Nonuniform polarized states of ferroelectric nanoparticles in a dielectric matrix

V N Nechaev¹, A V Viskovatykh² and A V Shuba¹

¹Military Educational and Scientific Centre of the Air Force N.E. Zhukovsky and Y.A. Gagarin Air Force Academy, Starich Bolshevikov Str, 54a, 394064, Voronezh, Russia
²Russian Scientific Center of Roentgenoradiology (RSCRR), Profsoyuznaya Str., 86, 117997, Moscow, Russia

E-mail: ostrogyvsk@mail.ru

Abstract. In the framework of the phenomenological theory of phase transitions (PT) Landau are showed that in nanoscale ferroelectrics (FE), a phase transition to a non-uniform polar state is possible. As a result of solving the eigenvalue problem for the equilibrium equation of polarization and electrostatic equations, a wave vector is defined, that characterizes a non-uniform phase in a thin ferroelectric film (FEF), temperature ranges of the «domain-like» phase are found, depending on the characteristic size of the FE inclusion and its surface properties. The possibility of controlling the domain structure in ferroelectric particles (FEP) using an external electric field is shown.

1. Introduction

High permittivity and polarization, and ability to control the operating parameters of the material by an external electric field or mechanical stresses, determine the wide use of nanocomposite materials (NCMs) based on FE in various devices and microwave technology, optoelectronics, information storage devices, pyro-receivers, humidity sensors and incite the researches, that needed to create a reliable model for predicting their properties [1–2]. In [3, 4] it was shown, that in dielectric (DE) matrix with FE inclusions, the formation of «domain-like» states in the polar phase is possible. In a thin FEF with a PT to the polar phase, the appearance of a spatially modulated state is also possible [5]. The use of the term «domain-like» state to characterize an inhomogeneous state is due to the fact that, unlike the usual domain structure, in this case there are no distinct boundaries separating the polar regions. Another type of inhomogeneous states was investigated when modeling the properties of relaxors [7].

We emphasize that a nonuniform state in the work means not only a state with a spatial dependence of the order parameter, that takes a place for any limited samples, but a state in which the polarization vector changes direction. The purpose of this work is to determine the temperature ranges of existence of inhomogeneous polarization states in thin FEF and in FE-DE nanocomposites, to study the conditions of their occurrence in a second-order phase transition depending on the size and shape of sample, its surface properties.

The sensitivity of the problem to consideration of electrostatic depolarizing fields makes it important to find the exact solution for polarization. As a rule, various approximations are used in studies of the properties of thin FEFs or NCMs with FE inclusions to consideration of electrostatic depolarizing fields [8–11]. For example, in the works [8–10], the Ritz direct variation method has been used, in
[11] the depolarizing field \( E_d \) is approximated by the formula \( E_d = -(P - P_{mean}) / \varepsilon \), where \( P_{mean} \) is the polarization average over the film thickness, \( \varepsilon \) is the permittivity. Note that a similar problem of magnetic fields consideration exists in the theories of magnetic films and domain structures [12,13].

An alternative to such approaches for NCM may be a numerical method, where the required accuracy can always be achieved by increasing the number of iterations. [3]. In the particular case for thin FEF it is possible, without any assumptions, to find the solution of the problem analytically, up to final formulas, which are analyzed numerically [5].

2. The features of PT in thin FEF
2.1. The system of relations, describing the PT
Consider a thin FEF with thickness \( l \) and perpendicular to the film plane ferroactive axis that is coincides with the 0z axis. The free energy of such a film is written in the form [14]:

\[
F = \int_V \left( -\frac{\alpha}{2} P^2 + \frac{\beta}{4} P^4 + \frac{\kappa}{2} \nabla P \cdot \mathbf{E} \cdot \mathbf{P} \right) dV - \int_{V_{\infty}} \frac{\varepsilon}{8\pi} \mathbf{E}^2 dV + \int_S \frac{\alpha_s}{2} \mathbf{P}^2 dS, \tag{1}
\]

where \( \mathbf{P} = (0, 0, P) \) is the vector of polarization; \( \alpha = \alpha_0 (T_C - T) \) and \( \beta \) are the Landau coefficients in the expansion of free energy [15], \( T_C \) is the Curie temperature of homogeneous infinite crystal; \( \kappa \approx \alpha_0^2 \), \( \kappa \) is the correlation constant, \( \alpha_0 \approx 3 \cdot 10^{-8} \) cm is the lattice parameter; \( \mathbf{E} \) is the electrostatic field strength, induced by a change of film polarization; \( \varepsilon \) is the contribution to the permittivity (mainly electronic), not considering the order parameter influence; \( \alpha_s \) is the coefficient at the lowest degree \( \mathbf{P} \) in the expansion of surface; \( V \) is the film volume; \( V_{\infty} \) is the volume around the film, included \( V \); \( S \) is the film surface.

