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Temperature dependences of the critical parameters of an inhomogeneous superconducting layer surrounded by non-superconducting layers

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The superconducting state of an inhomogeneous in thickness layer, adjacent to non-superconducting layers that influence it, is considered. Within the framework of the Ginzburg–Landau (GL) theory a technique has been formulated that allows one to estimate the critical parameters of the superconducting layer for the described problem. In the expansion of free energy in powers of the order parameter modulus an additional term and more accurate dependences of the expansion coefficients on temperature are taken into account, which allows quantitative estimates to be made over a wider temperature range than the classical GL theory. Using the technique, the temperature dependences of the critical current density and the critical magnetic field of the layer were simulated. It is shown that simultaneous consideration of the inhomogeneity of the superconducting layer in thickness and the influence of adjacent layers on its state in the calculation makes it possible to significantly improve the estimate of the critical current density in comparison with experimental data. In this case, temperature dependence type of the critical current density changes with distance from the critical temperature.

Keywords: superconducting films, critical current, Ginzburg–Landau theory, inhomogeneity.

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1. Introduction

The Ginzburg–Landau (GL) theory is of great importance for modern condensed matter physics [1–5]. The advantage of this theory is that it can be modified for a huge number of problems: for example, it can be used to study the behavior of Abrikosov vortices in various superconductors and superconducting structures [6–8]. Besides, it can be used to study both static and dynamic states using time-dependent GL equations [4,9–11].

Today, the GL theory is often used in modeling the actual objects made of superconducting materials [6,7,9,11–15]. They may include superconducting films and layers. Based on them it is possible to create electronic elements, as well as various sensors [16–19]. Superconducting layers can be an integral part of lamellar structures, for example, conductive tapes containing superconducting material [20–23]. The GL theory is often used when calculating the parameters of superconducting films and layers. However, it shall be considered that the superconducting state of the film or the layer highly depends on many factors, such as the presence of defects and inhomogeneity through thickness, as well as the environment of the film/layer, either it is an oxide layer on the film surface or adjacent layers in the lamellar structure. All this shall be considered when calculating the critical parameters. The described factors can be taken into account using generalized GL equations, which consider the inhomogeneity of properties through the thickness of the film/layer [24,25], as well as through the use of general boundary conditions for the order parameter, which describes the influence of the external environment [26].

The literature describes simple equations obtained under the GL theory, which make it possible to estimate the critical magnetic field and current (GL depairing current) of ultrathin plates with a thickness much less than both the coherence length ξ and the London penetration depth of the magnetic field λ [27]. The considered limit allows us to make the assumption that the order parameter Ψ does not change through the plate thickness, this significantly simplifies the GL equations and makes it possible to obtain simple analytical expressions for the depairing current and the critical magnetic field. Note that such assumption is not applicable for plates with a thickness about ξ (see, for example, the distributions of the order parameter from the paper [28]), and especially for plates with large thickness. Based on this, simple analytical expressions for the critical magnetic field and depairing current are not applicable for plates/layers with a thickness about ξ or more.

This paper presents calculations of critical parameters for an inhomogeneous superconducting layer with thickness about ξ and λ, for which, using specially derived boundary conditions for the order parameter, the influence of neighboring non-superconducting layers is introduced. The inhomogeneity of the superconducting layer is included in the modified GL equations. When deriving the modified equations in the expansion of free energy in powers of the order parameter modulus an additional term $|\Psi|^6$ and more accurate dependences of the expansion coefficients on temperature are taken into account, which allows quantitative estimates to be made using these equations over a wider temperature range than the classical GL theory.

2. Model description

In this paper we consider the superconducting layer with thickness of D (the length and width of the layer are much greater than its thickness), bordering on identical non-superconducting layers and inhomogeneous through thickness (in this problem formulation inhomogeneous along the axis x). The geometry of the problem, as well as the directions of the transport current I_t flowing through the layer and the external magnetic field $\mathbf{H}$ are shown in Figure 1. The Cartesian coordinate system (x, y, z) is introduced as shown in the Figure. The layer boundaries correspond to $x = 0$ and $x = D$. In the presented geometry the vector potential has the form $\mathbf{A} = \mathbf{e_y} A(x)$.

