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PHENOMENOLOGICAL APPROACH TO THE DESCRIPTION OF PHASE TRANSITIONS IN SOLIDS

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Abstract. A general model approach to the problem of describing the competition and coexistence of different phases of a condensed state is considered on the basis of Landau's theory of second-order phase transitions. We show that the multicomponent order parameter leads to a more complex pattern of phase transitions and the appearance of regions in the phase diagram in which different spatially ordered states can compete or coexist. The solution of the necessary equations of the Ginzburg-Landau theory was carried out by the variational method. The model considered in this paper is applicable to the analysis of phase transitions in solids with different electrical properties (transitions to the superconducting state, metal-dielectric and metal-semiconductor transformations) and magnetic states (paramagnet-ferromagnet, paramagnet-antiferromagnet). The proposed approach makes it possible to numerically simulate the free energy of a solid near the phase transition points. The necessary conditions and limits of applicability of the analyzed computational model are indicated.

Keywords: second-order phase transition, order parameter, phenomenological approach, competition and coexistence of phases

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ФЕНОМЕНОЛОГИЧЕСКИЙ ПОДХОД К ОПИСАНИЮ ФАЗОВЫХ ПЕРЕХОДОВ В ТВЕРДЫХ ТЕЛАХ

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Аннотация. В работе рассмотрен общий модельный подход к проблеме описания конкуренции и сосуществования различных фаз конденсированного состояния на основе теории фазовых переходов второго рода Ландау. Показано, что многокомпонентный параметр порядка приводит к более сложной (по сравнению с однокомпонентным) картине фазовых переходов и возникновению областей на фазовой диаграмме, в которых различные пространственно-упорядоченные состояния могут конкурировать или сосуществовать. Рассмотренная модель применима для анализа фазовых переходов в твердых телах с различными электрическими свойствами и магнитными состояниями. Предлагаемый подход позволяет численно моделировать свободную энергию твердого тела вблизи точек фазового перехода. Указаны необходимые условия и границы применимости анализируемой расчетной модели.

Ключевые слова: фазовый переход второго рода, параметр порядка, феноменологический подход, конкуренция и сосуществование фаз

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Introduction

Modern condensed matter theory [1, 2] often considers separate or simultaneous coexistence of different states (or phases) [3, 4]. Individual phase transitions in solids associated with dramatic transformations in their electrical and magnetic properties are not explained within the framework of existing models of first and second-order phase transitions. Detailed consideration of this problem at the microscopic level requires rather complex computational schemes [5, 6], since there are no universal methods for solving and analyzing the resulting nonlinear equations. The experimental approach to the problem deals with quantities only indirectly related to a specific microscopic mechanism and macroscopic quantities characterizing the behavior [7, 8]. For this reason, the phenomenological approach developed by Ginzburg and Landau has proved extremely fruitful; it is based on Landau's general thermodynamic theory of second-order phase transitions [9] and is universal for metals, semiconductors and dielectrics.

This paper reports on a phenomenological approach to describing second-order phase transitions with coexistence and competition of various ordered states.

We constructed a technique for calculating the free energy near the phase transition points applying the variational method to the Ginzburg–Landau equation. Computer simulation of thermodynamic parameters was performed and the results obtained were compared with experimental data.

Statement of the physico-mathematical problem

Let us consider the fundamentals of the Landau theory on second-order phase transitions, which is based on expansion of free energy in powers of the order parameter near the phase transition point, where the order parameter is small. The applicability of the theory is limited by the proximity to the critical temperature of the phase transition: $T_C - T \ll T_C$.

According to the theory of second-order phase transitions, the expansion of free energy density in powers of the order parameter Ψ can be written in the following form [9, 10]:

$$F_1 = F_0 + \alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4, \tag{1}$$

where F_1, F_0 are the free energies of the body at low temperatures in the absence of an external magnetic field and in the normal state at $T > T_C$, respectively; α, β are some phenomenological expansion coefficients characterizing the material.

These phenomenological parameters are expressed in terms of observed macroscopic quantities.

Let us define such a value of the order parameter at which the free energy reaches a minimum:

$$\frac{dF_{s0}}{d|\Psi|^2} = 0 \Rightarrow |\Psi_0|^2 = -\frac{\alpha}{\beta}.$$

Because the order parameter must vanish at $T = T_C$, it is different from zero and at $T < T_C$, then the coefficient $\alpha = 0$ at $T = T_C$ and $\alpha < 0$ at $T < T_C$. In the first order with respect to $(T_C - T)$, we can write $\alpha = \tilde{\alpha}(T - T_C)$, where $\tilde{\alpha}$ does not depend on proximity to T_C. The coefficient β can be assumed to be positive and independent of temperature [11]. This will lead to a minimum of the functional at $T < T_C$ and a non-zero order parameter Ψ. On the other hand, at $T > T_C$, the minimum is reached at a zero value of the order parameter, which corresponds to the normal state of the sample.

