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SUPERCONDUCTIVITY

Distribution of Pairing Functions in Superconducting Spin Valve SF1F2

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Abstract—The distribution of the spin-singlet component, the short-range spin-triplet component with zero projection, and the long-range spin-triplet component with projection ±1 of the superconducting pairing function has been obtained for different regimes of switching of a spin valve with a three-layer heterostructure (superconductor/ferromagnet/ferromagnet). The distribution of the components is discussed as the main reason for the behavior of the superconducting transition temperature as a function of the angle between the magnetic moments of the ferromagnetic layers in these regimes.

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1. INTRODUCTION

The superconducting transition temperature T_c was analyzed [1] for a three-layer heterostructure SF1F2, where S is a singlet superconductor and F1, F2 are ferromagnetic metals, in which the long-range triplet superconducting component is formed for noncollinear orientation of the magnetizations of the F layers. The asymptotically exact numerical method was used for calculating T_c as a function of the three-layer structure parameters, such as mutual orientation of magnetizations, transparency of boundaries, and layer thickness [2]. Earlier, it was shown in [3] that T_c of the semi-infinite heterostructure SF1F2 can be a nonmonotonic function of angle α between the magnetizations of two F layers in contrast to the monotonic behavior of the $T_c(\alpha)$ dependence obtained for the FSF model of the superconducting spin valve [4]. The existence of an anomalous dependence of the spin-triplet correlations on angle α in the FFS structure in the ballistic case was predicted in [5] (the layer thickness was much smaller than the correlation length of the material of these layers). In this research, we consider the distribution of amplitudes of spin-singlet and spin-triplet pair correlations as functions of the layer thickness for different values of angle α between magnetizations in the SF1F2 structure in order to determine how and which of the distributions affects the superconducting transition temperature T_c.

2. MODEL AND NUMERICAL METHOD

Let us first find the dependence of T_c of the SF1F2 structure (Fig. 1) on angle α between the exchange fields of two F layers.

Suppose that the S layer of thickness d_S lies in the region $-d_S < x < 0$, the middle layer F1 of thickness d_{F1} lies in the region $0 < x < d_{F1}$, and the outer layer F2 of thickness d_{F2} lies in the region $d_{F1} < x < d_{F1} + d_{F2}$. The x axis is assumed to be normal to the plane of the layers. The exchange field of the middle layer F1 lies in

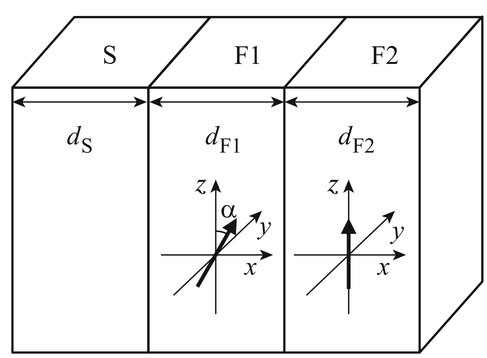

Fig. 1. Three-layer heterostructure SF1F2. The SF1 contact boundary corresponds to coordinate $x = 0$. Bold arrows in F layers indicate the direction of **h** exchange fields lying in yz plane.

the yz plane, $\mathbf{h} = (0, h\sin\alpha, h\cos\alpha)$, while the exchange field of the outer layer F2 is directed along the z axis, $\mathbf{h} = (0, 0, h)$. Angle α varies from zero (parallel configuration, P) to π (antiparallel configuration, AP).

Structure SF1F2 is considered in the "dirty" limit in which the state of the superconducting condensate is described by Usadel equations. In the vicinity of T_c, the Usadel equations are linearized and contain only the anomalous Green function $\hat{f}$ [1]:

$$\frac{D}{2}\nabla^2\hat{f} - |\omega|\hat{f} - \frac{i\,\mathrm{sgn}\,\omega}{2}\{\hat{\tau}_0(\mathbf{h}\hat{\boldsymbol{\sigma}}), \hat{f}\} + \Delta\hat{\tau}_1\hat{\sigma}_0 = 0. \quad (1)$$

Here, D is the diffusion constant, $\hat{f}$ is a 4×4 matrix, $\omega = \pi T_c(2n + 1)$ is the Matsubara frequency, where n is an integer, $\hat{\tau}_i$ and $\hat{\sigma}_i$ are the Pauli matrices in the Nambu–Gor'kov space and the spin space, respectively, and $\hat{\tau}_k\hat{\sigma}_l$ is the direct product of matrices. Order parameter Δ is real-valued in the superconducting layer and is zero in the ferromagnetic layer. Diffusion constant D is assigned with the appropriate subscript S or F when Eq. (1) is applied to the superconducting or ferromagnetic layer, respectively.

