

Movement of the interphase boundary in KNbO_3 under pressure

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The study of the movement of the paraelectric-ferroelectric interphase boundary in KNbO_3 under hydrostatic pressure is provided in the framework of the mean-field theory. The analytical solution for the parameters of motion of the interphase boundary is applied for the calculations of the width and velocity of the latter at different pressures. The calculations are based on the experimental data for the Curie-Weiss constant and for the parameters of the Landau-Ginzburg expression for the free energy. The response to hydrostatic pressure and the tricritical point were calculated nonempirically.

I. INTRODUCTION

A broad family of perovskite-type oxides with chemical formula ABO_3 (A , B metals) includes many practically important materials which may undergo a sequence of ferroelectric phase transitions of both first and second order. The relation between the chemical composition and the macroscopic properties of ferroelectrics is by no means straightforward, and the demand for *ab initio* quantitative predictions is considerable.

Whereas most of the *ab initio* calculations performed up to date concentrate on the description of bulk equilibrium paraelectric or ferroelectric phases (see, e.g., Refs. 1–5), it is not less important for technological applications to be able to predict the behavior of the interphase boundary, i.e., kinetic aspects of the ferroelectric transitions (see, e.g., Refs. 6–8). The kinetics of a phase transition may be influenced via the adjustment of external thermodynamic parameters, such as temperature, external fields, and composition. Of these three parameters, the effect of concentration on the phase transition kinetics is a delicate matter which demands the additional experimental (or calculated from first principles) data due to the inherent modifications of the electronic structure on doping. The magnetic field response of the electronic structure of perovskite compounds is again very complicated, and the theoretical study of this response should be complemented by the detailed experimental measurements. The investigation of the behavior of the ferroelectric phase transition under pressure is highly attractive owing to the possibility to predict theoretically the parameters of the pressure response at relatively small pressures. These parameters may be extracted from the equation of states of the perovskite

under investigation on the assumption of the linear response.

The utmost sensitivity of ferroelectric properties to pressure and hence volume is well known from experiments⁹ as well as first-principles calculations.^{1–3} One of the most pronounced pressure effects on the ferroelectric properties is the large shift of phase transition temperatures.⁹ The growth and kinetics processes at symmetry-breaking first-order phase transitions are associated with the migration of interphase boundaries separating two coexisting phases. Hydrostatic pressure can also be a powerful tool of controlling the phase transition order: first-order phase transitions can be transformed into second-order one with increasing pressure.¹⁰

Most of the hydrostatic pressure measurements of ferroelectric phase transitions have been aimed at the study of the static properties of ferroelectrics.⁹ We assume that pressure may also essentially influence the phase transition kinetics which depend strongly on the phase transition temperature. The picture of the temperature-induced phase transition kinetics at ferroelectric phase transitions should be complemented by the investigation of the pressure effect on the interphase boundary propagation.

The present paper concentrates on the study of the hydrostatic pressure effect on the phase transition kinetics in ferroelectric KNbO_3 . We discuss the interfacial kinetics within an exactly soluble mean-field model which is the time-dependent Ginzburg-Landau theory.¹¹ We propose here to use this model for studying the pressure-induced motion of the interphase boundary in KNbO_3 . The calculations are done on the basis of the experimental data, with some important missing parameters being calculated nonempirically in the framework of the full-potential linear muffin-tin orbital (LMTO) method.¹²

II. MODEL FOR THE INTERPHASE BOUNDARY MOTION

The present mean-field approach is based on the application of the time-dependent Ginzburg-Landau theory for first-order phase transitions. For ferroelectrics, the order parameter is polarization P . Under the assumption of noncritical dependence of the Landau-Khalatnikov transport coefficient Γ on temperature and pressure, the movement of the interphase boundary is determined by the equation

$$\dot{P} = -\Gamma(\delta G/\delta P), \quad (1)$$

where G is the Gibbs energy, and the functional derivative $\delta G/\delta P$ is a term tending to restore the value P to its thermal equilibrium value. In the framework of the Landau theory of phase transitions, G may be expressed in a power series of polarization:

$$G = \int \left[g_0(p, T) + D(\nabla P)^2 + \frac{1}{2}AP^2 - \frac{1}{4}BP^4 + \frac{1}{6}CP^6 \right] dV, \quad (2)$$

