogeneous* nonsymmetrical phase, so that Eq. (28) is meaningless for $L < 4r_{ct}$.

The finiteness of the region of the nonsymmetrical phase at HTL means that the transition TPS $\leftrightarrow$ symmetrical phase is discontinuous, i.e., there is an entropy jump (latent heat) at the transition. According to Eqs. (25) and (13), the value of the latent heat is

$$T\Delta S = -T\frac{dF_{etp}}{dT} = -TL\frac{\alpha'\eta_t^2}{2}\xi_{ein} = -T\frac{\alpha'\eta_t^2}{4}\sqrt{r_{ct}L}, \tag{29}$$

i.e., the entropy of TPS is less than that of the symmetrical phase, and there is a release of heat at phase transition from the symmetrical phase to TPS.

To consider the appearance of the region of the symmetrical phase, we have to equate the equilibrium energies of TPS [Eq. (25)] and homogeneous state [Eq. (14)], so that the condition of LTL (see also Fig. 1) reads

$$-L\alpha_t\eta_t^2\xi_e^2 + \frac{\alpha_t\eta_t^2}{4}r_{ct} = -L(-\alpha)^{3/2}/3\gamma^{1/2}. \tag{30}$$

Using Eq. (13), we express α through ξ_e and introduce a new variable defined as $\xi_e = 1 - \zeta_e$ in terms of which we have

$$-\eta_t^2(1-\zeta_{ein})^2 + \frac{\eta_t^2}{4L}r_{ct} = -\alpha_t^{1/2}(3 - 4\zeta_{ein})^{3/2}/3\gamma^{1/2}. \tag{31}$$

Near the LTL, $\zeta_e \ll 1$, and one can expand the r.h.s. in series of powers of ζ_{ein} up to ζ_{ein}^2 and use Eqs. (4) and (5) to obtain

$$\zeta_{ein} = \sqrt{\frac{3r_{ct}}{4L}} \tag{32}$$

or

$$l_{2ein} = \sqrt{\frac{3r_{ct}L}{4}}. \tag{33}$$

We see that the dependence $l_{in} \propto L^{1/2}$ remains for LTL also, although the numerical coefficient is different. Rewriting Eq. (13) in terms of ζ_e, we find

$$\alpha_2 = \alpha_t\left(-3 + 2\sqrt{\frac{3r_{ct}}{L}}\right). \tag{34}$$

Now we calculate the latent heat at transition between TPS and the homogeneous nonsymmetrical phase,

$$T\Delta S = -T\frac{d(F_{enhc} - F_{etp})}{dT} = -T\frac{\alpha'\eta_t^2}{12}\sqrt{3r_{ct}L}, \tag{35}$$

i.e., the entropy of the homogeneous nonsymmetrical phase is less than that of TPS, and there is a release of heat at phase transition from TPS to the homogeneous nonsymmetrical phase.

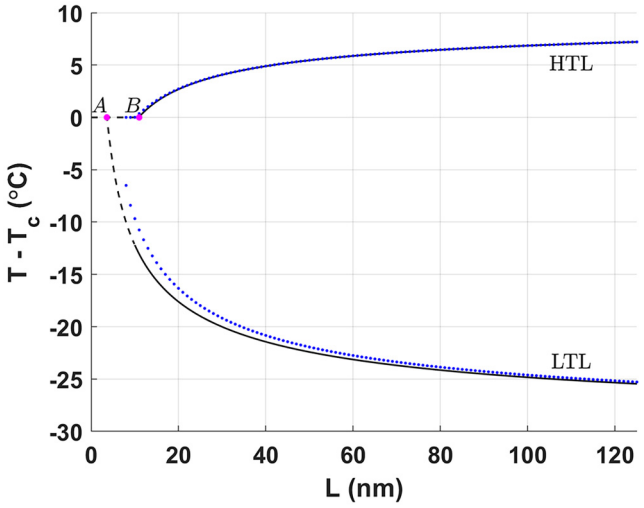

FIG. 2. *T- L* phase map showing theoretical HTL and LTL (solid lines), according to Eqs. (28) and (34), for material constants close to those of $BaTiO_3$ (see the text) along with their numerically computed counterparts (blue dots, see Sec. V).