Passing in the functional (1) to independent functions – polarization \( \mathbf{P}(\mathbf{r}) \) and electric potential \( \varphi(\mathbf{r}) \), considering \( \mathbf{E} = -\nabla \varphi \), we obtain a closed coupled system of equations [5]:

\[
\begin{cases}
-\kappa \Delta P - \alpha P + \beta P^3 = -\partial \varphi_i / \partial z \\
\varepsilon_c \partial \varphi_e = 0
\end{cases}
\]

for internal FEF region, \( \varphi_i \) is the electric potential; \( \partial \varphi_i / \partial z = 0 \) for external FEF region \( \varphi_e \) is the electric potential (2)

and boundary conditions

\[
\begin{align}
\kappa \partial P / \partial z + \alpha_s P \big|_{z=0,l} &= 0, \\
\varphi_i \big|_{z=0,l} &= \varphi_e \big|_{z=0,l} \\
\varepsilon_c \partial \varphi_i / \partial z - 4\pi \mathbf{P} \big|_{z=0,l} &= \varepsilon_e \partial \varphi_e / \partial z \big|_{z=0,l} \\
\varepsilon_e \partial \varphi_e / \partial z \big|_{z=\pm\infty} &= 0,
\end{align}
\]

where \( \varphi_i \), \( \varphi_e \) and \( \varepsilon_c \), \( \varepsilon_e \) are the electric potential and permittivity for internal and external FEF region respectively.

2.2. Solving a boundary value eigenvalue problem
Considering that a second-order PT occurs by the mechanism of stability loss of the paraelectric phase, to determine PT temperature, it suffices to find the appearance point of a nonzero solution of the boundary value problem (2) – (7) in the linearized view – without \( \beta P^3 \) term in (2). The symmetry of the problem makes it possible to use the Fourier transform of \( x \), \( y \) variables to find unknown functions \( P(x, y, z) \) and \( \varphi(x, y, z) \).

Equations for the Fourier transforms \( \tilde{P}(k_x, k_y, z) \) and \( \tilde{\varphi}(k_x, k_y, z) \) arising from equations (2), (3) and have the form
\[ \left\{ \begin{array}{ll}
\kappa d^2 \ddot{P} / dz^2 + (\alpha - k_{\perp} \kappa) \ddot{P} = d \ddot{\phi}_l / dz \\
\ddot{\phi}_l / dz^2 = k_{\perp}^2 \ddot{\phi}_l + 4 \pi / \varepsilon \cdot d \ddot{P} / dz \\
d^2 \ddot{\phi}_e / dz^2 = k_{\perp}^2 \ddot{\phi}_e
\end{array} \right. \]  
(8)

where \( k_{\perp}^2 = k_{\parallel}^2 + k_{\perp}^2 \). The solution of equations (8), (9) must satisfy additional conditions arising from the boundary conditions (4) – (7) of the original problem.

Solving the system of equations (8), we obtain the equation

\[ \kappa d^4 \dddot{P} / dz^4 + (\alpha - 2k_{\perp}^2 \kappa - 4 \pi / \varepsilon) \cdot d^2 \dddot{P} / dz^2 - k_{\perp}^2 (\alpha - k_{\perp} \kappa) \dddot{P} = 0, \]  
(10)

which solution will be found in the form

\[ \dddot{P}(k_{\perp} \cdot z) = C_1 e^{\lambda_1 z} + C_2 e^{\lambda_2 z} + C_3 e^{-\lambda_1 z} + C_4 e^{-\lambda_2 z}, \]  
(11)

where \( C_1, \ C_2, \ C_3, \ C_4 \) are the arbitrary constants, which can be found from the boundary conditions, \( \pm \lambda_1, \pm \lambda_2 \) are the roots of characteristic equation:

\[ \kappa \lambda^4 + (\alpha - 2k_{\perp}^2 \kappa - 4 \pi / \varepsilon) \lambda^2 - k_{\perp}^2 (\alpha - k_{\perp} \kappa) = 0. \]  
(12)