The expansion of the Gibbs free energy in powers of Ψ should be considered in the general case of an inhomogeneous body in an external magnetic field [11]:

$$G_{sH} = G_n + \int\left[\alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{1}{4m}\left|-i\hbar\nabla\Psi - \frac{2e}{c}\mathbf{A}\Psi\right|^2 + \frac{(\mathrm{rot}\,\mathbf{A})^2}{8\pi} - \frac{\mathrm{rot}\,\mathbf{A}\cdot\mathbf{H}}{4\pi}\right]dV,$$

where m is the free electron mass; $\mathbf{H}$ is the strength of the external magnetic field; the penultimate term determines the magnetic energy density (here rot$\mathbf{A}(\mathbf{r})$ gives the magnetic field strength at a given point of the body); the term with a gradient term represents the kinetic energy density of electrons; integration is carried out over the entire volume.

Let us find such equations with respect to $\Psi(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ that would give the minimum value of free energy. To do this, it is necessary to solve variational problems:

$$\delta_{\Psi^*}G_{sH} = 0,\ \delta_{\Psi}G_{sH} = 0,\ \delta_{\mathbf{A}}G_{sH} = 0.$$

The first of these variations leads to the well-known first-order Ginzburg-Landau equation from superconductivity theory and the corresponding boundary condition [10]:

$$\begin{gathered}\alpha\Psi + \beta|\Psi|^2\Psi + \frac{1}{4m}\left(-i\hbar\nabla - \frac{2e}{c}\mathbf{A}\right)^2\Psi = 0,\\ \left(i\hbar\nabla + \frac{2e}{c}\mathbf{A}\Psi\right)\mathbf{n} = 0.\end{gathered} \tag{2}$$

where $\mathbf{n}$ is the unit vector of the normal to the surface of the superconductor.

The variation with respect to Ψ leads to a complex conjugate equation. Let us obtain an equation with respect to the vector potential **A**; for this purpose, it is necessary to solve the last of the given variational problems:

$$\mathbf{j}_s = -\frac{i\hbar e}{2m}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) - \frac{2e^2}{mc}\mathbf{A}\left|\Psi\right|^2, \tag{3}$$

what is the second equation of the Ginzburg–Landau theory [10].

Main computational results

The calculations presented in the previous paragraph satisfactorily describe the transition between the two phases. If more phases compete or coexist, the structure of functional (1), which is the basis of the phenomenological description, should differ from the one considered earlier. The form of the order parameter itself should also be different.

Notably, the structure of the order parameter can be obtained from the microscopic theory of the phenomenon, as it was done for the Ginzburg–Landau functional in the meanfield formulation introduced by Bardeen, Cooper and Schrieffer for an attractive pairing interaction (which corresponds to a one-component complex order parameter) [12].

In general, the order parameter can be given as

$$\Psi(\mathbf{R},\mathbf{k}) = \sum_s \Psi_s(\mathbf{R})\varphi_s(\mathbf{R},\mathbf{k}),$$

where $\Psi_s(\mathbf{R})$ are the expansion coefficients of the order parameter with respect to the complete orthonormal system of functions $\varphi_s(\mathbf{R},\mathbf{k})$ obtained from the microscopic description of the body state.

The dependence of the expansion coefficients on the radius vector **R** allows to describe the inhomogeneities in the structure of the material.

Let the state of a solid be described by a two-component order parameter, as obtained, for example, in [13]. The expansion of the free energy density in powers of the order parameter in this case is represented as $f = f_0 + f_g + f_m$ [14], where

$$f_0 = \sum_{s'} A_{ss'}\Psi_s^*\Psi_{s'} + \frac{1}{2}\sum_{s't'} B_{ss'tt'}\Psi_s^*\Psi_{s'}^*\Psi_t\Psi_{t'}$$

is an expansion of free energy density in the second and fourth power of the order parameter.

Here, the matrices $A_{ss'}$ and $B_{ss'tt'}$ are either determined from the microscopic description, or expressed in terms of quantities observed macroscopically. The elements of the matrix $A_{ss'}$, as in the case of the functional (1), should depend on the temperature of the sample, thus determining the temperature at which an ordered state is established. The gradient contribution follows the expression

$$f_g = \frac{\hbar^2}{4m}\sum_{ss'}\left[\hat{D}\Psi_s\right]^+ M_{ss'}\left[\hat{D}\Psi_{s'}\right],$$

where the elements of the matrix $M_{ss'}$ are also determined by microscopic theory or expressed based on macroscopic observables; the operator $\hat{D} = -i\nabla - \frac{2e}{\hbar c}\mathbf{A}$.