The phase map according to Eqs. (28) and (34) is presented in Fig. 2 for material constants of $BaTiO_3$ close to those given in Pertsev *et al.* (1998) and Hlinka *et al.* (2006) excluding the value of β that, as is noted above, is put to zero for the sake of illustration. Specifically, we employed $\alpha = 6.6 \times 10^5 (T - T_c)\,\mathrm{J\,m\,C^{-2}}$, $\gamma = 4 \times 10^{10}\,\mathrm{J\,m^9\,C^{-6}}$, $q = 1.2 \times 10^{10}\,\mathrm{J\,m\,C^{-2}}$, $\delta = 5 \times 10^{-11}\,\mathrm{J\,m^3\,C^{-2}}$, and $Q = 2.4 \times 10^{11}\,\mathrm{J\,m^{-3}}$. The value of T_C does not matter in our analysis. In the region where L is comparable with r_{ct}, this map is contradictory: between the points A and B, the phase transition from the symmetrical phase occurs at $\alpha = 0$, i.e., with the loss of stability of the symmetrical phase with respect to *homogeneous* order parameter, while for the same interval of L, the transition from the homogeneous nonsymmetrical phase is into an *inhomogeneous* state (TPS). This means that somewhere below the line segment AB there should be a line of phase transitions between a newborn homogeneous nonsymmetrical phase and TPS, which is absent at the map. This failure of the approximation of infinitely thin boundary is natural when the boundary thickness (r_{ct}) becomes comparable with L. The region of such small Ls is of interest, and some preliminary results were reported by us in Levanyuk *et al.* (2020), but we left them beyond the paper not to overload it and because of the preliminary nature of the results.

IV. GINZBURG–LANDAU ONE-DIMENSIONAL MODEL

A. Governing equations

From Eq. (1) with $\beta = 0$ and the condition of mechanical equilibrium, we obtain equations for equilibrium distributions of η and u. They are

$$\alpha\eta_e + \gamma\eta_e^5 - \delta\frac{d^2\eta_e}{dx^2} + 2q\eta_e u_e = 0, \tag{36}$$

$$d\sigma/dx = 0 \quad \text{or} \quad \sigma = const, \tag{37}$$

where σ is given by Eq. (16). Therefore,

$$Qu_e + q\eta_e^2 = C. \tag{38}$$

The constant C can be found from the condition of clamping (Onuki *et al.*, 2007). Averaging Eq. (16) over the sample and taking into account that, because of the clamping the average of u_e, i.e., $\langle u_e \rangle = 0$, one finds $C = q\langle\eta_e^2\rangle$ and

$$u_e = q\frac{\langle\eta_e^2\rangle - \eta_e^2}{Q}. \tag{39}$$

Substituting this into Eq. (36), one has

$$\alpha^+\eta_e - \frac{2q^2}{Q}\eta_e^3 + \gamma\eta_e^5 - \delta\frac{d^2\eta_e}{dx^2} = 0, \tag{40}$$

where

$$\alpha^+ = \alpha + 2q^2\langle\eta_e^2\rangle/Q. \tag{41}$$

B. Large length approximation

A solution of Eq. (36) is known for an infinite system, for $0 < \alpha^+ < \alpha_t$, and the condition that both η and $d\eta/dx$ tend to zero as $x \to \pm\infty$ (Falk, 1983). We will present the η profile in our finite system truncating this solution. We will argue that this provides a good approximation for the η profile in the case of sufficiently large L. To show this, let us discuss the form of this solution. It reads

$$\eta = \eta_0\left(\frac{1}{1 + p(\sinh(gx))^2}\right)^{1/2}, \tag{42}$$

where

$$\eta_0 = \eta_t\left(1 - \sqrt{\Delta}\right), \tag{43}$$

$$p = 2\frac{\sqrt{\Delta}}{1 + \sqrt{\Delta}}, \tag{44}$$

$$g = \sqrt{\alpha^+/\delta} = \sqrt{\alpha_t/\delta}\sqrt{1 - \Delta}, \tag{45}$$

$$\Delta = \frac{\alpha_t - \alpha^+}{\alpha_t}. \tag{46}$$

Solution [Eq. (42)] is presented in Fig. 3 for $\beta = 0$ and other material constants close to those of $BaTiO_3$ (Pertsev *et al.*, 1998; Hlinka *et al.*, 2006). For very small values of Δ, it can be interpreted as a region of the nonsymmetrical phase surrounded by the infinite symmetrical one. Pay attention that the values of Δ which

correspond to macroscopic widths of this region are extremely small. This is not completely unexpected: recall that $\alpha^\star$ of Eqs. (22) and (23) which plays the same role in defining the value of η in Sec. II as α^+ in this section [cf. Eqs. (40) and (22)] was found to be exactly equal to α_t in all temperature region of TPS. But this "exactly" refers to an approximate treatment. Naturally, in a more precise treatment where no assumptions are made, the difference between α_t and an analog of $\alpha^\star$, i.e., α^+, is no more zero but is very small. Let us discuss Eq. (42) more formally considering the case $p \neq 0$. Because of extreme smallness of Δ, we can put: $g = r_{ct}^{-1}$, $\eta(0) = \eta_t$, and $p = 2\sqrt{\Delta}$. It is seen from Eq. (42) that, starting from η_0 at $x = 0$, the value of η almost does not change with x until $p(\sinh(gx))^2$ term becomes comparable with unity. The point $x = x_0$ where $p(\sinh(gx_0))^2 = 1$ can be considered as corresponding to the half-width of the maximum. Since $p \ll 1$, this occurs when $\sinh(gx) \gg 1$, i.e., $\sinh(gx) \simeq \exp(gx)/2$ so that