The inhomogeneity of the superconducting layer in the model is due to the change in the electron mean free path l through its thickness. The distribution of the mean free path length is given by the expression

$$l(x) = l_0\left(1 - \eta\left(\frac{x}{D} - 0.5\right)^2\right), \tag{1}$$

where l_0 — the mean free path in the center of the layer, and η — a parameter showing the difference between the mean free path in the center of the layer and the value at its boundaries. If $\eta = 0$, then $l(x) = l_0$, which corresponds to the case of a homogeneous superconducting layer. Information described above makes it clear that η characterizes the degree of inhomogeneity of the layer.

The choice of dependence $l(x)$ in the form (1) is due to the following considerations. In the center of the superconducting layer or film the parameters of the material are close or even coincide with those characteristic of this material in the bulk of the massive superconductor. When approaching the boundaries of the layer, due to technological reasons, caused, in particular, by the presence of an interface between different materials, the layer properties change. Structural and elemental analysis of superconducting films shows that at interfaces with the substrate and the external environment, the composition of the superconducting layer can coincide with the composition of the material from which it is made, while the atoms forming the material can be disordered (see, for example, [29]). Based on the disorder of the crystal lattice at the film boundaries, the proposed model makes the assumption that the mean free path decreases when approaching the film boundaries (see expression (1)).

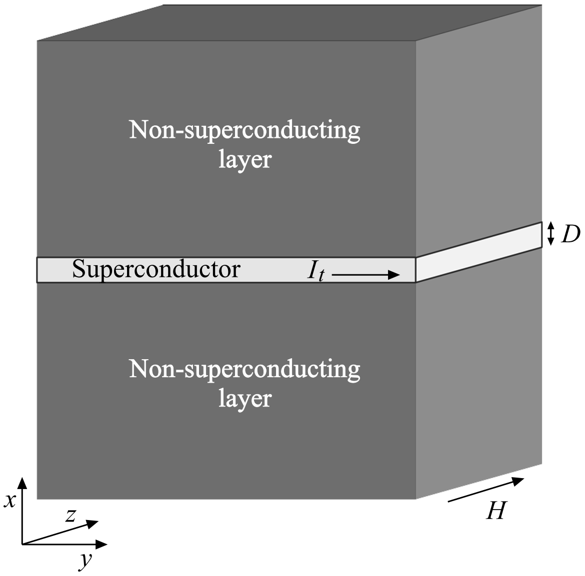

Figure 1. Geometry of the problem.

To derive the GL equations for the described problem, let's consider the free energy functional:

$$F_1 \propto \int_0^D \Bigg[-a_1(T)|\Psi(x)|^2 + \frac{a_2(T)}{2}|\Psi(x)|^4 - \frac{a_3(T)}{3}|\Psi(x)|^6 + b(T,x)\left(\left|\frac{\partial\Psi}{\partial x}\right|^2 + \frac{4e^2}{c^2}A(x)^2|\Psi(x)|^2\right) + \frac{(\partial A/\partial x - H)^2}{8\pi}\Bigg]dx, \tag{2}$$

where Ψ — order parameter, e — electron charge, c — speed of light, T — temperature of the superconducting layer, $a_{1,\ldots,3}(T)$ and $b(T, x)$ — coefficients in the expansion of the free energy functional. According to microscopic calculations under the Bardeen–Cooper–Schriefer (BCS) theory, the temperature dependences $a_{1,\ldots,3}(T)$ have the following form [30]:

$$a_1 = \alpha_1\left(1 - \frac{T}{T_{\mathrm{cm}}}\right)\left(1 + 0.5\left(1 - \frac{T}{T_{\mathrm{cm}}}\right)\right),$$
$$a_2 = \alpha_2\left(\frac{T}{T_{\mathrm{cm}}}\right)^2, \ a_3 = \alpha_3\left(\frac{T}{T_{\mathrm{cm}}}\right)^4, \tag{3}$$

where $\alpha_{1,\ldots,3}$ — coefficients whose numerical values can be calculated, T_{cm} — the critical temperature of the massive superconductor from which the layer is made.

In turn, the expansion coefficient $b(T, x)$ in the „dirty limit“ $l \ll \xi_0$, where ξ_0 — the coherence length in a pure superconductor in the BCS theory is proportional to the electron mean free path l [31]. Taking into account the assumption about the form of the dependence $l(x)$ (1), $b(T, x)$ will have the form

$$b(T,x) = b_{\mathrm{cn}}\left(\frac{T_{\mathrm{cm}}}{T}\right)^2\left(1 - \eta\left(\frac{x}{D} - 0.5\right)^2\right), \tag{4}$$

where b_{cn} — coefficient independent of T and x.

