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The influence of magnetic fields on the interphase boundary dynamics of ferroelectric phase transitions

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Abstract. A general description of the thermo-induced dynamics of the interphase boundaries in ferroelectrics is proposed. The influence of applied magnetic fields on the velocity and width of the interphase boundaries is considered.

Dielectric measurements (Wagner and Bäuerle 1981; Lawless *et al* 1982) have shown that there is a considerable effect of the applied magnetic field on the phase transition temperature in ferroelectric perovskites. The cause of this influence is the magnetoelectric effect (Astrov 1960, Folen *et al* 1961, Clin *et al* 1988). This effect is caused microscopically by the influence of the magnetic field on the orbital wave functions determining the polarizability (Wagner and Bäuerle 1981). Since many ferroelectric phase transitions, in particular in perovskites, are first-order ones, it is worthwhile to consider such peculiarities of the first-order phase transitions as growth processes related to the dynamics of the interphase boundaries and the influence of magnetic field on them. The temperature-induced kinetics of the first-order ferroelectric phase transitions has been extensively studied in perovskites both experimentally (Surowiak *et al* 1978a, b, Yufatova *et al* 1980, Dec 1986, 1988, 1989, Dec and Yurkevich 1990) and theoretically (Gordon 1983, 1986, 1987, 1991). Recently the first attempt at studying the magnetic-field-induced kinetics of the ferroelectric phase transitions has been made by Gordon and Wyder (1992). However, the case under consideration is restricted by the overdamped motion of the interphase boundary. In this work we propose a general description of the thermally induced interphase boundary motion and study the influence of the applied magnetic field on the ferroelectric interphase boundaries.

We start from the Ginzburg–Landau functional of the total free energy for uniaxial ferroelectrics

$$F[P(x,t)] = \int \left[D\left(\frac{\partial P}{\partial x}\right)^2 + f(P)\right] \mathrm{d}x \qquad (1)$$

where P is the polarization, $f(P)$ is the free-energy density for a uniform system undergoing a first-order phase transition:

$$f(P) = \tfrac{1}{2}aP^2 - \tfrac{1}{4}bP^4 + \tfrac{1}{6}cP^6 \qquad (2)$$

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where coefficients b and c are positive, D is the positive coefficient of the inhomogeneity term, coefficient a is a temperature-dependent one: $a = a'(T - T_0)$, and T_0 is the stability limit of the paraelectric phase.

Up to date the dynamics of ferroelectric interphase boundaries has been considered with the help of the time-dependent Ginzburg–Landau equation for the evolution of spontaneous polarization (Gordon 1983, 1986). In this case we have the following equation:

$$\partial P/\partial t = -\Gamma\, \delta F/\delta P \tag{3}$$

where Γ is the Landau–Khalatnikov transport coefficient, which sets the time scale of the relaxation process and is assumed to depend non-critically on temperature; the term including the functional derivative $\delta F/\delta P$ is one tending to restore the value of P to its thermal equilibrium value; F is given by (1) and (2). However, this equation gives the overdamped motion of the interphase boundary. To consider a more general case we take into account the kinetic energy density. Then the Euler–Lagrange equation is given as follows:

$$2D\, \partial^2 P/\partial x^2 - \rho\, \partial^2 P/\partial t^2 - aP + bP^3 - cP^5 = 0. \tag{4}$$

The Lagrangian density $L = K - F$, where K is the kinetic energy. We take K as follows:

$$K = \tfrac{1}{2}\rho(\partial P/\partial t)^2. \tag{5}$$

We present the kinetic energy as the energy of oscillations of ions. It is assumed that the polarization in a ferroelectric is due to the displacement of a definite ion (Ginzburg 1960). $P = nez$ and $\rho = m/ne^2$, where z is the displacement of the ion, e is the effective charge, m is the effective mass, and n is the number of ions in unit volume. For the sake of simplicity we neglect the energy of elastic oscillations and elastic energy in (5) (see Gordon 1991).