Green's function $\hat{f}$ can be decomposed into the following components:

$$\hat{f} = \hat{\tau}_1(f_0\hat{\sigma}_0 + f_3\hat{\sigma}_3 + f_2\hat{\sigma}_2). \quad (2)$$

Here, f_0 is the singlet component, f_3 is the triplet component with zero projection on the z axis, and f_2 is the triplet component with projection ± 1 on the z axis (realized only for $\alpha \neq 0, \pi$).

In view of the existing symmetry of components (3) given below, it is sufficient to consider only the positive Matsubara frequencies, $\omega > 0$:

$$\begin{aligned} f_0(-\omega) &= f_0(\omega), & f_0 &\text{ real}, \\ f_3(-\omega) &= -f_3(\omega), & f_3 &\text{ imaginary}, \\ f_2(-\omega) &= -f_2(\omega), & f_2 &\text{ imaginary}. \end{aligned} \quad (3)$$

The problem of calculating T_c can be reduced to an effective system of equations in a singlet component in layer S. The system of equations includes the self-consistent equation, the Usadel equations, and the boundary conditions to them:

$$\Delta \ln\frac{T_{cS}}{T_c} = 2\pi T_c \sum_{\omega>0}\left(\frac{\Delta}{\omega} - f_0\right), \quad (4)$$

$$\frac{D}{2}\frac{d^2 f_0}{dx^2} - \omega f_0 + \Delta = 0, \quad (5)$$

$$\frac{df_0}{dx} = 0|_{x=-d_S}, \quad -\xi_S\frac{df_0}{dx} = Wf_0|_{x=0}. \quad (6)$$

Here, T_{cS} and $\xi_S = \sqrt{D_S/2\pi T_{cS}}$ are the superconducting transition temperature and the coherence length of the isolated layer S, respectively. This is the problem for which a multimode method was worked out in [2] and later used for the structure F1SF2 [4] and the semi-infinite spin valve SF1F2 [3]. We must only determine the exact expression for W in Eq. (6) by solving the boundary value problem for the heterostructure SF1F2.

The following characteristic wavevectors were obtained from Usadel equations (1):

$$k_\omega = \sqrt{\frac{2\omega}{D}}, \quad k_h = \sqrt{\frac{h}{D}}, \quad \tilde{k}_h = \sqrt{k_\omega^2 + 2ik_h^2}. \quad (7)$$

The solution of Eq. (1) in layer S (A and B are purely imaginary quantities) can be presented in the form

$$\begin{pmatrix} f_0(x) \\ f_3(x) \\ f_2(x) \end{pmatrix} = \begin{pmatrix} f_0(x) \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ A \\ B \end{pmatrix}\frac{\cosh[k_\omega(x + d_S)]}{\cosh(k_\omega d_S)}. \quad (8)$$

The singlet component $f_0(x)$ in layer S has the same form as in [2].

The solution to Eq. (1) in the middle layer F1 (C_1 and S_1 are purely imaginary quantities, $C_3 = -C_2^*$, $S_3 = -S_2^*$) has the form

$$\begin{aligned} \begin{pmatrix} f_0(x) \\ f_3(x) \\ f_2(x) \end{pmatrix} &= C_1\begin{pmatrix} 0 \\ -\sin\alpha \\ \cos\alpha \end{pmatrix}\cosh(k_\omega x) \\ &+ C_2\begin{pmatrix} 1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix}\cosh(\tilde{k}_h x) \\ &+ C_3\begin{pmatrix} -1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix}\cosh(\tilde{k}_h^* x) + S_1\begin{pmatrix} 0 \\ -\sin\alpha \\ \cos\alpha \end{pmatrix}\sinh(k_\omega x) \\ &+ S_2\begin{pmatrix} 1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix}\sinh(\tilde{k}_h x) + S_3\begin{pmatrix} -1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix}\sinh(\tilde{k}_h^* x). \end{aligned} \quad (9)$$

The solution to Eq. (1) in the outer layer F2 (E_1 and H_1 are purely imaginary quantities, $E_3 = -E_2^*$, $H_3 = -H_2^*$) has the form

$$\begin{aligned} \begin{pmatrix} f_0(x) \\ f_3(x) \\ f_2(x) \end{pmatrix} &= E_1\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\cosh(k_\omega x) + E_2\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}\cosh(\tilde{k}_h x) \\ &+ E_3\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}\cosh(\tilde{k}_h^* x) + H_1\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\sinh(k_\omega x) \\ &+ H_2\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}\sinh(\tilde{k}_h x) + H_3\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}\sinh(\tilde{k}_h^* x). \end{aligned} \quad (10)$$