This contribution takes into account not only the external magnetic field, but also the internal one. Finally, the energy density of the magnetic field is expressed as

$$f_m = \frac{z_0}{8\pi}(\mathrm{rot}\,\mathbf{A})^2.$$

Producing a variation of the functional, we obtain a system of two equations (for the case of a two-component order parameter) of the form

$$\sum_{s'} A_{s'} \Psi_{s'} + \sum_{s't'} B_{s't'} \Psi_{s'}^* \Psi_t \Psi_{t'} + \sum_{s'} M_{s'} \left(-i\nabla - \frac{2e}{\hbar c} \mathbf{A} \right)^2 \Psi_{s'} = 0$$

and boundary conditions

$$\sum_{s'} M_{ss'} \left(i\nabla + \frac{2e}{\hbar c} \mathbf{A} \right)^2 \Psi_{s'} \mathbf{n} = 0.$$

The resulting system of equations can lead to several nontrivial solutions, which may differ, for example, by the relative phase of the components of the order parameter. These minima are completely determined by the relationship between the elements of the matrices $A_{ss'}$, $B_{ss'tt'}$ and $M_{ss'}$, as described, for example, in [14, 15].

On the other hand, the appearance of an ordered state can be described by the standard expansion of free energy in even powers of a given order parameter:

$$f = a_1 \psi^2 + \frac{1}{2} b_1 \psi^4.$$

Another ordered state can be described similarly:

$$f = a_2 \alpha^2 + \frac{1}{2} b_2 \alpha^4.$$

Here, the coefficients a_i determine the transition temperature from the ground state to the ordered one, similar to the coefficient α in expansion (1). The competition of two ordered states produces a non-zero value of the gradient contribution, which leads to the appearance of an additional term $b_{12} \boldsymbol{\psi}^2 \boldsymbol{\alpha}^2$.

Thus, the functional describing the coexistence and competition of two ordered states can be written as

$$f = a_1 \psi^2 + a_2 \alpha^2 + \frac{1}{2} b_1 \psi^4 + \frac{1}{2} b_2 \alpha^4 + b_{12} \psi^2 \alpha^2. \quad (4)$$

The coefficients a_1 and a_2 can be written as follows [11]:

$$a_1 = -a' \tau', \; a_2 = -a'' \tau'', \; \tau' = \frac{T_1 - T}{T_1}, \; \tau'' = \frac{T_2 - T}{T_2}.$$

where T_1, T_2 are the temperatures of transitions to the corresponding ordered states, below which the order parameters $\boldsymbol{\psi}$ and $\boldsymbol{\alpha}$ may be different from zero.

The above expansion makes sense only in the vicinity of a small region of the phase diagram, where the lines of curves T_1 and T_2 either intersect or pass close to each other.

In the more general case of a multicomponent order parameter, we can adopt formulas similar to (3), setting the forms for various types of ordered states and their coexistence and competition [16–20].

The model considered above is applicable exclusively for micro- and macrobodies, since it does not take into account the contribution of surface tension, which is significant for nanoparticles [21, 22]. The size and shape of the surface make a fairly large contribution to the total energy in nanomaterials [23, 24] and considerably affect the thermodynamic parameters of phase transitions [23, 25, 26]. As found in [27–29], the contribution of surface energy for homogeneous solid particles can be neglected at sizes greater than 200 nm in each of the spatial directions, since the contribution of the surface to the total energy of the system in this case does not exceed 2%.

Analysis of the model and computational results

Let us consider what a functional with a two-component order parameter similar to Eq. (3) can lead to. For this purpose, we examine whether it has any minima and monitor the variation in the topology of free energy isolines. Fig. 1 shows the free energy isolines (3) $f(\psi,\alpha) = const$.