Taking into account the damping term with $(1/\Gamma)\, \partial P/\partial t$ we obtain the following equation of motion:

$$2D\, \partial^2 P/\partial x^2 - \rho\, \partial^2 P/\partial t^2 - (1/\Gamma)\, \partial P/\partial t - aP + bP^3 - cP^5 = 0. \tag{6}$$

For $\rho = 0$ we have the usual time-dependent Ginzburg–Landau equation describing the overdamped motion of the phase boundary (Gordon 1983). Substituting $s = x - vt$ into (6) we have

$$2\Gamma(D - \rho v^2/2)\, \mathrm{d}^2 P/\mathrm{d}s^2 + v\, \mathrm{d}P/\mathrm{d}s - \Gamma(aP - bP^3 + cP^5) = 0. \tag{7}$$

The partial solution of (7) is known (Gordon 1983). The ferroelectric interphase boundary is given by

$$P = P_0/[1 + \exp(-s/\Delta)]^{1/2} \tag{8}$$

where

$$P_0^2 = (b/2c)[1 + (1 - 4ac/b^2)^{1/2}]. \tag{9}$$

Here we have new expressions for the interphase boundary width Δ and its velocity v:

$$\Delta = \tfrac{3}{4}\left\{D/a'(T_c - T_0)[1 - 3\delta/8 + (1 - 3\delta/4)^{1/2}](1 + \rho q^2/2)\right\}^{1/2} \tag{10}$$

$$v = qD^{1/2}/(1 + \rho q^2/2)^{1/2} \tag{11}$$

where

$$q = 2\Gamma[a'(T_c - T_0)]^{1/2}\{\delta - \tfrac{2}{3}[1 + (1 - 3\delta/4)^{1/2}]\}/[1 - 3\delta/8 + (1 - 3\delta/4)^{1/2}]^{1/2} \tag{12}$$

where

$$\delta = (T - T_0/(T_c - T_0) \tag{13}$$

and T_c is the phase transition temperature.

The dependences of the interphase boundary width Δ and velocity v on the dimensionless temperature δ are shown in figures 1 and 2. These expressions are different from ones obtained for the overdamped case (Gordon 1983), in which for $(\rho q^2/2 \ll 1)$ we obtain

$$\Delta = \tfrac{3}{4}\{D/a'(T_c - T_0)[(1 - 3\delta/8) + (1 - 3\delta/4)^{1/2}]^{1/2}\} \tag{14}$$

and

$$v = qD^{1/2}. \tag{15}$$

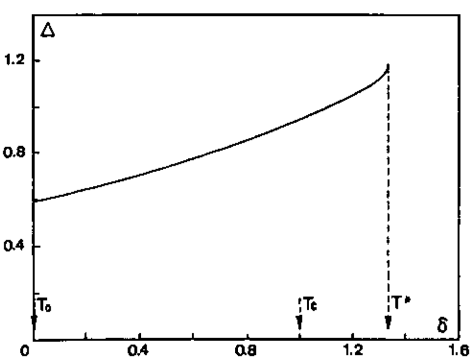

Figure 1. The temperature dependence of the interphase boundary width Δ. The width is given in units of $\frac{3}{4}[D/a'(T_c - T_0)]^{1/2}$ as a function of the dimensionless temperature $\delta = (T - T_0)/(T_c - T_0)$.

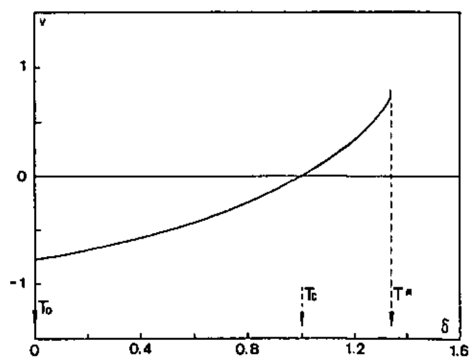

Figure 2. The temperature dependence of the interphase boundary velocity v. The velocity is presented in units of $2\Gamma[Da'(T_c - T_0)]^{1/2}$ as a function of the dimensionless temperature $\delta = (T - T_0)/(T_c - T_0)$.