where p , V , and T are pressure, volume, and temperature, respectively; g_0 is the Gibbs energy density for the paraelectric phase. A , B , and C are the Landau expansion coefficients, and D is the essentially positive coefficient of the gradient term. A first-order phase transition takes place when all Landau coefficients are positive. In (2), we implied the absence of piezoelectric effects in the paraelectric phase for cubic perovskites. Several recent nonempirical calculations (see, for example, Refs. 4 and 5) demonstrated the overwhelming importance of coupling to both isotropic and anisotropic strain. As shown in Ref. 13 the strain effect in perovskite-type ferroelectrics can be phenomenologically taken into account by renormalizing the coefficient B from Eq. (2). Thus, the experimentally obtained coefficient B already contains the strain contributions.

The high-temperature paraelectric phase may exist at temperatures above, and becomes absolutely unstable versus ferroelectric transition below, T_0 , that is, the stability limit of the paraelectric phase. Correspondingly, the ferroelectric phase becomes absolutely unstable above its stability limit T^* . In case of a first-order transition, these two temperature regions overlap: $T_0 < T^*$, giving rise to the temperature hysteresis: the system may pass through the same temperature remaining in the paraelectric state (on cooling), or in the ferroelectric state (on heating). The phase transition at some temperature T , where $T_0 < T < T^*$, develops as the growth of one phase at the expense of another one, with the interphase boundary moving. The equilibrium between two phases at the Curie temperature T_C is possible only if their free-energy densities are equal.

Analogously, upper and lower critical values and hysteresis exist with respect to pressure: the pressure p_c inducing the phase transition at a given temperature is

within limits $p_0 < p_c < p^*$, p_0 being the lower pressure limit for the stability of the paraelectric phase, p^* , the higher pressure limit for the stability of the ferroelectric phase.

The actual state of the material is determined by the topology of the free-energy surface in the (p, T) space. For temperatures $T_0 < T < T_C$ (or pressures $p_0 < p < p_c$), the paraelectric phase corresponds to a local minimum of the free-energy surface and hence is metastable, whereas the ferroelectric phase corresponds to the global minimum and is stable. At $T_C < T < T^*$ ($p_c < p < p^*$), the paraelectric phase is stable and the ferroelectric phase metastable.

The stability limit of the paraelectric phase with respect to temperature or pressure (T_0, p_0) is determined by the condition $A = 0$, or equivalently $(\frac{AC}{B^2})_0 = 0$; the stability limit of the ferroelectric phase follows from $(\frac{\partial g}{\partial P} = 0, \frac{\partial^2 g}{\partial P^2} = 0)$ and yields $(\frac{AC}{B^2})^* = \frac{1}{4}$; finally, the temperature T_C and pressure p_c at which the phase transition occurs are determined from $(\frac{\partial g}{\partial P} = 0, g = g_0)$ and hence $(\frac{AC}{B^2})_c = \frac{3}{16}$.

At $B = 0$, the region (in temperature or pressure) where two phases coexist shrinks to zero, thus determining the tricritical point (p_t, T_t) : $T_0 \rightarrow T_C = T_t \leftarrow T^*$, $p_0 \rightarrow p_c = p_t \leftarrow p^*$. This means that the phase transition in temperature changes from first order to second order at pressure p_t , as is known to be the case in perovskites.^{9,14-16,18,19}

The interphase boundary may remain quite sharp unless the temperature or pressure get sufficiently near the tricritical point, when the boundary becomes dispersed by spatially large fluctuations. The temperature difference between the phase transition temperature T_C and the temperature corresponding to the stability limit of the paraelectric phase, T_0 , decreases with increasing pressure; this is a manifestation of the fact that the phase transition changes from first order to second order with pressure. Such a situation may be described with the following pressure dependence of B apart from the tricritical point,

$$B = b(p_t - p). \quad (3)$$

The linear dependence of B on pressure corresponds to the first-order term in the pressure expansion series in analogy with the temperature dependence of the coefficient A in the Landau theory of phase transitions.

Considering low pressures and taking into account that paraelectric KNbO₃ has a cubic structure, we can express the coefficient A according to Ref. 9,

$$A = \beta(T - T_0) + 2\Xi p. \quad (4)$$

Here Ξ is a function of elastic and electrostrictive coefficients. Coefficient $\beta = 1/2c$, where c is the Curie-Weiss constant, depends neither on temperature nor pressure, as has been established for KNbO₃ in Ref. 14.