As a result of the free energy functional (2) variation with respect to the order parameter and vector potential, and taking into account the form of expansion coefficients (3) and (4), the GL equations are obtained in the form

$$\psi - 2p(T)q(T)\psi^3 + p(T)q^2(T)\psi^5 + \left(1-\eta\left(\frac{x_\xi}{d}-0.5\right)^2\right)\frac{\partial^2\psi}{\partial x_\xi^2} - \frac{2\eta}{d}\left(\frac{x_\xi}{d}-0.5\right)\frac{\partial\psi}{\partial x_\xi} - \frac{U^2}{\kappa_0^2}\psi\left(1-\eta\left(\frac{x_\xi}{d}-0.5\right)^2\right) = 0, \quad (5)$$

$$\frac{\partial^2 U}{\partial x_\xi^2} - 2p(T)q(T)\frac{\psi^2}{\kappa_0^2}U\left(1-\eta\left(\frac{x_\xi}{d}-0.5\right)^2\right) = 0, \quad (6)$$

where

$$p(T) = \frac{0.367101}{(1-T/T_{\text{cm}})(1+0.5(1-T/T_{\text{cm}}))},$$

$$q(T) = 1-\sqrt{1-2.724043(1-T/T_{\text{cm}})(1+0.5(1-T/T_{\text{cm}}))},$$

ψ — normalized order parameter: $\psi = \Psi/\Psi_0$, $\Psi_0 = \sqrt{a_2(1-\sqrt{(1-4a_1a_3/a_2^2)})/2a_3}$ — order parameter in massive superconductor if external magnetic field is absent [30], κ_0 — GL parameter in the center of the superconducting layer. Instead of the dimensional values of the coordinate x and potential A the dimensionless variables x_ξ and $U(x_\xi)$ were introduced, respectively

$$x_\xi = \frac{x}{\xi_{\text{cn}}}, \quad U = \frac{2\pi\kappa_0\xi_{\text{cn}}}{\phi_0}A,$$

where ϕ_0 — magnetic flux quantum, ξ_{cn} — GL coherence length of a homogeneous superconductor or GL coherence length at the center of an inhomogeneous superconductor, while

$$\xi_{\text{cn}} = \sqrt{b_{\text{cn}}\left(\frac{T_{\text{cm}}}{T}\right)^2/a_1} = \frac{\xi_{\text{cn}0}}{(T/T_{\text{cm}})\sqrt{(1-T/T_{\text{cm}})(1+0.5(1-T/T_{\text{cm}}))}}, \quad (7)$$

$\xi_{\text{cn}0}$ — coherence length in the center of the layer at $T = 0$. In other parts of the superconducting layer, the dependence of the coherence length on temperature is similar to (7).

When deriving the equations, the calibration of the vector potential $\operatorname{div}\mathbf{A} = 0$ was used.

Note that during deriving equations (5) and (6) the use of the free energy functional (2) with temperature dependences of the expansion coefficients in the form (3) and (4) allows us to carry out quantitative estimates using these equations at temperatures $T > 0.7T_{\text{cm}}$ [30].

Since the transport current I_t in the layer creates a magnetic field

$$H_I = \frac{2\pi}{c}I_t, \quad (8)$$

then the total field near its surfaces is equal to $H \pm H_I$, and the boundary conditions for equation (6) have the form

$$\left.\frac{\partial U}{\partial x_\xi}\right|_{x_\xi=0} = h - h_i,$$

$$\left.\frac{\partial U}{\partial x_\xi}\right|_{x_\xi=d} = h + h_i, \quad (9)$$

where

$$h = \frac{H}{H_\xi}, \quad h_I = \frac{H_I}{H_\xi}, \quad H_\xi = \frac{\phi_0}{2\pi\kappa_0^2\xi_{\text{cn}}^2}.$$

Let us discuss in more detail the boundary conditions for equation (5). Consider the free energy functional F_2:

$$F_2 \propto F_1 + \gamma|\Psi(0)|^2 + \gamma|\Psi(D)|^2. \quad (10)$$

The last two terms by analogy with [26] describe the contribution of the energy of the superconducting layer surfaces to its free energy. In turn, γ — coefficient in the expansion of the energy of the superconducting layer surfaces in powers of the order parameter. For this paper we assume that the layer surfaces (corresponding to $x = 0$ and $x = D$) are the same.