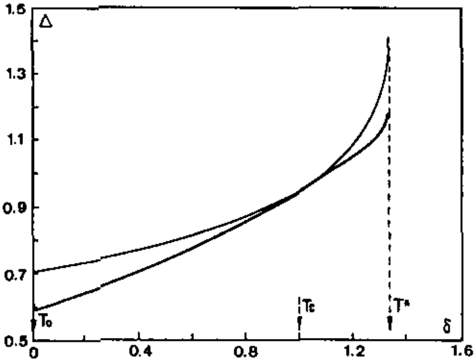

Figure 3. A comparison of the temperature dependences of the interphase width for the overdamped case and the general one (thick curve).

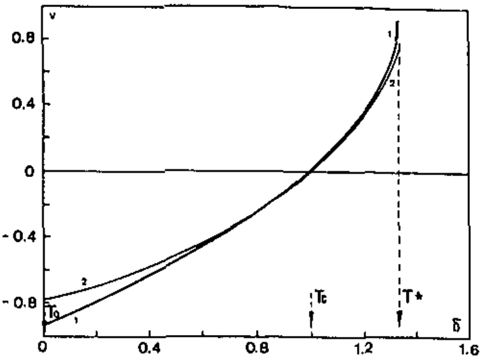

Figure 4. A comparison of the temperature dependences of the interphase velocity for the overdamped (curve 1) and general (curve 2) cases.

For a comparison we plot the temperature dependences of the interphase boundary width and velocity for the overdamped and general cases. In figure 3 it is seen that the width in the general situation (equation (10)) (the thick full curve) is more narrow than for the overdamped case and its temperature increase is less sharp. In figure 4 the strong differences between the two velocities take place near the stability limits of the paraelectric and ferroelectric phases. The temperature growth of the velocity in the general case (equation (11)) (curve 2) is less sharp than for the overdamped situation (curve 1).

Solution (8) was also derived for non-linear lattices with dissipation by Gordon and Genossar (1984) and by Takeno and Kisoda (1988) (stable, self-sustained lattice kinks intrinsic to the dissipated lattice system). Gordon and Genossar (1984) took into account the inertia effects for different types of non-linear lattices. This solution is a kink-type solitary wave which presents the interphase boundary separating paraelectric and ferroelectric phases. It describes the propagation of the interphase boundary leading to the phase transition.

We shall consider the dynamic aspects of the phase transition as a growth in the presence of an applied magnetic field H. To study the magnetic-field-induced dynamics of the interphase boundary we add the terms containing the magnetic field influence to the free-energy density (Wagner and Bäuerle 1981). Then dynamic equations (6) and (7) are given as follows:

$$2D\,\partial^2 P/\partial x^2 - \rho\,\partial^2 P/\partial t^2 - (1/\Gamma)\,\partial P/\partial t - aP + bP^3 - cP^5 - gPH^2 - hPH^4 = 0 \tag{16}$$

and

$$2\Gamma(D - \rho v^2/2)\,\mathrm{d}^2 P/\mathrm{d}s^2 + v\,\mathrm{d}P/\mathrm{d}s - \Gamma(aP - bP^3 + cP^5 + gPH^2 + hPH^4) = 0. \tag{17}$$