The present form of the coefficient A in Eq. (2) is correct in ferroelectrics for which the temperature of the stability limit of the paraelectric phase decreases linearly with increasing pressure. This is true, for example, in perovskites.^{9,14}

$$T_0(p) = T_0(0) - \frac{2\Xi p}{\beta}. \quad (5)$$

It follows from Eq. (2) that the dielectric susceptibility ϵ obeys the Curie-Weiss law. From the known data for perovskites at a constant temperature, the Curie-Weiss law can be written as follows:¹⁵

$$\frac{1}{\epsilon} = 2\Xi(p - p_0) \quad (6)$$

$$p_0 = -\frac{1}{2} \frac{\beta[T - T_0(0)]}{\Xi}. \quad (7)$$

Using the above pressure dependences, we consider the pressure-controlled interfacial dynamics at ferroelectric phase transitions. Taking a variation of the functional (2) and substituting the result into Eq. (1), we obtain for the uniaxial case the equation of motion for the polarization:

$$\dot{P} + \Gamma(AP - BP^3 + CP^5) - 2\Gamma DP_{xx} = 0. \quad (8)$$

Here a subscript means a derivation with respect to this variable. Equation (8) is the mean-field representation of the nonequilibrium interphase boundary kinetics. A steady-state solution of Eq. (8) may be found according to Ref. 11. The substitution $x \rightarrow s + vt$ introduces the coordinate system which moves along with the interphase boundary. The profile of the polarization front in the moving system is defined by

$$2\Gamma DP_{ss} + vP_s - \Gamma(AP - BP^3 + CP^5) = 0, \quad (9)$$

with the solution having the kink form

$$P = P_0 \left[1 + \exp\left(\frac{s}{\Delta}\right) \right]^{-0.5}, \quad (10)$$

which clearly represents the boundary between the ferroelectric phase ($P \rightarrow P_0$ for $s \rightarrow -\infty$) and the paraelectric phase ($P \rightarrow 0$ for $s \rightarrow \infty$). P_0 is the equilibrium value of polarization

$$P_0^2 = \frac{B}{2C} \left[1 + \left(1 - \frac{4AC}{B^2} \right)^{0.5} \right] \quad (11)$$

and Δ is the width of the interphase boundary given by

$$\Delta^2 = \frac{(3DC)}{B^2} [1 - 2\alpha + \sqrt{1 - 4\alpha}]^{-1}, \quad (12)$$

where

$$\alpha = \frac{AC}{B^2} = \frac{(p - p_0)}{(p_t - p)^2} \frac{b^2}{2\Xi C},$$

which moves with the velocity v :

$$v = \left(\frac{2D}{C} \right)^{0.5} \frac{\Gamma B}{3} (8\alpha - 1 - \sqrt{1 - 4\alpha}) \times [1 - 2\alpha + \sqrt{1 - 4\alpha}]^{-0.5}. \quad (13)$$

We restricted ourselves to the steady-state solution of (8), where the interphase boundary moves with a constant velocity v given by (13), but does not change its shape. The velocity v is determined by balancing the energy

acquired from the new phase with the energy lost from dissipation. At the equilibrium which should be reached for $t \rightarrow \infty$, the static form of the interphase boundary in the original coordinate system is

$$P = P_0 \left[1 + \exp\left(\frac{x - x_0}{\Delta}\right) \right]^{-0.5}, \quad (14)$$

as can be directly seen from the substitution of (14) into (8). The static shape of the interphase boundary (14) results from the competition of two terms: the homogeneous part of the Gibbs energy tends to bring the system to the paraelectric or ferroelectric state, while the inhomogeneous part of Eq. (2) enhances the tendency to the nonuniform state. Thus, the boundary preserves its equilibrium shape while moving. The ferroelectric phase transition proceeds at a finite rate by means of the phase transition front, which separates stable and metastable regions of the crystal specimen. The driving force of the interphase boundary movement is the tendency of the system to lower its Gibbs energy through a kinetic relaxation towards equilibrium. Analyzing (13) under isobaric conditions, we can conclude that the interphase boundary velocity may be positive or negative, depending on whether $T < T_C$ or $T > T_C$. The velocity v depends therefore on whether the sample is being cooled or heated.