As a result of variation of the free energy functional (10) with respect to the order parameter, the generalized boundary conditions can be obtained in the form:

$$\left.\frac{d\psi}{dx_\xi}\right|_{x_\xi=0} = \frac{\psi(0)}{\Lambda(1-0.25\eta)},$$

$$\left.\frac{d\psi}{dx_\xi}\right|_{x_\xi=d} = -\frac{\psi(d)}{\Lambda(1-0.25\eta)}. \quad (11)$$

Here

$$\Lambda = \frac{1}{\gamma}\sqrt{b_{\text{cn}}\left(\frac{T_{\text{cm}}}{T}\right)^2 a_1}$$

is length dimension parameter, which, by analogy with [26], will be called as the extrapolation length.

The analysis of equations (11) shows the following. If we take $\eta = 0$, then the boundary conditions take the form that is used for calculations in the case of homogeneous films (see, for example, [32–34]). If the extrapolation length is $\Lambda = \infty$, then the boundary conditions (11) take the form that does not take into account the influence of adjacent layers [28,35]. Additionally, it is worth mentioning that the paper [26] indicates the need to use in calculations the general boundary conditions for the order parameter for high-temperature superconductors (HTSC). This is due to the fact that usually the coherence length for these materials is short compared to low-temperature superconductors. In this case, according to [26], at the superconductor boundary the extrapolation length is $\Lambda \propto \xi$, which leads to small values of Λ for HTSC, and it becomes necessary to apply the general boundary conditions to the order parameter. In the case of inhomogeneous superconducting layers at their boundaries the mean free path decreases relative to

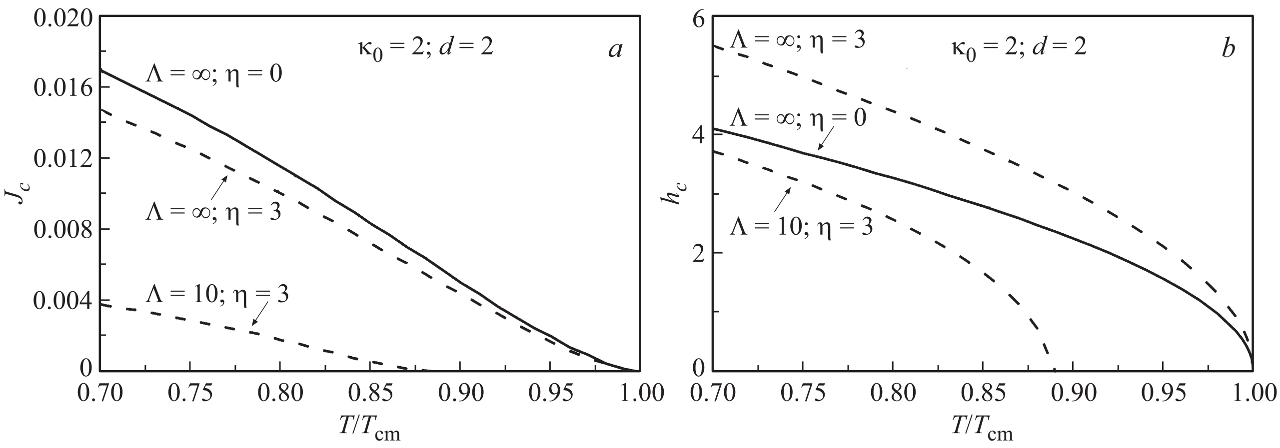

Figure 2. Dependencies: *a* — critical current density J_c and *b* — critical magnetic field h_c vs. ratio T/T_{cm} for homogeneous ($\eta = 0$, solid lines) and inhomogeneous ($\eta = 3$, dashed lines) superconducting layers with thickness $d = 2$. The shown dependencies also correspond to both case of the adjacent layers effect ($\Lambda = 10$), and to effect absence ($\Lambda = \infty$). GL parameter in the center of the layer $\kappa_0 = 2$, T_{cm} — critical temperature of massive superconductor.

its value in the bulk of the layer due to the disorder of atoms at the boundary (see, for example, [29]). Due to this, within the framework of the „dirty limit" the value of ξ at the boundary decreases relative to its value in the bulk. This leads to decrease in Λ value and the need to take into account the general boundary conditions for the order parameter not only for layers of HTSC materials, but also for layers of low-temperature superconductors.