$$x_0 = r_{ct} \ln\left(2/\sqrt{\Delta}\right)/2. \tag{47}$$

This explains extremely small values of Δ corresponding to macroscopic values of x_0. When $x - x_0$ is larger than several r_{ct}, the value of η decays exponentially,

$$\eta \cong \frac{2^{1/2}\eta_0}{\Delta^{1/4}} \exp(-x/r_{ct}). \tag{48}$$

Thus, for $\Delta \ll 1$, the profile of η can be presented as a very flat plateau with a steep decent to practically zero. The width of the decent (the "boundary") being equal to several r_{ct} (see Fig. 3) is much less than the plateau width. We see, therefore, that at $\Delta \ll 1$ one can interpret $2x_0$ as approximate width of nucleus or, rather, a

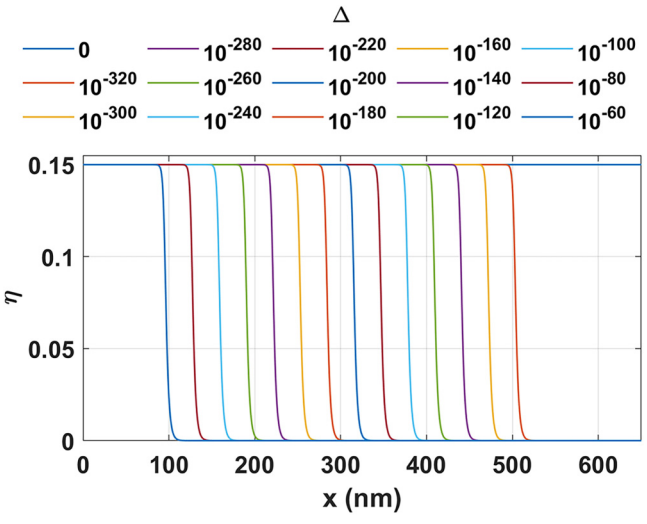

FIG. 3. η profiles, according to Eq. (42), for various values of Δ. Note almost 300 orders of magnitude of change in Δ when the width of the region of nonsymmetrical phase changes about five times. This agrees with Eq. (47) and is commented in the text.

region of the nonsymmetrical phase with the thickness of interphase boundary of the order of r_{ct}, which is much smaller than the nucleus width.

We propose to truncate the solution for infinite space to represent TPS in a finite system. This is very good approximation if, e.g., we present TPS where the region of the nonsymmetrical phase occupies the center of the sample, and there are two regions of the symmetrical phase, to the left and to the right from the center. Any homogeneous boundary condition will be fulfilled in this case with exponentially small error if the borders of the system are not too close to the interphase boundaries. Another possibility is to truncate the solution at points $x = 0$ at Fig. 3 and at some other point $(x = L)$ and fix the boundary conditions as

$$\frac{d\eta}{dx}(0, L) = 0. \tag{49}$$

Equation (49) is evidently satisfied at $x = 0$ and is approximately satisfied at $x = L$ if this point is not close to the interphase boundary. This is easy to accomplish at HTL where the nonsymmetrical phase occupies the minor part of the system but is also possible at LTL though here the nonsymmetrical phase occupies the main part of the system. Indeed, according to Eq. (33), the width of the region of the symmetrical phase at LTL is $\sqrt{3r_{ct}L/4}$. This is more than the boundary width (r_{ct}) and the point $x = L$ is located in the region of exponential "tail" of η distribution if

$$L \gg r_{ct}. \tag{50}$$

Figure 3 illustrates why the approximation of infinitely thin boundary works very well. Indeed, the width of the region of the nonsymmetrical phase is extremely sensitive to the value of Δ: to pass from the infinite width at $\Delta = 0$ to a width of 0.5 μ, the change in Δ of only 10^{-320} (!) is needed while the width of the interphase boundary is practically independent of Δ down to L comparable with $r_{ct} = 2.7$ nm for our material constants (Fig. 3). That is why the condition of the large length approximation given by Eq. (50) is also the condition of approximation of infinitely thin boundary used in Sec. III.