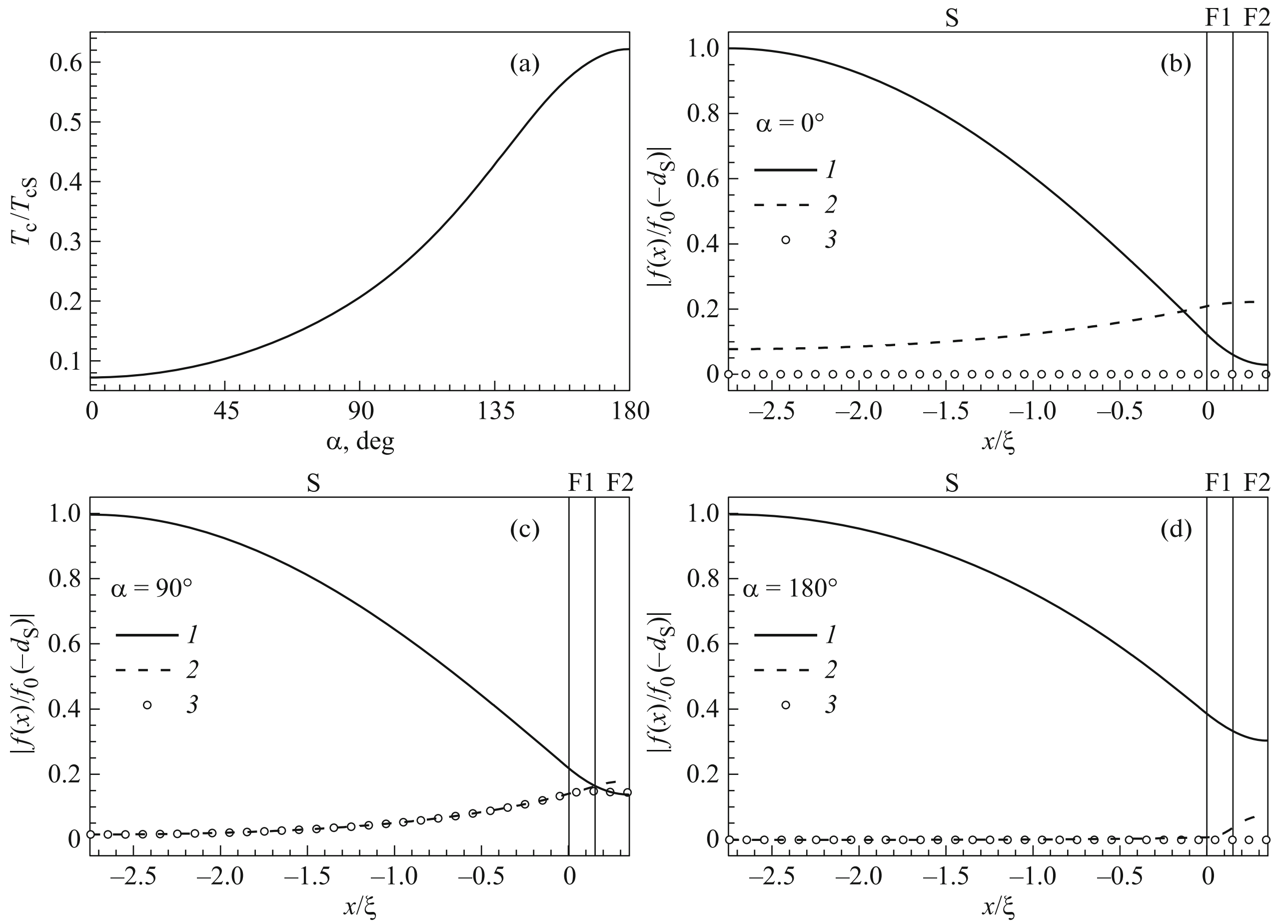

Fig. 2. (a) Superconducting transition temperature T_c as a function of angle α in the direct regime. The spin singlet $|f_0(x)/f_0(-d_S)|$ (curve *1*) and spin triplet $|f_3(x)/f_0(-d_S)|$ (curve *2*) and $|f_2(x)/f_0(-d_S)|$ (curve *3*) distributions of the superconducting pairing components in direct regime for (b) parallel, (c) orthogonal, and (d) antiparallel orientations of the magnetizations of ferromagnetic layers for $n = 2$.