III. CALCULATIONS OF THE PRESSURE DEPENDENCE OF THE INTERPHASE WIDTH AND VELOCITY FOR KNbO_3

Some explanatory comments are essential here to underline the distinguishing features of our approach in comparison with others, including first-principles, calculations devoted to the study of ferroelectric transitions for perovskites. The main aim of our paper is to describe the kinetics of phase transitions but not their thermodynamics. The kinetic properties of the system are much more sensitive to external conditions than thermodynamic ones. Thus special attention has to be attached to the choice of the model Ginzburg-Landau functional describing the phase transition as well as to the evaluation of the adjustable parameters appearing in this functional.

In a first-principles approach, the hierarchy of the different phases of the substance undergoing phase transition is usually studied in terms of thermodynamic potentials. Thus, the thermodynamic factor is declared to be the main one that determines the energetically favorable state. In order to construct thermodynamic potentials the preliminary modeling of the functional has to be done. For example, in the first-principles theory of ferroelectric phase transitions two main parameters describing the phase transition are accounted. They are the atomic displacements and strain deformations from the equilibrium cubic structure (see Ref. 5). The energy surface is represented by a low-order Taylor expansion with respect to these parameters. This expansion is performed together with the necessary symmetry conditions

that have to be put on the appearing terms. Several advantages of such a first-principles approach are obvious. The main one is the possibility to account for both microscopic and macroscopic phase transition parameters as well as their interaction. On the other hand, the use of the Taylor expansion, although it represents a regular procedure with principally controlled accuracy, leads to a dramatic increase of the number of first-principles calculations. This disadvantage becomes crucial if somebody wishes to construct the Φ^6 model functional, which includes up to sixth-order terms in microparameters and macroparameters of a phase transition. From the point of view of the common theory of phase transitions formulated in the Landau approach these terms are of special meaning. Only their inclusion allows one to describe in a proper way the first-order phase transition of ABO_3 perovskites between two thermodynamically stable states. Otherwise, restricting by the terms in the order lower than six in the power series on the parameters that describe the first-order phase transition, the coexistence of two stable states cannot be described. This result is well known and is discussed elsewhere (see, for example, Ref. 20). Thus, including such terms in the Ginzburg-Landau functional to describe first-order phase transitions is an essential and principal feature of the phenomenological Landau theory. Now, the question arises about the physical meaning of the results that may be obtained by first-principles calculations of ABO_3 perovskites, based on the Taylor expansion of the energy up to the fourth order with respect to microparameters and macroparameters.

The phases recognized as coinciding with experimentally observed cannot be considered as thermodynamically stable phases. They are not realized as a result of existing first-order phase transitions. Although the embryos of these phases may be obtained in theoretical simulations, the question about their thermodynamic stability or metastability remains open. Really, in a completely first-principles approach only supercells of limited sizes, traditionally small enough, are calculated. These supercells, even if their structure is the same as experimentally observed, have to be assumed and described as metastable embryos, which represent the short-range-ordered structure, but not the long-range-ordered one.

At variance with the Taylor expansion, the phenomenological Landau theory represents the Ginzburg-Landau functional as a polynomial function of parameters that are responsible for a phase transition,²¹ with the necessary accounting of the symmetry properties of the initial and final phases of the first-order phase transition.^{20,22} If we are going to investigate the kinetics of paraelectric-ferroelectric first-order phase transitions, two simplifications are possible. The main one accounts for the only macroscopic parameter that is responsible for the transformation (polarization, in the case of paraelectric-ferroelectric phase transition). The second one is making use of experimental data on the coefficients of the Ginzburg-Landau functional. This allows us to account for effectively also strain effects, because the coefficients of the functional are renormalized. This result is well known and was discussed, for example, in

Ref. 13. Furthermore, the measurements of the tricritical point in $KNbO_3$ are not available, to the best of our knowledge. That is why we are forced to combine the phenomenological approach with the first-principles calculations allowing us to estimate the missing data.