C. Method to find the high- and low-temperature limits of two-phase state

We begin by calculating (Gradshtein *et al.*, 1996)

$$\langle \eta_e^2 \rangle = \frac{1}{L}\eta_t^2 \int_0^L \frac{1}{1 + 2\sqrt{\Delta}(\sinh(gx))^2} dx$$
$$= \frac{\eta_t^2}{2gL\sqrt{1-2\sqrt{\Delta}}} \ln \frac{1 + \sqrt{1-2\sqrt{\Delta}}\tanh gL}{1 - \sqrt{1-2\sqrt{\Delta}}\tanh gL}. \tag{51}$$

Since Δ is expressed through α and $\langle \eta_e^2 \rangle$ [see Eq. (46)], we have now a transcendental equation for function $\langle \eta_e^2 \rangle = \langle \eta_e^2 \rangle(\alpha)$ or $\alpha(\langle \eta_e^2 \rangle)$. It may seem that the minimum of the first or maximum of the second function corresponds to the beginning of the region of the two-phase state. This is not necessarily so. The corresponding solution for $\eta(x)$ may well correspond also to an unstable metastable state. A reliable way to find the temperature of formation of the two-phase state is to calculate its energy and to

find the temperature where this energy is zero, i.e., it is equal to the energy of the symmetrical phase. We shall do this later and now we try to simplify Eq. (51). Since Δ is extremely small, we neglect it in the nominator of the logarithm's argument and expand the square root in the denominator. Also, we use an approximate formula $\tanh x \simeq 1 - 2\exp(-2x)$ that is valid for $x \gg 1$ or for $L \gg r_{ct}$, which, as we argued in Sec. IV B, is the condition of our approximation. As a result, we obtain

$$\langle \eta_e^2 \rangle = \frac{\eta_t^2 r_{ct}}{2L} \ln \frac{2}{\sqrt{\Delta} + 2\exp(-2L/r_{ct})}, \tag{52}$$

where the exponential term is neglected in the nominator and is conserved in the denominator since both this term and $\sqrt{\Delta}$ tend to zero at $L \to \infty$. For what follows, it is convenient to present Eq. (52) as

$$\alpha = \alpha_t - 2q^2 \langle \eta_e^2 \rangle / Q - 4\alpha_t \left(\exp\left(-\langle \eta_e^2 \rangle 2L/(\eta_t^2 r_{ct}) \right) - \exp(-2L/r_{ct}) \right)^2. \tag{53}$$

To calculate the energy of TPS, we first substitute Eq. (39) into Eq. (1) with $\beta = 0$; and by replacing in this equation η by η_e and integrating over x, we obtain

$$F_e = \int_0^L \left(\frac{1}{2}\alpha^+ \eta_e^2 - \frac{q^2}{2Q}\eta_e^4 + \frac{\gamma}{6}\eta_e^6 + \frac{\delta}{2}\left(\frac{d\eta_e}{dx}\right)^2 - \frac{q^2}{2Q}\langle \eta_e^2 \rangle \eta_e^2 \right) dx. \tag{54}$$

Note now that

$$\int_0^L \frac{\delta}{2}\left(\frac{d\eta_e}{dx}\right)^2 dx = -\int_0^L \frac{\delta}{2}\eta_e \frac{d^2\eta_e}{dx^2} dx + \frac{\delta}{2}\eta_e(L)\frac{d\eta_e}{dx}(L), \tag{55}$$

where the last term does not disappear because of the violation of the boundary condition at $x = L$ within our approximation. Being exponentially small for large L, this term does not influence the results and will be omitted in what follows. Using Eqs. (40) and (55), one can eliminate from the integrand in Eq. (54) the terms with α^+ and δ to obtain

$$F_e = L\frac{q^2}{2Q}\left(\langle \eta_e^4 \rangle - \frac{\langle \eta_e^6 \rangle}{\eta_t^2} - \langle \eta_e^2 \rangle^2 \right). \tag{56}$$

It is straightforward to calculate $\langle \eta_e^4 \rangle$ and $\langle \eta_e^6 \rangle$ with the help of Gradshtein *et al.* (1996). Within the same approximation as for Eq. (52), we obtain

$$F_e = \frac{\alpha_t \eta_t^2 r_{ct}}{4}\left(\frac{\Delta + 4\sqrt{\Delta}\exp(-2L/r_{ct})}{\left(\sqrt{\Delta} + 2\exp(-2L/r_{ct})\right)^2} - \frac{r_{ct}}{L}\ln^2 \frac{2}{\sqrt{\Delta} + 2\exp(-2L/r_{ct})} \right). \tag{57}$$

D. High-temperature limit of two-phase state (HTL)

Here, within our approximation, the width of the region of the non-symmetrical phase (x_0) is much less than L which, according to Eq. (47), means that $\sqrt{\Delta_{1\,in}} \gg 2\exp(-2L/r_{ct})$. Then, Eq. (57) simplifies to

$$F_e = \frac{q^2 r_{ct} \eta_t^4}{4Q}\left(1 - \frac{r_{ct}}{L}\ln^2 \frac{2}{\sqrt{\Delta}} \right). \tag{58}$$

The free energy is zero if

$$\sqrt{\Delta_{1\,in}} = 2\exp(-L^{1/2}/r_{ct}^{1/2}) \tag{59}$$

and

$$\langle \eta_{e1\,in}^2 \rangle = \eta_t^2 \sqrt{\frac{r_{ct}}{4L}} \tag{60}$$

[see Eq. (52)]. All the exponential terms in Eq. (53) can be neglected, and with the help of Eq. (60), we recover Eq. (28).