The boundary conditions at the free boundary of F2 can be written as

$$\frac{df_i}{dx} = 0\Big|_{x=d_{F1}+d_{F2}}. \tag{11}$$

The boundary conditions at the SF1 and F1F2 contact boundaries have the form [6]

$$\left(f_i + \gamma_B \xi \frac{df_i}{dx}\right)\Big|_{\text{left}} = f_i\big|_{\text{right}}, \qquad \left(\gamma\xi\frac{df_i}{dx}\right)\Big|_{\text{left}} = \left(\xi\frac{df_i}{dx}\right)\Big|_{\text{right}}, \tag{12}$$

where γ_B and γ are spin-independent proximity parameters

$$\gamma_{BSF1} = R_{BSF1}A_B/\rho_S\xi_S, \quad \gamma_{SF1} = \rho_{F1}\xi_{F1}/\rho_S\xi_S, \quad \gamma_{BF1F2} = R_{BF1F2}A_B/\rho_{F1}\xi_{F1}, \quad \gamma_{F1F2} = \rho_{F2}\xi_{F2}/\rho_{F1}\xi_{F1}; \tag{13}$$

R_{BSF1}, R_{BF1F2} and A_B are the resistances and area of the SF1 and F1F2 contact boundaries, respectively; ρ_S, ρ_{F1}, and ρ_{F2} are the resistivities of layers S, F1, and F2, respectively.

The following simple formulation is used for numerical calculations in this work: all contact boundaries are transparent ($\gamma_B = 0$), the diffusion constants and resistivities are identical ($\gamma = 1$), and the magnitudes of the exchange fields in both F layers are identical.

Joining the Usadel solutions in the layers with the help of boundary conditions (11) and (12), we obtain 15 equations. The equation containing the singlet component derivative on the S side of SF1 contact boundary ($x = 0$) has the form

$$\xi_S \frac{df_0}{dx}\Big|_{x=0} = \tilde{k}_h S_2 - \tilde{k}_h^* S_3. \tag{14}$$

The remaining 14 linear equations form a system in the 14 coefficients in Eqs. (8)–(10). This system of equations has a nonzero solution, because $f_0(0)$ derived from Eq. (8) appears on the right-hand side of the system of equations. Function $W(\alpha)$ in Eq. (6) can be