Keeping in mind the above-mentioned circumstances we can analyze the pressure dependences of the width and velocity of the interphase boundary under isothermal conditions. For our calculations we used the following experimental data for $KNbO_3$ at room temperature: $c = 2.4 \times 10^5$ K, $T_0 = 377^\circ\text{C}$, $C(p = 1 \text{ bar ambient pressure}) = 5.4 \times 10^{-22}$ CGSE, and $B_0 = 10^{-12}$ CGSE.⁸

The calculations of the coefficient Ξ and the tricritical point for perovskite-type $KNbO_3$ have been performed based on full-potential LMTO calculations using Methfessel's code.¹² With the choice of the basis set as in Ref. 3 we have carried out the calculations of the total energy at the set of different volumes for the paraelectric phase [see Fig. 1(a)] and three ferroelectric phases [differences of en-

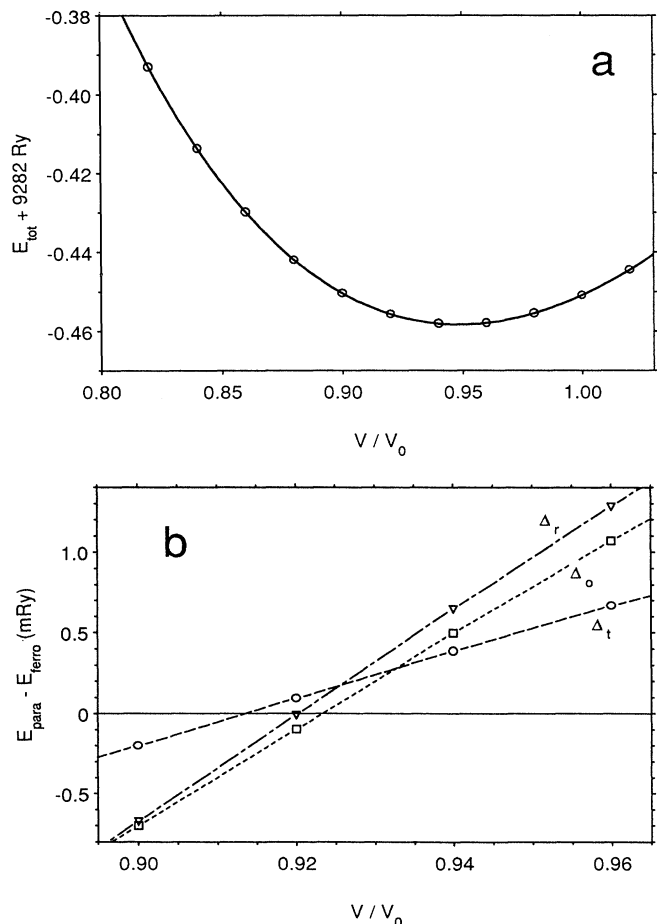


FIG. 1. (a) Total energies of the paraelectric phase in $KNbO_3$ as functions of the relative volume V/V_0 , where V_0 is the experimentally measured equilibrium volume of the paraelectric phase with the lattice parameter 3.997 \AA . (b) The differences of total energies for the paraelectric and three ferroelectric phases: $\Delta_t = E_{\text{para}} - E_{\text{tetra}}$; $\Delta_o = E_{\text{para}} - E_{\text{ortho}}$; $\Delta_r = E_{\text{para}} - E_{\text{rhomb}}$.

ergies from that of the paraelectric phase are shown in Fig. 1(b)]. In these calculations, we concentrated on the off-center displacements of the Nb atom as the primary feature of a ferroelectric transition. First, we have found the equilibrium off-center displacements for tetragonal, orthorhombic, and rhombohedral ferroelectric phases to be 0.022, 0.028, and 0.033 of the “theoretical” lattice constant, correspondingly. (“Theoretical” volume, as is typical when using the local density approximation, is underestimated by $\sim 5\%$ as compared to the “experimental volume” which corresponds to the lattice parameter of cubic perovskite cell extrapolated to zero temperature, $a=3.997 \text{ \AA}$.) We then scaled this displacement along with the unit cell dimensions while fitting the total energy versus volume dependence, in order to obtain the coefficient Ξ ,

$$\Xi = \left\{ -\frac{1}{V} \left(\frac{d^2 E}{dV^2} \right)^{-1} \right\},$$

where $\{\dots\}$ stands for the averaging over a set of volumes. For the paraelectric phase, we obtained $\Xi = 0.47 \times 10^{-3} \text{ kbar}^{-1}$. The measurements aimed at obtaining this parameter experimentally are expected to be rather difficult; therefore, nonempirical calculations of this value are crucially important for our high-pressure interphase simulations.