Then, we find the Fourier transform \( \dddot{\phi}_l \):

\[ \dddot{\phi}_l(k_{\perp} \cdot z) = C_1 (\lambda_1^2 + b) e^{\lambda_1 z} + C_2 (\lambda_2^2 + b) e^{\lambda_2 z} - C_3 (\lambda_1^2 - b) e^{-\lambda_1 z} - C_4 (\lambda_2^2 + b) e^{-\lambda_2 z}, \]  
(13)

where \( a = \kappa / k_{\perp}^2, \ b = (\alpha - 4 \pi / \varepsilon) / k_{\perp}^2 - \kappa. \)

Equation (9) to determine \( \dddot{\phi}_e \) is solved independently of the other system equations. For the region \( z \leq 0 \) we get

\[ \dddot{\phi}_e(k_{\perp} \cdot z) = C_5 e^{\lambda_{\perp} z}. \]  
(14)

Using boundary conditions for \( \dddot{P}, \dddot{\phi}_l, \) and \( \dddot{\phi}_e \), we obtain a system of five homogeneous algebraic equations to determine \( C_1, \ C_2, \ C_3, \ C_4, \ C_5 \) [5], which has nonzero solutions only if its determinant

\[ \Delta = \frac{\alpha \lambda + \kappa \lambda \text{th}(\lambda_1 l/2)}{\alpha \lambda + \kappa \lambda \text{th}(\lambda_2 l/2)} - \frac{\lambda_1 (\lambda_1^2 + b)(\lambda_1 + k_{\perp} \text{th}(\lambda_1 l/2) e_e / e)}{\lambda_2 (\lambda_2^2 + b)(\lambda_2 + k_{\perp} \text{th}(\lambda_2 l/2) e_e / e) - 4 \pi / \varepsilon} \]  
(15)

is equal zero. The equation \( \Delta(T, k_{\perp} l, e, e_e, \alpha \lambda) = 0 \) is implicit dependence of the PT temperature \( T_f \) on the FEF parameters \( l, \ e, \ e_e, \ \alpha \lambda \) and on wave vector \( k_{\perp} \), characterizing inhomogeneous polarized state, to study which is really only numerically. The dependence of PT temperature \( T_f \) on wave vector \( k_{\perp} \), determining the spatial modulation of the polar phase for different film thicknesses, is shown on Fig. 1. For draw graphics, the parameters of a triglycine sulfate (TGS) crystal were used: \( T_C = 322 K, \) \( \alpha_0 = 3.92 \cdot 10^{-3} \text{ K}^{-1}, \ \beta = 8 \cdot 10^{-10} \text{ unitsESU} [16]. \)

2.3. Results analysis

It should be at once noted that the behavior of all film characteristics will be qualitatively different for different signs \( \alpha_{\lambda} \) (figure 1). This difference is described in detail in [17, 18] for the simplest situation when there is need not to consider electric or magnetic fields: if \( \alpha_{\lambda} > 0 \) the temperature \( T_f \) decreases, polarization profile as a function of coordinate is a convex up function; if \( \alpha_{\lambda} < 0 \) – convex down situation. In both cases \( T_f \rightarrow T_c \) at \( l \rightarrow \infty \). When consider the depolarizing field in the FE phase, the PT can occur in a uniform (if the film parameters allow) or nonuniform state.

Figure 1 shows that in sufficiently thin films \( (l < 30 \cdot 10^{-8} \text{ cm}) \) the PT takes place according to the «classical type»: the functions \( T = T_f(k_{\perp}) \) steadily decrease with increasing \( k_{\perp} \) from \( k_{\perp} = 0 \). If
$l \geq 30 \cdot 10^{-8}$ cm the PT occurs in spatially modulated nonuniform state with nonzero wave vector $k_\perp$, depending on parameters $l$, $\varepsilon$, $\varepsilon_e$, $\alpha_s$. The PT to the nonuniform state takes place regardless of the sign parameter $\alpha_s$.