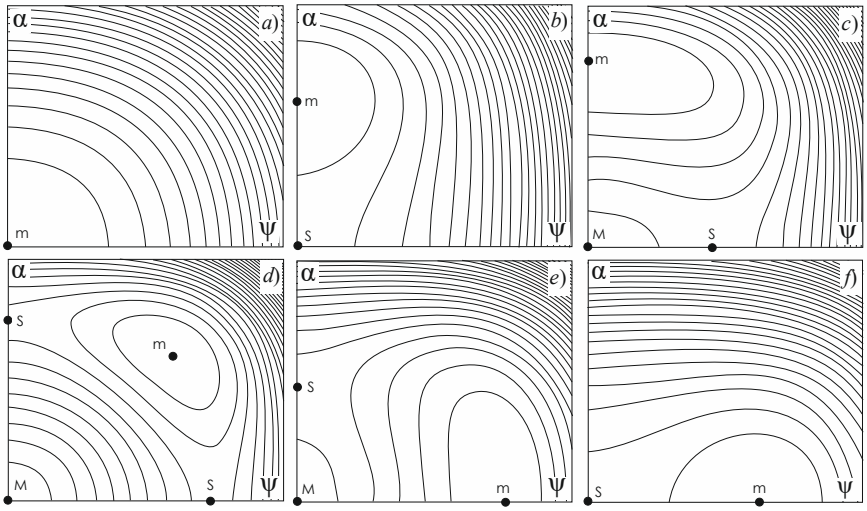

Fig. 1. Topology of free energy isolines along the coordinates ψ and α (horizontal and vertical axes, respectively), showing possible states in the phase diagram: normal phase (*a*); α-phase without ψ-phase (*b*) and with its fluctuations (*c*); coexistence of α and ψ-phases (*d*); ψ-phase with fluctuations of α-phase (*e*), and ψ-phase (*f*). Maxima *M*, minima *m* and free energy saddles *S* are shown by bold dots

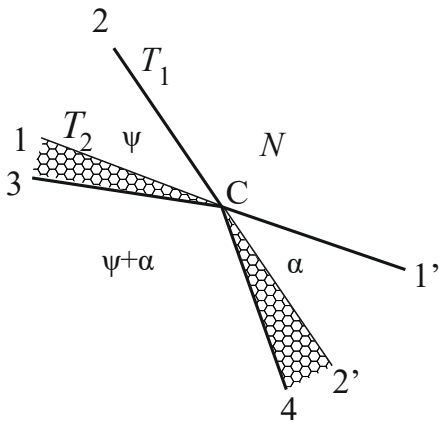

Fig. 2. Fragment of the phase diagram of the solid state in the vicinity of the transition lines: the boundaries in which an ordered state may appear are shown by straight lines 1 − 1′ and 2 − 2′ (*N* is a normal state without ordering); the letters ψ, α, ψ + α denote the corresponding phases and their coexistence (the shaded regions correspond to well-developed fluctuations of one phase in the presence of another). The phase transition lines are highlighted with bold

In the normal phase, at $T > T_1$ and $T > T_2$, the free energy has a minimum at $\psi = 0$, $\alpha = 0$ (see Fig. 1,*a* and Fig. 2, the region *N*, to the right of the polyline 2-*C*-1′), which shifts along the axis α to the point $\psi = 0$, $\alpha = \sqrt{-a_2/b_2}$ upon transition to the region with $T < T_2$ and $T < T_1$ into the α-phase (see Fig. 1,*b* and Fig. 2, the region α in the sector 2′-*C*-1′). This minimum, however, is the only singular point of free energy only in the upper part of the α-phase rather than in the entire region of its existence. After the line $T < T_1$ is crossed a saddle point is added to the minimum that determines the thermodynamically stable α-state at $\psi = \sqrt{-a_1/b_1}$, $\alpha = 0$, where the free energy has a minimum with respect to the variable ψ at $\alpha = 0$ (Fig. 1, *c* and Fig. 2, shaded triangle 2′*C*4).

On the other hand, upon transition from the normal state to the region with $T > T_2$ and $T < T_1$ into the ψ-phase, the minimum shifts along the axis ψ to the point $\alpha = 0$, $\psi = \sqrt{-a_1/b_1}$ (see Fig. 1,*f* and the region ψ in the sector 2-*C*-1 in Fig. 2). After the line $T < T_2$ is crossed, this minimum is also supplemented by a saddle point with the coordinates $\alpha = \sqrt{-a_2/b_2}$ and $\psi = 0$ (see Fig. 1,*e* and Fig. 2, shaded triangle 1*C*3). Finally, a region where the α- and ψ-phases coexist can be detected in the phase diagram (Fig. 1,*d* and the region ψ + α below the polyline 3-*C*-4).

Apparently, in this case the phase transition does not occur at temperatures T_1 and T_2. These temperatures mark the boundaries within which an ordered state may appear, determining the regions with well-developed fluctuations of the competing existing ordered state and the emerging order in the regions with phase competition (see Fig. 1, *c* and *e*), . The phase transition to the coexistence region occurs at a lower temperature (lines 3-*C* and 4-*C* in Fig. 2) and is characterized by the topology of free energy isolines, as in Fig. 1,*d*. We should note that the regions of four different phases of matter converge at point *C* in Fig. 2.

Conclusion

To summarize, adopting the theory of second-order phase transitions as a basis for phenomenological consideration of competing and coexisting phases for selecting the appropriate order parameter, which can be obtained from microscopic description of the state of matter, allows to qualitatively characterize the experimentally observed states of condensed media.

The phenomenological approach turns out to be simpler in calculations than the microscopic description, but it does not allow to determine the mechanisms that induce ordering in the system. The applicability limits of the considered approach are the proximity to the phase transition boundary, the region where the first two terms in the expansion of free energy in powers of the order parameter are sufficient.

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