As is seen from Fig. 1(b), the cubic phase remains stable against any ferroelectric transformation for $V/V_0 < 0.9135$. Larger volume favors ferroelectric transitions first into the tetragonal phase, and then, for $V/V_0 > 0.9253$, the rhombohedral phase becomes energetically favorable over both the tetragonal and orthorhombic phases. For $V/V_0 > 0.9326$, i.e., covering the region of both “theoretical” and “experimental” lattice volumes, the well-known hierarchy of stabilities of three ferroelectric phases is established. As the temperature increases, the substance is expected to undergo a transition from rhombohedral to orthorhombic, then to tetragonal, and finally to the cubic paraelectric phase. When an external pressure is applied, the sequence of transitions initially remains the same, but the temperature intervals needed to pass the system through the sequence of transitions are gradually decreased, as is qualitatively evident from ever shrinking energy differences between phases. This is consistent with the trends in the phase transition temperatures of KNbO_3 on doping with Ta, that suppresses the ferroelectric state as an ultimate effect (see, e.g., Ref. 17), as well as with the data on phase transition temperatures as functions of pressure in $\text{K}(\text{Ta},\text{Nb})\text{O}_3$.¹⁴

At $V/V_0 < 0.9326$ our calculation shows that the sequence of phases is changed: the rhombohedral phase tends to undergo, on increasing the temperature, a transition first to the tetragonal and then to the orthorhombic phase. For pressures corresponding to this volume region, it is possible to determine the interphase boundary as that between cubic (paraelectric) and orthorhombic (ferroelectric) phases. On further increasing the pressure to that corresponding to $V/V_0 = 0.9232$, the total energy of the orthorhombic phase becomes equal to that

of the cubic phase at zero temperature, and the cubic-to-orthorhombic phase transition is no longer possible. The pressure related to this critical volume is therefore the tricritical pressure p_t . From the pressure-volume relation

$$dE/dV = -p,$$

which is shown in Fig. 2 for the cubic phase (corresponding curves for all phases are indistinguishable in this scale) and assuming that the thermal expansion coefficients for both phases are equal, it was found to be $p_t = 58.5 \text{ kbar}$.

We failed to find any experimental reports for tricritical pressure in KNbO_3 , but the estimated value seems to be reasonable, compared with $p_t=34 \text{ kbar}$ for BaTiO_3 .¹⁸ The difference $T_C - T_0$ for KNbO_3 is three times larger than that for BaTiO_3 (see, for example, Ref. 8). Consequently, a higher pressure should be required to reach the tricritical point.

It is worth noting that our results concerning the exact energetics of three ferroelectric phases with respect to the nonpolar one, and correspondingly the exact estimation of the tricritical pressure, may be somehow affected by the lattice strain, if the latter is properly taken into account in the geometry-optimizing calculations. The effect of the strain is expected to be most pronounced for the tetragonal phase, as follows from total-energy calculations for KNbO_3 (Ref. 3) and BaTiO_3 ,¹ and would bring the ground-state energy of the tetragonal phase closer to that of the rhombohedral phase at least near zero pressure. It is not as clear, however, how the energy differences shown in Fig. 1(b) will be changed over the broader range of volumes. Strictly speaking, one should also take into account electrostrictive effects in Ξ by optimizing the Nb displacement independently for each volume. The calculations which account for these additional factors are in progress and will be published elsewhere.

We estimated the coefficient D according to Ref. 23: $D = \frac{\pi}{15} d^2$, where d is the lattice parameter. The $d(p)$ dependence was also extracted from the data of the full po-

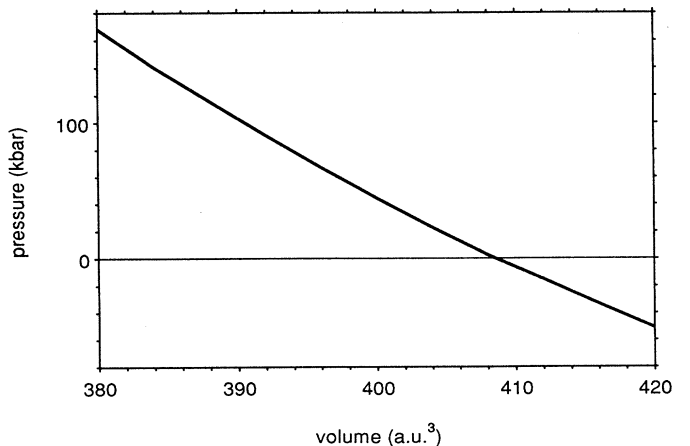


FIG. 2. The equation of states for the paraelectric phase in KNbO_3 .