E. Low-temperature limit of two-phase state (LTL)

It is seen from Fig. 3 that $\Delta_{2\,in} \ll \Delta_{1\,in}$. So that it could very well be erroneous to neglect from the beginning the exponent in Eqs. (52) and (57). That is why we introduce a new variable (ψ) instead of Δ,

$$\sqrt{\Delta} = 2\psi \exp(-2L/r_{ct}). \tag{61}$$

Then, Eq. (52) acquires a form convenient near LTL,

$$\langle \eta_e^2 \rangle = \eta_t^2 \left(1 - \frac{r_{ct}}{2L}\ln(1+\psi) \right). \tag{62}$$

The free energy of the two-phase state [Eq. (57)] can be now presented in the following form:

$$F_{etph}/L = -\frac{q^2\eta_t^4}{2Q}\left(1 - \frac{\psi^2 - 2\psi}{4(1+\psi)^2}\frac{r_{ct}}{L} - \frac{r_{ct}}{2L}\ln(1+\psi) + \frac{r_{ct}^2}{4L^2}\ln^2(1+\psi) \right). \tag{63}$$

Transition to the two-phase state occurs when its free energy given by Eq. (63) is equal to the energy of the single-domain state in the clamped system [Eq. (15)]. To express this energy in terms of Δ or ψ, we first express α in these terms. Using Eqs. (41) and (62), we obtain after some algebra,

$$\alpha = -3\alpha_t - \alpha_t\Delta + 2\alpha_t \frac{r_{ct}}{L}\ln(1+\psi) \simeq -3\alpha_t + 2\alpha_t \frac{r_{ct}}{L}\ln(1+\psi). \tag{64}$$

The possibility to neglect the term with Δ is evident after inspecting Fig. 3 but will be also justified later. The equilibrium free energy of

the homogeneous state can now be written as

$$F_{enhc}/L = -(-\alpha)^{3/2}/3\gamma^{1/2} = -\frac{q^2\eta_t^4}{2Q}\left(1 - \frac{r_{ct}}{L}\ln(1+\psi) + \frac{r_{ct}^2}{6L^2}\ln^2(1+\psi)\right), \quad (65)$$

where it is taken into account that $\frac{r_{ct}}{L}\ln(1+\psi) \ll 1$ will be shown after finding ψ. From $F_{enhc} = F_{etph}$, we obtain for $\psi = \psi_{2\,in}$ using Eqs. (63) and (65),

$$\ln(1+\psi_{2in}) = \sqrt{\frac{\psi_{2in}^2 - 2\psi_{2in}}{(1+\psi_{2in})^2}\frac{3L}{r_{ct}}}. \quad (66)$$

This equation has no solution at $\psi_{2in} < 2$, but supposing that $\psi_{2\,in} \gg 1$, we find

$$\psi_{2in} = \exp\left(\sqrt{\frac{3L}{r_{ct}}}\right) \quad (67)$$

justifying the assumption. Also,

$$\Delta_{2\,in} = 4\exp\left(2\left(\frac{3L}{r_{ct}}\right)^{1/2} - 4L/r_{ct}\right). \quad (68)$$

We also see that the neglection of the term with Δ in Eq. (64) was justified and $\frac{r_{ct}}{L}\ln(1+\psi) = \left(\frac{3r_{ct}}{L}\right)^{1/2}$, i.e., is indeed small for very large L though, because of the square root, the condition of L being large is more restrictive here than for HTL. From Eq. (64) we obtain Eq. (34).

V. NUMERICAL SIMULATIONS

The condition of applicability of our long-length approximation [Eq. (50)] is rough. We can acquire a realistic idea about the level of precision of our approximation by performing numerical solutions for the same problem with different Ls. The coefficients in the Landau free energy are chosen to be the same or close to those for $BaTiO_3$ in Pertsev *et al.* (1998) and Hlinka *et al.* (2006) with the exclusion of the coefficient of η^4 that is put to be equal to zero in order to have a tricritical transition in the clamped system if the homogeneity is imposed as we supposed in the analytical part. In the numerical calculations, the distribution of η and the displacement U have been obtained on a grid consisting of 0.05 nm (0.02 nm if $L \leq 50$ nm) cells by solving the governing equations using an iterative scheme, namely, Newton's method (Quarteroni *et al.*, 2014). We solve Eqs. (36) and (37) for η and the longitudinal displacement U given that $u = dU/dx$. Specifically, we have

$$\alpha\eta_e + \gamma\eta_e^5 + 2q\eta_e\frac{dU_e}{dx} - \delta\left(\frac{d^2\eta_e}{dx^2}\right) = 0 \quad (69)$$