The real phase transition temperature $T_{\beta}$ and the wave vector of the static polarization $k_\perp$ coincide with the point of maximum $T_{\beta} = T_f^{\text{max}}$ on the dependences $T = T_f(k_\perp)$ (figure 1). This temperature as a function of $l$ at various parameters $\alpha_s$ on the FEF surface is shown in figure 2.

![Figure 1](image1.jpg)

**Figure 1.** The dependences $T_f$ on $k_\perp$ at different $l$ : $a - \alpha_s = 0.75 \cdot 10^{-8}$ cm, $b - \alpha_s = -0.75 \cdot 10^{-8}$ cm.

![Figure 2](image2.jpg)

**Figure 2.** The dependences $T_{\beta}$ on $l$ at different $\alpha_s$ : $a - \alpha_s > 0$, $b - \alpha_s < 0$.

It is shown, if $\alpha_s > 0$, then with increasing film thickness $l$ the temperature $T_{\beta}(l)$ increases and tends to $T_c$ (figure 2a). The curve $T = T_{\beta}(l)$ is clamped between the lines $T = T_f(l)$ and $T = T_c$, which are its asymptotes. The increase of $T_{\beta}(l)$ with an enlarge $l$ is explained by a decrease of the relative contributions of the correlation's and surface energies compared with other contributions to the free energy (1). The decrease of $T_{\beta}(\alpha_s)$ with an enlarge $\alpha_s$ ($\alpha_s > 0$), naturally due to an increase in positive surface energy. Note that the dependence $T = T_{\beta}(l)$ qualitatively coincides with the dependence of the PT temperature in a uniform state on the film thickness [18]. The dependence $T = T_{\beta}(\alpha_s)$ be also traced in figure 2a: with increase of parameter $\alpha_s$ the PT temperature to nonuniform state decreases, that is naturally, since in this case the surface works as a factor preventing the PT.
In the case the surface stimulates the transition to the FE phase, the parameter $\alpha_s < 0$ (figure 2b) and for small values of the parameter $|\alpha_s| < 1.2 \times 10^{-8}$ cm there is also a non-linear behavior of the function $T = T_\alpha(l)$, but its growth with increasing film thickness is weaker than with $\alpha_s > 0$, due to the negative contribution of the surface to the free energy (1). With decreasing parameter $\alpha_s < 0$ the influence of surface energy grows and already at $|\alpha_s| \geq 1.2 \times 10^{-8}$ cm the temperature $T_\alpha$ practically does not depend on the film thickness (for the thicknesses used in the numerical calculations) – the surface tightens the PT into the up temperature region and fully controls the existence of the polar phase. The fundamental difference of behavior $T_\alpha(l)$ in this case is that $T_\alpha > T_i > T_c$ and deviation $T_\alpha$ from the temperatures $T_i$, $T_c$ increases with increasing parameter $|\alpha_s|$.

The width $\Delta T = T_\alpha - T_i(0)$ of the temperature existence of the nonuniform phase depends on $l$ (figure 3). When $\alpha_s < 0$ (figure 3b) $\Delta T$ significantly lower than similar values for $\alpha_s > 0$ (figure 3a), what, apparently, to be related to the above features of the PT for this situation [19].

2.4. Effect of shielding the surface charges

In a real situation, the environment of the film has a non-zero conductivity, and the larger it is, the stronger the surface charges are shielded. If we consider the characteristic shielding length $L$, then (14) and (15) will take the form

$$\tilde{\alpha}_s(k_{\perp}, z) = C_s e^{\kappa_{\perp} z} \left(1 - e^{-2k_{\perp}(L+z)}\right).$$

$$\frac{\alpha_s + \kappa_1 \text{th}(\lambda_1 l/2)}{\alpha_s + \kappa_2 \text{th}(\lambda_2 l/2)} - \frac{\lambda_1 (\alpha_1^2 + b \lambda_1 \text{th}(\lambda_1 l/2) \left(1 + e^{-2k_{\perp} L} \right) e_{\perp}/e)}{\lambda_2 (\alpha_2^2 + b \lambda_2 \text{th}(\lambda_2 l/2) \left(1 + e^{-2k_{\perp} L} \right) e_{\perp}/e)} - 4\pi/e = 0. \tag{17}$$