Let us discuss the change in the ratio of the superconducting layer thickness D and the coherence length ξ with a change in temperature $(D/\xi(T))$. As it was mentioned above, the parameters of the superconducting layer vary through its thickness, so we will consider the value of the coherence length averaged through the layer thickness

$$\langle\xi\rangle(T) = \frac{1}{D}\int_0^D \xi(x, T)dx,$$

where

$$\xi(x, T) = \xi_{cn}(T)\sqrt{\left(1 - \eta\left(\frac{x}{D} - 0.5\right)^2\right)}.$$

The dependence $\xi_{cn}(T)$ is determined by ratio (7). The relationship that is valid for the „dirty limit" $\xi \propto \sqrt{l}$ is also taken into account here. Note that when conducting experiments, as a rule, the average value ξ is determined for the film/layer. In this paper we consider the superconducting layer with thickness $D = 2\xi_{cn0}$. Calculations were made for the degree of heterogeneity $\eta = 3$ and at temperatures $T > 0.7T_{cm}$. At the boundaries of the temperature interval under consideration, the ratio $D/\langle\xi\rangle(0.7T_{cm}) \approx 0.96$ and decreases with temperature increasing. For the layer homogeneous through thickness (case $\eta = 0$) $D/\xi(0.7T_{cm}) \approx 0.82$ and also decreases with T increasing. Thus, the relation $D < \xi(T)$ for the simulated superconducting layer is satisfied over the entire temperature range under consideration.

It is worth noting that all the length and thickness values given below are presented in units of the coherence length at the center of the superconducting layer at zero temperature ξ_{cn0}, and the magnetic field values are in units of $H_{\xi_{cn0}}$ (see (9)). In particular, the layer thickness is $d = D/\xi_{cn0}$. The use of such units makes it easier to compare the properties of inhomogeneous superconducting layers with the properties of homogeneous ones, in which $\eta = 0$. The current values within the model are represented in terms of H_I (8) and therefore, like the magnetic field, are expressed in units of $H_{\xi_{cn0}}$. The critical current density J_c is defined as H_I of critical current divided by the superconducting layer thickness. The iterative procedure for solving the system of equations (5) and (6) with boundary conditions (9) and (11) is similar to that described in the paper [34].

3. Results of numerical calculations

Figure 2, *a* shows the critical current density J_c versus temperature for a superconducting layer with thickness $d = 2$. The influence of boundaries is taken into account through the parameter Λ. Next, two cases are considered: neighboring layers do not affect the superconducting layer ($\Lambda = \infty$), and neighboring layers affect ($\Lambda = 10$). The extrapolation length $\Lambda = 10$ is taken as an example. Smaller values of the extrapolation length correspond to a stronger influence of the adjacent layers on the superconducting state of the layer. So, in this case, the effects described below and associated with the influence of layers will be more pronounced. The superconducting layer itself can be homogeneous ($\eta = 0$, in Figure 2, *a* corresponds to the solid curve) and inhomogeneous ($\eta = 3$, dashed lines in Figure 2, *a*).

Let us first consider the homogeneous and the inhomogeneous layer without taking into account the influence of adjacent layers ($\Lambda = \infty$, $\eta = 0$ and 3). As can be seen from