and the mechanical equilibrium equation given as

$$\frac{d^2U_e}{dx^2} + \frac{2q}{Q}\eta_e\frac{d\eta_e}{dx} = 0. \quad (70)$$

Taking into account the boundary conditions on U_e and η_e, $U_e = 0$ and $d\eta_e/dx = 0$ at $x = 0$ and $x = L$, one obtains the complete set of equations to solve $\eta_e(x)$ and $U_e(x)$ for various system sizes and temperatures. Computations were initiated from a low enough temperature, e.g., $T_s = 90\,^\circ C$, at which the homogeneous nonsymmetrical phase is the equilibrium solution, starting from the zero vector for U and a vector of uniformly distributed random numbers between 0.12 and 0.15 for η as the initial guess. Equations (69) and (70) are solved sequentially until a pre-set convergence criterion, e.g., a maximum of 10^{-12} in the infinity norm of the difference of η profiles obtained in consecutive iterations, is reached. Following that, the thus obtained solution is then provided as the initial guess for the next temperature $T_s + dT$ where $dT = 0.1\,^\circ C$. The calculations were performed up to the temperature, T_{max}, at which the homogeneous symmetric phase is the only solution. The temperature interval from T_s to T_{max} constitutes the heating cycle of the computations. After reaching the peak temperature T_{max}, temperature was decreased all the way down to T_s in steps of $dT = 0.1\,^\circ C$, and this run constitutes the cooling cycle. At each temperature, the energy of the system is calculated by inserting the solutions for $\eta_e(x)$ and $U_e(x)$ into Eq. (71),

$$F = \int_0^L \left(\frac{\alpha}{2}\eta^2 + \frac{\gamma}{6}\eta^6 + q\eta^2 u + \frac{Q}{2}u^2 + \frac{\delta}{2}\left(\frac{d\eta}{dx}\right)^2\right)dx. \quad (71)$$

HTL was determined from the heating cycle as the first, i.e., lowest, temperature at which the energy of the system becomes equal to zero. Meanwhile, the LTL was determined as the temperature at which the energy of the homogeneous nonsymmetric phase obtained in the heating cycle is equal to that of the TPS obtained in the cooling cycle. The main difficulty of the numerical simulations is that the equations provide solutions for both equilibrium and metastable states. For comparison with the theory, the latter presents no interest and thus such solutions, e.g., η profiles with several IBs, were discarded. Additionally, since the presence of a single boundary is a necessary but not a sufficient condition for equilibrium, for a temperature inside the interval of existence of TPS, we consider the η profile as equilibrium if the same profile is reproduced both at heating and at cooling cycles. Profiles of η corresponding to equilibrium solutions are provided in Figs. 4(a)–4(f) for various T and L. The transition from the non-symmetrical phase to the two-phase state is consistent with the solution form given by Eq. (42) down to the lengths comparable with r_{ct}, see Fig. 3.

We see from Fig. 4 that the profiles of η assumed in the approximation of infinitely thin boundaries in the analytical treatment are reproduced well for fairly large L only [see Fig. 4(f)], while the temperatures of HTL and LTL are in good agreement with this approximation down to much smaller lengths (Fig. 2). This might be explained by the fact that it is