The numerical solution of equation (17) is presented in figure 4. It shows that with increasing shielding (decreasing characteristic length $L$) the effect of the depolarizing field decreases and the PT temperature increases. Width $\Delta T$ in case $\alpha_s > 0$ about twice more (figure 4a), then in case $\alpha_s < 0$ (figure 4b). The shift of the temperature $T_\alpha$ caused by electric fields in the second case is larger (2.6 K) than in the first one (2.3 K).
3. Nonuniform polar states in FE nanoparticles

3.1. The system of relations, describing the PT

Consider the problem of the PT in the FE inclusion surrounded by a DE matrix. Let the FE P has the shape of a rotation ellipsoid with an elongation coefficient $a/b$ (a and b are major and minor semi-axes). DE matrix has the shape of a cube with c edge. The FE is uniaxial with the polar axis, parallel to the coordinate axis $Oz$ and b. This problem can be solved numerically only. The system of equations for the FE-DE composite in an external electric field of a strength $dE$ similar to (2) – (3), except for the appearance $dE$ in the right-hand side of the first equation (2). The boundary conditions on the $\gamma$ surface of the FEP will take the form

$$\kappa \frac{\partial P}{\partial n} - \alpha_s P|_\Gamma = 0, \quad \phi_e|_\Gamma = \phi_e^0, \quad \nu \frac{\partial \phi_i}{\partial n} - 4\pi P \cdot n|_\Gamma = \nu_e \frac{\partial \phi_e}{\partial n}|_\Gamma.$$  \hspace{1cm} (18)

The boundary conditions, respectively, on the lower, upper, and lateral faces of the composite are

$$\phi_e|_{D_1} = 0, D_1 : \{ |x|, |y| \leq c/2, z = -c/2 \} ; \quad \phi_e|_{D_2} = -E_d \cdot c, D_2 : \{ |x|, |y| \leq c/2, z = c/2 \} ;$$

$$\frac{\partial \phi_e}{\partial n}|_{D_3} = 0, D_3 : \{ x, y \leq c/2, |z| = -c/2 \},$$  \hspace{1cm} (19)

where $n$ is the unit vector of the outer normal to the surface. The nonlinear boundary value problem (2), (3), (18), (19) has solved numerically by the finite element method in the software package Comsol Multiphysics.

3.2. Results analysis of the of numerical calculations

In figure 5 the polarization profiles in the FEP ($\tau = 5$) are shown. As in the case of the FEF (figure 1), for the FEP of size $a \leq 30 \cdot 10^{-8}$ cm the PT occurs to polar phase in accordance with classical notions: at the definite temperature, that is different from $T_c$ and depends on the FEP size, the polarization appears, which monotonously increases with distance from the PT point (figure 5a). For the FEP of size $a > 30 \cdot 10^{-8}$ cm the PT takes place to the polar nonuniform «domain-like» state, characterized by the regions with contrary polarization vector directions (figure 5b). Splitting into domains occurs in a direction perpendicular to the polar axis. In the direction of the polar axis, no splitting into domains is observed due to the increase in electrostatic energy. There is a central region (domain) with the maximum polarization at the center of the FEP decreasing in absolute value to the domain periphery. The dependence of the polarization on the coordinates, along with the behavior in external electric field, is one of the main differences between such regions and real domains. The next domain covers the central domain, and so on. The conditional boundaries of domains in the FEP are represented by concentric circles at the section by a plane perpendicular to the ferroactive axis. In each next region (domain) after the central one, the maximum polarization in absolute value is less, than that in the previous one.
Figure 5. Distribution profiles $P$ along $a$ in the FEP with $\tau = 5$ at different temperatures:

$$a - a = 3\text{nm}, \alpha_s^{-1} = 0; b - a = 9\text{nm}, \alpha_s^{-1} = 0.$$  

As mentioned above, the cause of the PT to nonuniform state is the same as the reason for splitting the infinite FE into domains: the tendency of the system to reduce a free energy by reducing the electrostatic energy of the depolarizing field. Firstly, this fact is proved by the strong dependence of the PT behavior on the size and shape of the FEP (figures 5a, b) [3]. Secondly, the direct proof of the role of the depolarizing field is the study of structural PT in which these is no the long-range electrostatic fields in the dielectric phase [20].