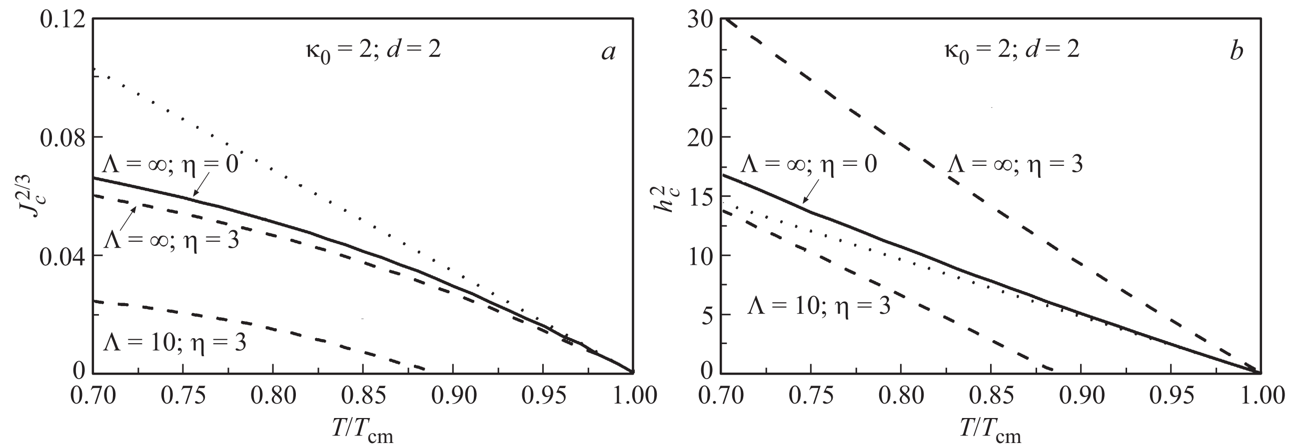

Figure 3. Dependencies $J_c^{2/3}$ (*a*) and h_c^2 (*b*) on the ratio $T/T_{\rm cm}$ for homogeneous ($\eta = 0$, solid lines) and inhomogeneous ($\eta = 3$, dashed lines) superconducting layers with thickness $d = 2$. The shown dependencies also correspond to both case of the adjacent layers effect ($\Lambda = 10$), and to effect absence ($\Lambda = \infty$). GL parameter in the center of the layer $\kappa_0 = 2$, $T_{\rm cm}$ — critical temperature of massive superconductor. Dashed lines are introduced to show the deviation of solid lines from the linear law.

the graph that the inhomogeneity accounting significantly reduces the value of the critical current density, while the value of the critical temperature does not change, which is consistent with what was obtained earlier [36]. If we take into account the influence of adjacent layers ($\Lambda = 10$), then we can see that the values of the critical current density and critical temperature greatly decrease compared to the case $\Lambda = \infty$.

Figure 2, *b* shows the critical magnetic field h_c versus temperature for the layer with thickness $d = 2$. The homogeneous layer ($\eta = 0$), as well as an inhomogeneous layer ($\eta = 3$) were considered, with and without consideration of adjacent layers influence. A regularity is observed: the greater the degree of inhomogeneity is, the higher the value of the critical magnetic field is. This result for inhomogeneous films was obtained in [36]. If we take into account the influence of adjacent layers, then the value of the critical field decreases compared to the case where such influence is not taken into account. Thus, the heterogeneity of the layer and the adjacent layers have a multidirectional effect on the critical magnetic field.

The experiments described in the literature show that GL theory gives good estimates of the critical magnetic field parallel to the film surface, they coincides with experimental data [27,37]. On the other hand, estimates of the GL depairing current are significantly overestimated compared to experimental data, even for films in vortex-free state [38].

Let us discuss the quantitative change in critical parameters J_c and h_c under the influence of inhomogeneity and adjacent layers. Simultaneous consideration of these factors in the model leads to a noticeable decrease in the value of the calculated critical current (critical current density) in comparison with the case of homogeneous layer/film not considering the influence of boundaries (Figure 2, *a*). Thus, the results of the calculations described in this paper show that consideration in the model of the simultaneous influence of adjacent layers and layer/film inhomogeneity can significantly improve the estimate of the critical current under the GL theory compared to experimental data. The combined influence of boundaries and inhomogeneity of thin films/layers on their superconducting state may be one of the factors that explains the significant difference between the GL depairing current and the measured values of the critical current for films/layers made of type I superconductors, as well as films/layers made of type II superconductors, thin enough so that vortices do not penetrate into them. Identification of the reasons leading to significant overestimation of the critical current under the GL theory is an important aspect for assessing the accuracy of calculations of the critical current of actual superconducting structures.