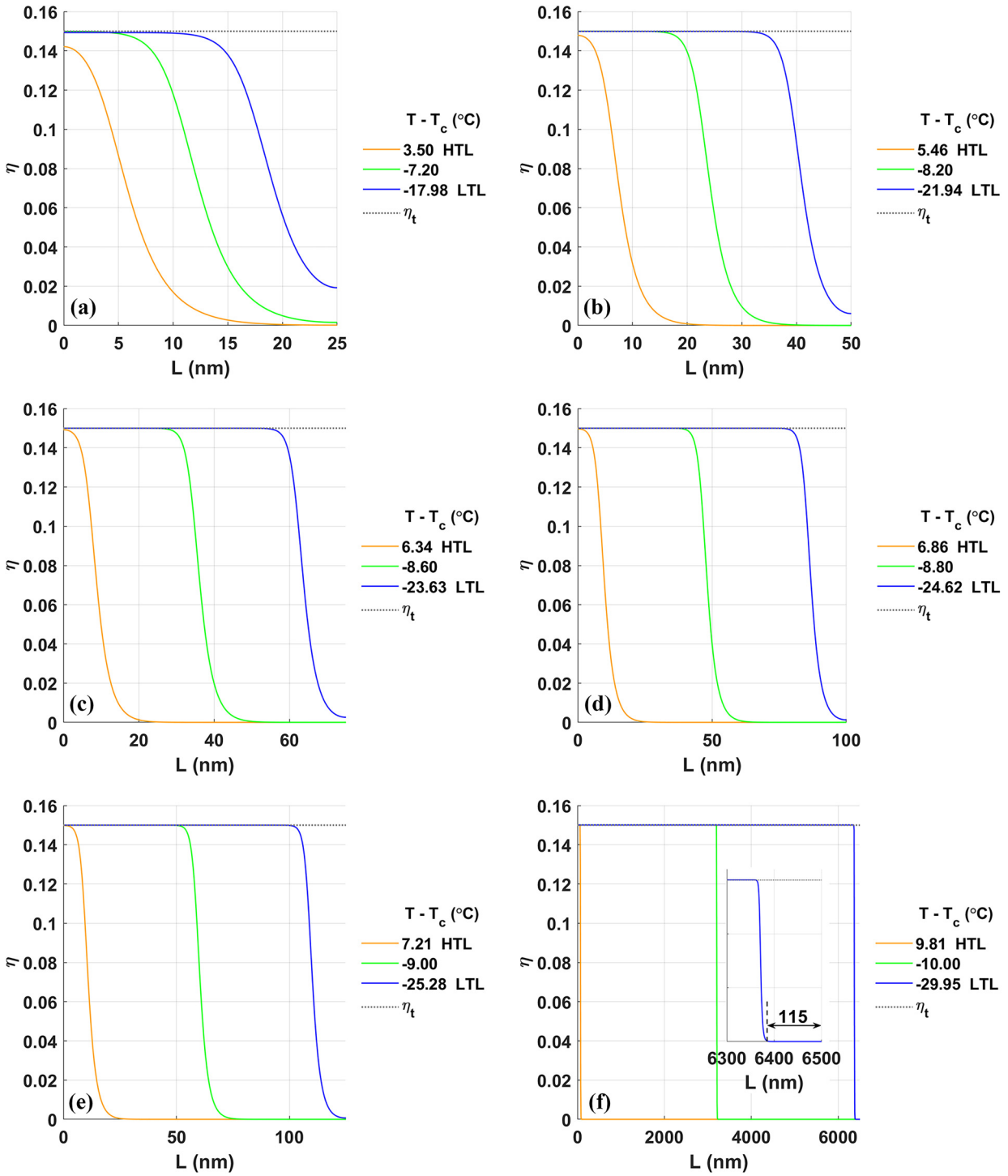

FIG. 4. The computed η profiles at HTL (blue line), LTL (orange line), and at the midway of these two limiting temperatures (green line) for L values of (a) 25 nm, (b) 50 nm, (c) 75 nm, (d) 100 nm, (e) 125 nm, and (f) 6500 nm. In (a)–(f), dotted black line displays η_t. In (f), the inset shows the details of the η profile at LTL where the width of the region of the symmetrical phase determined from Eq. (33) as 115 nm is shown to emphasize accordance of the large length approximation [Eq. (33)] with the numerical result.

the energy corresponding to a η profile and not its exact form that influences the HTL and LTL. We intentionally do not present the data for the smallest lengths of order of r_{ct}. The reason we do so is that the character of the non-symmetrical phase dramatically changes at small lengths where our analytical theory becomes inapplicable. After some preliminary analysis, we noticed that the study of what the non-symmetrical phase transforms to at small lengths deserves a separate investigation whose results would overload the content of the current paper and will be presented elsewhere.

VI. CONCLUSIONS

In summary, we analyzed the formation of the two-phase state taking into account the existence of interphase boundaries within Ginzburg–Landau or Landau-type models of the two-phase state arising in clamped systems with the material exhibiting first-order phase transition in a free state. We restricted ourselves to the one-dimensional case where available analytical formulas for space distribution of the order parameter can be used to a very good approximation for systems whose length is much larger than the order parameter correlation radius at the temperature of first-order transition in the corresponding free system. The main result of the paper is that the initial size of new phase at phase transitions to two-phase state from both the symmetrical and homogeneous non-symmetrical phases is proportional to $L^{1/2}$, where L is the system size. The analogy with the Landau–Lifshitz–Kittel law for dependence of domain width on the slab thickness is evident. Both phase transitions prove to be discontinuous, unlike in the earlier works, with the latent heat proportional to $L^{1/2}$ as well. The high- and low-temperature limits of the two-phase state shift with respect to the results of the Landau-type model which neglect energy of the interphase boundaries. These shifts increase with the diminishing of L and go to zero for infinite lengths (L) but relatively slowly, proportionally to $L^{-1/2}$ that makes this shift observable even for not very small lengths, e.g., for micrometer lengths in the system with structural phase transitions. These results were obtained analytically using the Landau-type approach in the simplified form when the thickness of the interphase boundary is neglected and a more consistent Ginzburg–Landau model considering gradients of the order parameter. In the latter case, the analytical results were possible to obtain analytically within an approximation valid for sufficiently large L. The results coincide with those obtained within the simplified approach. The deviations from the analytical results for the high- and low-temperature limits of the two-phase state obtained with the use of simplified approach or the large L approximation were found in numerical simulations at L about 10 nm if the material constants close to those of $BaTiO_3$ are used. A more detailed study of systems with small lengths, including finding the expected "critical length" below which no two-phase state forms, is left out of the paper so as not to overload it.