With an increase in the size of the FEP, the analysis of the temperature evolution of «domain-like» states becomes more complicated, the number of domains increases. Table 1 shows the temperature intervals for the existence of various polar states, which successively replace each other and for which different number of domains is characteristic.

Table 1. Temperature ranges of domains in the FE nanoparticle (K).

| $a$ (nm) | $\tau$ | $\alpha_s$ (nm) | $T_f$ (K) | Number of domains in FE particle |
|----------|--------|-----------------|-----------|---------------------------------|
|          |        |                 |           | 1     | 2     | 4     | 3     | 2     |
| 3        | 5      | $\infty$       | 251       | 0-251 |       |       |       |       |
| 6        | 5      | $\infty$       | 288       | 0-196 | 197-288 |       |       |       |
| 6        | 3      | $\infty$       | 273       | 0-120 | 120-273 |       |       |       |
| 9        | 5      | $\infty$       | 300       | 0-197 | 198-242 | 243-251 | 252-287 | 288-300 |
| 9        | 5      | 0.6             | 304       | 0-224 | 225-271 | 272-274 | 275-290 | 291-304 |

Figure 6 shows the polarization profiles for different $\alpha_s$. In the general case, with decreasing $|\alpha_s|$, the PT of the FE-DE system to the «monodomain» structure occurs through the several nonuniform states with different number of domains. For large absolute values of negative values $\alpha_s$ ($|\alpha_s| \geq 6\text{nm}$ for $a = 9\text{nm}, T = 256\text{K}$ and $|\alpha_s| \geq 1.5\text{nm}$ for $a = 9\text{nm}, T = 290\text{K}$) there is a deviation from the rule «from a large number of domains to a «monodomain» state with decreasing parameter $|\alpha_s|$» (table 2).

Table 2. Influence of the parameter $|\alpha_s|$ on the domain structure (nm).

| $a$ (nm) | $\tau$ | $T_f$ (K) | Number of domains in FE particle |
|----------|--------|-----------|---------------------------------|
|          |        |           | 1     | 2     | 4     | 3     | 2     |
| 6        | 5      | 240       | $\leq 0.75$ |       |       |       | 0.75-3 |
| 9        | 5      | 256       | $\leq 0.3$  | 0.33-1.5 | 3-3.75 | $\geq 6$ |
| 9        | 5      | 290       | $\leq 0.25$ | 0.25-0.43 | 0.5-1.0 | 1.5-30 |
Note, when $|\alpha_s|$ decreases, the «multidomain» states, which the system undergoes by cooling from the dielectric phase, are repeated (figures 6a, b). For $a = 9\text{nm}$, $\tau = 5$ at $T = 290\text{K}$ failed to observe the polar state with four domains. It is possible due to the small interval of values $|\alpha_s|$.

The features of the polarization distribution, naturally, should influence the temperature dependences of the physical properties of researched materials. We shall discuss some possibilities of experimental observation of the manifestation of the nonuniform «domain-like» structure. At first, the new nonuniform state of the system should be reflected in its behavior in external electric field. The typical behavior of the temperature dependence of the dielectric permittivity for such systems is a sharp maximum at the PT temperature and its value strongly depends on the external field $E_d$, significantly decreasing with its growth. In the case of the PT in uniform state, the behavior of the dielectric permittivity differs radically (figure 7). In the temperature region of the nonuniform phase, there are several maxima, apparently related to the restructuring of the quasi-domain structure in a strong external field, and significant dielectric permittivity values between them, which is also associated with the presence of a nonuniform structure.

**Figure 6.** Distribution profiles $P$ along $a$ in the FEP ($\tau = 5$) for a different $|\alpha_s|$: $a - \alpha = 6\text{nm}$, $T = 240\text{K}$; $b - a = 9\text{nm}$, $T = 256\text{K}$.

**Figure 7.** Temperature dependence of dielectric permittivity of the FEP ($a = 9\text{nm}$, $\tau = 5$, $\alpha_s^{-1} = 0$) for different $E_d$.

**Figure 8.** Distribution profiles $P$ along $a$ in the FEP ($a = 6\text{nm}$, $\tau = 5$, $\alpha_s^{-1} = 0$) for different $E_d$. 