Additionally, we present information on the experimentally measured critical current density of thin superconducting films. The measured values depend on many factors, for example, the temperature at which the critical current is measured, the material from which the superconducting film/layer is made, the production technology of the structure under study, etc. In this regard, we will focus on thin films of niobium, the parameters of which are close to those that we used in the calculations presented in the article. Systematic studies of such films were described in papers [39,40]. The authors of the article [39] present the critical current density 7.5 MA/cm^2 measured for the thin superconducting niobium film ($D \approx \xi(0)$). The measurements were carried out at a temperature of 4.2 K, in turn, the critical temperature of the film was 6.7 K. Comparison of the measured current density with the calculated value of the depairing current density (15.9 MA/cm^2) showed that the latter was exceeded by more that two times. The authors associated this difference with the inaccuracy in determining the structure parameters used to calculate the depairing current, as well as the formation of a thin non-superconducting metal layer on its surface during film production. In paper [40] the authors also associated the decrease in the experimentally determined critical parameters of thin niobium films relative to the parameters for bulk samples with the presence of disordered metal layers at the superconductor-substrate interface. This is consistent with the conclusions made in this paper.

The influence of adjacent layers and inhomogeneity of films/layers on the value of the critical magnetic field are comparable in magnitude (Figure 2, b). This multidirectional influence leads to the fact that the resulting estimate of the critical magnetic field h_c does not change so much under the influence of the described factors.

In the immediate vicinity of the critical temperature T_c the critical current and field depend on temperature as $(T_c - T)^{3/2}$ and $(T_c - T)^{1/2}$, respectively [27,31]. Shown in Figure 3 dependencies $J_c^{2/3}$ (a) and h_c^2 (b) on temperature show that for the critical current densities such law is met at $T > 0.95T_c$, and for critical magnetic field — at $T > 0.9T_c$. Note also that in the considered temperature range $(T > 0.7T_{\text{cm}})$ upon movement from T_{cm} the form of dependence $J_c(T/T_{\text{cm}})$ changes more then form of dependence $h_c(T/T_{\text{cm}})$. At the same time, the influence of adjacent layers and heterogeneity does not change the form of the discussed dependencies. Moreover, the obtained form of the critical magnetic field versus temperature corresponds to that observed experimentally [37].

4. Conclusion

In the paper, within the framework of GL theory, a model was formulated that allows one to calculate the critical parameters of the superconducting layer with thickness about the coherence length ξ and the London penetration depth λ. The model takes into account factors such as the influence of adjacent layers and layer heterogeneity through thickness. Taking into account the additional term in the expansion of free energy and more accurate temperature dependences of the expansion coefficients when deriving the equations made it possible to expand the temperature range where the model gives quantitatively accurate estimates. The main results of the paper can be formulated as follows:

– it is shown that taking into account the influence of adjacent non-superconducting layers and inhomogeneity on the superconducting state of the layer significantly corrects the estimate of its critical current density, resulting in its decrease. At the same time, the value of the critical current density calculated taking into account the mentioned factors is closer to that measured experimentally than without taking them into account;

– in the case of critical magnetic field consideration of the influence of boundaries and inhomogeneity of the superconducting layer will affect the estimate h_c, but not as significantly as in the case of the critical current density;

– when moving away from the critical temperature T_c towards low temperatures, the form of the model temperature dependence h_c changes slightly, and strict compliance with the law $(T_c - T)^{1/2}$ is observed at $T > 0.9T_c$. In turn, the dependence J_c(T) changes significantly, and the law $(T_c - T)^{3/2}$ is applicable at $T > 0.95T_c$ only. The inhomogeneity of the superconducting layer and the adjacent non-superconducting layers do not change the form of temperature dependences J_c and h_c. The form $h_c(T)$ is consistent with what was observed experimentally.

Thus, this article shows that taking into account factors such as the influence of adjacent layers and inhomogeneity on the superconducting layer with thickness about ξ and λ significantly improves the estimate of the critical current density in comparison with experimental data, at the same time not significantly changing the estimate and qualitative behavior of the temperature dependence of the critical magnetic field, which, even without these factors consideration are consistent with experimental data.

The results of this paper will allow more accurate calculations of superconducting parameters for various films and superconducting structures (for example, structures S–I–S and S–N–S) from niobium and niobium-containing materials (NbC, Nb_3Sn, NbTi), as well as other similar materials. When using suitable calculation parameters, the method described in this paper can be used to simulate structures from HTSC materials with coherence length about several tens of nanometers (for example, $KBaBiO_3$).

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Conflict of interest

The authors declare that they have no conflict of interest.

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