Of course, in real systems, non-equilibrium (metastable) two-phase states may exist for a very long time, not only longer than the experiment times but often longer than historical epochs. Theoretical understanding of these states in martensites is quite advanced, see, e.g., Roitburd (1978), Khachaturyan (1983), and Onuki (2002), but not, e.g., in ferroelectric systems. A clear understanding of equilibrium two-phase states in ideal finite systems with weak first-order phase transitions seems to be a necessary precondition for successful attacks on many unsolved problems.

SUPPLEMENTARY MATERIAL

See the supplementary material for more general results for the case of $\beta \neq 0$ without derivation but only providing formulas.

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DATA AVAILABILITY

The data that support the findings of this study are available within the article and its supplementary material.

REFERENCES

Devonshire, A. F., "Theory of barium titanate—Part II," Philos. Mag. **42**, 1065–1079 (1951).
Falk, F., "Ginzburg–Landau theory of static domain walls in shape-memory alloys," Z. Phys. B Condens. Matter **51**, 177–185 (1983).
Gradshtein, I. S. and Ryzhik, I. M., *Table of Integrals, Series and Products CD-ROM* (Academic Press, Inc., 1996).
Hlinka, J. and Marton, P., "Phenomenological model of a 90° domain wall in $BaTiO_3$-type ferroelectrics," Phys. Rev. B **74**, 104104 (2006).
Khachaturyan, A. G., *Theory of Structural Transformations in Solids* (John Wiley, New York, 1983).
Koukhar, V. G., Pertsev, N. A., and Waser, R., "Thermodynamic theory of epitaxial ferroelectric thin films with dense domain structures," Phys. Rev. B **64**, 214103 (2001).
Lajzerowicz, J., "Domain wall near a first order phase transition: Role of elastic forces," Ferroelectrics **35**, 219–222 (1981).
Larkin, A. I. and Khmelnitskii, D. E., "Layered structure in ferroelectric photoconductors," Sov. Phys. JETP **28**, 1245–1250 (1969) [Zh. Eksp. Teor. Fiz. **55**, 2345 (1969)].
Levanyuk, A. P., Minyukov, S. A., and Misirlioglu, I. B., "Loss of elastic stability and formation of inhomogeneous states at phase transitions in thin films on substrates," Ferroelectrics **533**(1), 1–9 (2018).
Levanyuk, A. P., Minyukov, S. A., Misirlioglu, I. B., and Okatan, M. B., "Elastic instability in clamped crystalline structures undergoing symmetry changing structural phase transitions," in The 31st Annual Workshop 2020 Fundamental Physics of Ferroelectrics and Related Materials, Silver Spring, MD, 26–29 January 2020.
Onuki, A., *Phase Transitions Dynamics* (Cambridge University Press, 2002).
Onuki, A. and Minami, A., "Phase transition in compressible ising systems at fixed volume," Phys. Rev. B **76**, 174427 (2007).
Pertsev, N. A., Zembilgotov, A. G., and Tagantsev, A. K., "Effect of mechanical boundary conditions on phase diagrams of epitaxial ferroelectric thin films," Phys. Rev. Lett. **80**, 1988–1991 (1998).
Pertsev, N. A. and Koukhar, V. G., "Polarization instability in polydomain ferroelectric epitaxial thin films and the formation of heterophase structures," Phys. Rev. Lett. **84**, 3722–3725 (2000).
Quarteroni, A., Saleri, F., and Gervasio, P., *Scientific Computing with Matlab and Octave*, 4th ed. (Springer, 2014).
Roitburd, A. L., "Martensitic transformation as a typical phase transformation in solids," Solid State Phys. **33**, 317–390 (1978).

Strukov, B. A. and Levanyuk, A. P., *Ferroelectric Phenomena in Crystals* (Springer, Berlin, 1998).

Tselev, A., Strelcov, E., Luk'yanchuk, I. A., Budami, J. D., Tishler, J. Z., Ivanov, I. N., Jones, K., Proksch, R., Kalinin, S. V., and Kolmakov, A., "Interplay between ferroelastic and metal–insulator phase transitions in strained quasi-two-dimensional VO_2 nanoplatelets," Nano Lett. **10**, 2003–2011 (2010).

Wei, J., Wang, Z., Chen, W., and Cobden, D. H., "New aspects of the metal-insulator transition in single domain vanadium dioxide nanobeams," Nat. Nanotechnol. **4**, 420–424 (2009).

Wu, J., Gu, Q., Guiton, B. S., de Leon, N. P., Quyang, L., and Park, H., "Strain-induced self-organization of metal-insulator domains in single-crystalline VO_2 nanobeams," Nano Lett. **6**, 2313–2317 (2006).