In this case (at $T = T_c$, i.e. for $\delta = 1$) the interphase boundary has the width

$$\Delta = y[D/(1 + \rho x^2/2)]^{1/2} \tag{18}$$

where

$$x = [\Gamma b/(6c)^{1/2}][1 + B - (1 - B)^{1/2}]/[(5 - B)/4 + (1 - B)^{1/2}]^{1/2} \quad (19)$$

$$y = [(6c)^{1/2}/b][(5 - B)/4 + (1 - B)^{1/2}]^{-1/2} \quad (20)$$

$$B = (16c/b^2)(gH^2 + hH^4) \quad (21)$$

and moves with the velocity

$$v = x[D/(1 + \rho x^2/2)]^{1/2}. \quad (22)$$

According to Ginzburg (1960), $D \propto d^2$, where d is the lattice parameter. Since the lattice parameter d is not changed under the influence of the applied magnetic field, coefficient D is independent of the magnetic field strength. The transport coefficient Γ does not include the dependence of the phase transition temperature (Landau and Khalatnikov 1954). For this reason we assume that the magnetic field dependence of Γ is negligible.

Figures 5 and 6 show the magnetic field dependences of the width Δ and velocity v for $BaTiO_3$. Here $g = a'\alpha$ and $h = a'\beta$, $a' = 6.7 \times 10^{-5}$ K^{-1} (Grindlay 1970) where $\alpha = 6.27 \times 10^{-4}\, kT^{-2}$ (Wagner and Bäuerle 1981), $\beta = 6.28 \times 10^{-7}\, kT^{-4}$ (Wagner and Bäuerle 1981). We use $b = 9.7 \times 10^8$ MKS (Grindlay 1970) and $c = 3.9 \times 10^{10}$ MKS (Grindlay 1970); the magnetic field strength is given in Tesla (T). For strong damping ($\rho x^2/2 \ll 1$) we have

$$\Delta = yD^{1/2} \quad (23)$$

and

$$v = xD^{1/2}. \quad (24)$$

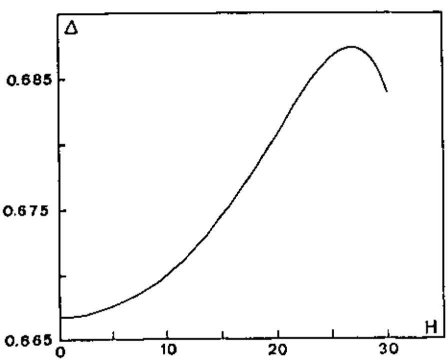

Figure 5. The magnetic field dependence of the interphase boundary Δ for $BaTiO_3$. The width is given in units of $(6Dc)^{1/2}/b$.

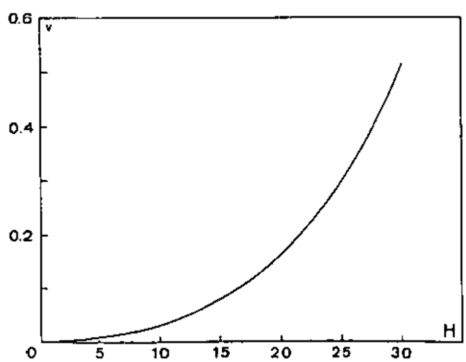

Figure 6. The magnetic field dependence of the interphase boundary velocity v for $BaTiO_3$. The velocity is presented in units of $\Gamma b(D/6c)^{1/2}$.

There is no significant difference between the magnetic field dependence of the interphase boundary velocity for the general and the overdamped cases (equation (24)), while the width of the interphase boundary gives a curve with a maximum (figure 5), when the magnetic field increases. In the overdamped case the width is widened when the applied magnetic field increases (equation (23)). The inertia effect hinders the growth of the interphase width and leads to its decrease.

An analogous consideration of the phase transition kinetics can be carried out for the Kittel model of antiferroelectricity. As was shown by Dec and Yurkevich (1990), the interphase boundary of the Kittel antiferroelectric may also be expressed as a kink solution (8) of the time-dependent Ginzburg–Landau equation. Consequently, the above presented results may be applied to antiferroelectrics.

Since the moving of the interphase boundary is related to the growth of ferroelectric and antiferroelectric crystals, the magnetic field effect can be used to govern the growth processes.

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