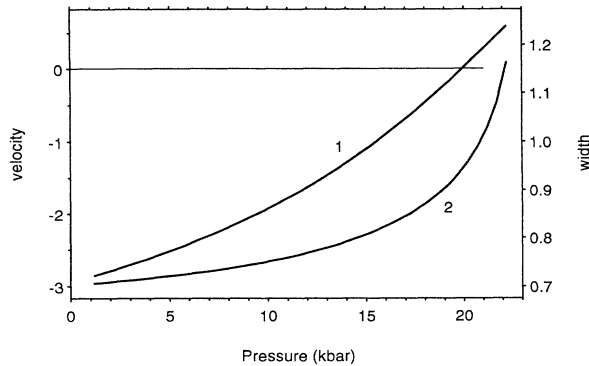


FIG. 3. Curve 1 is the interphase boundary velocity v [in units of $(\frac{2D}{C})^{0.5} \frac{E_B}{3}$] and curve 2 is the width Δ [in units of $(3DC)^{0.5} \frac{1}{B}$] as functions of pressure in KNbO_3 .

tential calculations by solving the equation of state. Using calculated $d(p)$, we see that within the pressure limits where both paraelectric and ferroelectric phases and hence the interphase boundary exist, the largest change in the unit cell size induced by pressure is about 6%.

It is seen from (12) that at $p = p_t$ the interphase boundary width Δ tends to infinity and thus at this pressure the first-order phase transition is transformed into a second-order one as it should take place at tricritical point. In Fig. 3 the pressure dependence of the width Δ [calculated along Eq. (12)] and velocity v [calculated along Eq. (13)] is shown over the whole range of pressures for which two phases may coincide; that was found to be $1.5 \text{ kbar} < p < 22.6 \text{ kbar}$. Both Δ and v are ever increasing functions of pressure. Since the width increases merely by a factor of 2, the interphase boundary remains well defined under typical hydrostatic pressures. The sign of the velocity specifies the direction in which the interphase boundary propagates, i.e., which one of two phases (paraelectric or ferroelectric) grows at the expense of the other. At $p = p_c = 19.9 \text{ kbar}$, the interphase boundary stops because the difference between the Gibbs energies of the two phases that is the driving force of the phase transition becomes zero. True equilibrium between two phases is possible only at $p = p_c$. The above-mentioned interfacial broadening results from the increase in the interphase boundary velocity. Analyzing the pressure dependence of the interface velocity for $p > p_c$ we obtain that $v \propto (p - p_c)^n$, where $n = 1.37 \pm 0.02$, and for $p < p_c$ we have $v \propto (p_c - p)^m$, where $m = 0.56 \pm 0.02$.

Experimental investigations of the temperature dynamics of interphase boundaries were carried out in ferroelectrics^{24–31} under isobaric conditions. These stud-

ies proved the theory of the temperature-induced interphase boundary dynamics, which was developed on the basis of the kink solution of the equation of motion for polarization. We made an extension of this theory for the case of the pressure-induced dynamics.

IV. CONCLUSION

We have presented a study of the pressure-induced movement of the ferroelectric phase transition boundary on the example of KNbO_3 . Our research is based on the exact solution of the time-dependent Ginzburg-Landau equation taking into account the hydrostatic pressure influence. The mean-field approximation describes well many static and dynamic phenomena in ferroelectrics, for example, in perovskites discussed here.⁹ For this reason, the theoretical results on the temperature-induced kinetics of perovskite ferroelectrics have been successfully used for the interpretation of experiments on the interphase boundary motion under isobaric conditions.^{26,32} Therefore, the application of the pressure-induced kinetics of ferroelectric phase transitions can also be useful for the interpretation of corresponding hydrostatic pressure measurements. We want to note that the not yet published, to our best knowledge, data on the tricritical pressure in KNbO_3 were extracted from the nonempirical calculations and may be obtained equally straightforwardly for other related systems. Experimental estimations of this important property are possible only when based on quite delicate high-pressure measurements.

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