It is shown that the domain-like structure is strongly dependent on temperature and parameter $\alpha_s$, but it is technically difficult to use these parameters for structure control. It is more convenient to control of the «nanodomain» structure with external electric field applied along the polar axis of the FEP (figure 8). With an increase in $E_z$, the region of the existence of the two-domain structure decreases, the transition to the single-domain state occurs at a higher temperature and a smaller absolute value of the polarization at the FEP center. In addition, at a direct transition from a two-domain structure to a single-domain structure, the width of the central domain in the presence of an electric field is larger, than that in the absence of a field.

3.3. Effect of screening of depolarizing field on the PT in the nanocomposite

The bound electric charges on the surface of the FEP are shielded to some extent. This effect can be consideration by imposing a boundary condition on the surface of the FEP with help a dielectric layer of thickness $h$. The thickness $h$ of this layer plays the role of the shielding length, similar $L$ in the FEF.

Figure 9 shows the dependences of the polarization distribution in the FEP for different temperatures, $h$ and boundary conditions. At $h < 3\text{nm}$ and $\alpha_s^{-1} = 0$, which corresponds to the Dirichlet boundary condition for $P$ at the FEP surface, the PT takes place in the single-domain state at $T = 306 \text{ K}$ in according to the «classical type»; then with the temperature decreases the average polarization increases.

At $h \geq 3\text{nm}$ and $\alpha_s^{-1} = 0$ the PT takes place to the nonuniform state, the temperature range $\Delta T$ of which expands with increasing $h$: $\Delta T = 304 - 302\text{K} = 2\text{K}$ at $h = 3\text{nm}$ (figure 9a) and $\Delta T = 302 - 292\text{K} = 10\text{K}$ at $h = 5\text{nm}$ (figure 9b). At $\alpha_s = -0.6\text{nm}$ and $h = 5\text{nm}$ (figure 9c), the PT also takes place to the FE phase on the «classical type».

![Figure 9](image_url)

**Figure 9.** Distribution profiles $P$ along $a$ in the FEP ($a = 9\text{nm}, \tau = 5$) for various temperatures:

- $a - a_s^{-1} = 0$, $h = 3\text{nm}$;
- $b - a_s^{-1} = 0$, $h = 5\text{nm}$;
- $c - a_s = -0.6\text{nm}$, $h = 5\text{nm}$.

The shielding of surface charges at the FE-DE interface leads to an increase in Curie temperature in the NCMs. Another mechanism of increasing the Curie temperature in the NCM due to the existence of an additional layer between the FE and the DE is considered in [21].

4. Conclusion

The temperature evolution of polar states can be investigated only in case of nonlinear approximation, which was done in this work with apply of numerical methods for an elliptical FE particle. Analysis of the results allows us to identify some general features typical of the PT in FEPs:

1. The presence of the following stages of the polarization profile evolution with distance from the PT point (if the particle parameter and the DE matrix parameters allow it):

   a) the PT to the nonuniform state and the subsequent increase of polarization vector in domains with its contrary direction (it's possible fast restructuring of domains, changing its number with a changing of temperature).
b) growing of the central domain to the formation of a uniform single-domain state;

в) increase in the average polarization in the single-domain region with decreasing temperature.

2. Nonmonotonic oscillating behavior of the average polarization of unit volume as a function of temperature.

3. The existence of a certain temperature range for a nonuniform state near the PT point, the width of which depends on the shape and size of the FEPs, a concentration of the FEPs and their relative position [22], the parameters of the boundary between the FE and DE.

4. The conditions for the occurrence of a nonuniform state substantially depend on the existence in the material of free charge carriers that shield the electric field, arising at the PT.

The detected features of the PT will manifest themselves experimentally, for example, in the temperature anomalies of the heat capacity, the dielectric permittivity and the kinetic coefficients. In the case of massive samples, this effect will also appear as nonuniform states near the surface.

Note that the formation of the domain structure of the FE phase of the NCM, in addition to those considered in this article, should certainly be influenced by the following parameters. This is the volume concentration of the FE phase and its distribution in the NCM. In this case, it is necessary to consider the mutual influence of FEP on the formation of domains, taking into account changes of the depolarizing field. [22]. The preparation technology, the existence and concentration of defects, the cooling rate of FE material can also make a significant contribution to the formation of a «domain-like» structure. All this complicates the analysis of such states and is the subject of future research.

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