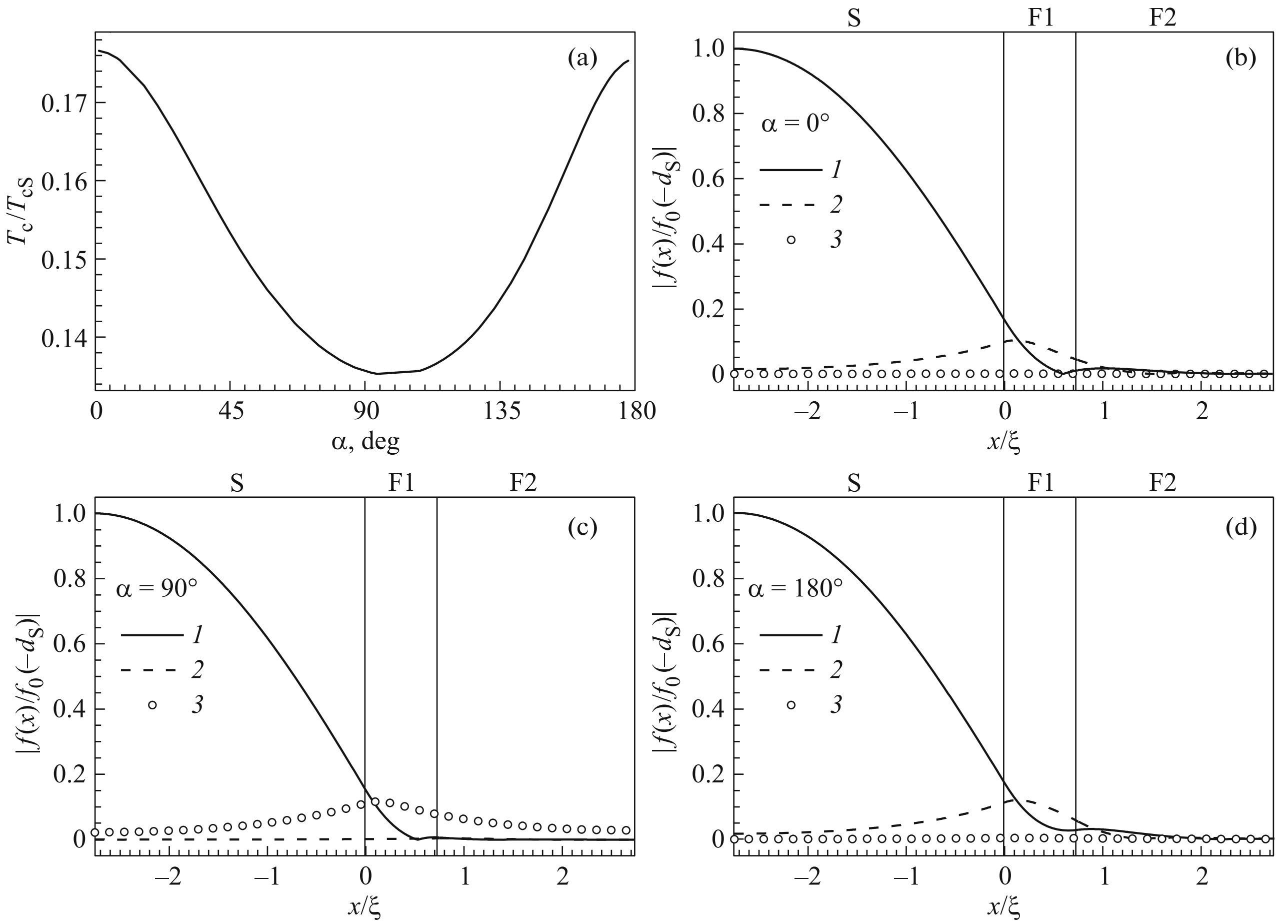

Fig. 3. (a) Superconducting transition temperature T_c as a function of angle α for the triplet regime. The spin singlet $|f_0(x)/f_0(-d_S)|$ (curve *1*) and the spin triplet $|f_3(x)/f_0(-d_S)|$ (curve *2*) and $|f_2(x)/f_0(-d_S)|$ (curve *3*) distributions of the superconducting pairing components in the triplet regime for (b) parallel, (c) orthogonal, and (d) antiparallel orientations of the magnetizations of ferromagnetic layers for $n = 2$.

derived in explicit form by substituting coefficient S_2 into Eq. (14). The single real-valued function $W(\alpha)$ contains the entire information about the two F layers.

3. DISCUSSION OF RESULTS

Figures 2–4 show the results of self-consistent numerical calculations of T_c as a function of angle α and distributions of the components of superconducting pairing function for different thicknesses of F layers in the three-layer heterostructure SF1F2.

Figure 2a shows the direct switching of the spin valve $[T_c^{AP}(\alpha = 180°) > T_c^{P}(\alpha = 0°)]$, which takes place for $d_{F1}/\xi_{F1} = 0.15$ and $d_{F2}/\xi_{F2} = 0.20$. Here and below, $d_S/\xi_S = 2.75$ is the thickness of the superconducting layer. When magnetizations of F1 and F2 layers are antiparallel, the main physical reason behind the difference in T_c^{AP} and T_c^{P} is the partial compensation of ferromagnetic exchange fields. The compensation quite adequately ensures the large difference between T_c^{AP} and T_c^{P} as long as the thickness of F layers is smaller than the coherence length. Both triplet pairing components f_2 and f_3 have a peak at the outer surface of the F2 layer (Figs. 2b–2d).

The triplet regime of the spin valve (T_c(noncollinear) < T_c^{P}, T_c^{AP}), which is realized for $d_{F1}/\xi_{F1} = 0.73$ and $d_{F2}/\xi_{F2} = 2$, is shown in Fig. 3a. In this regime, singlet component f_0 of the superconducting pairing oscillates. The peak of the distribution of the triplet components f_2 and f_3 is situated near the SF1 contact boundary (Figs. 3b–3d).

Figure 4a shows the inverse regime of the spin valve ($T_c^{P} > T_c^{AP}$), realized for $d_{F1}/\xi_{F1} = 1.1$ and $d_{F2}/\xi_{F2} = 0.3$. In this regime, the distribution of the triplet component with zero f_3 projection has a peak on the outer surface the F2 layer, while the peak of the distribution of long-range triplet component f_2 is situated near the SF1 contact boundary (Fig. 4c). For antiparallel configuration (Fig. 4d), the singlet component f_0 passes

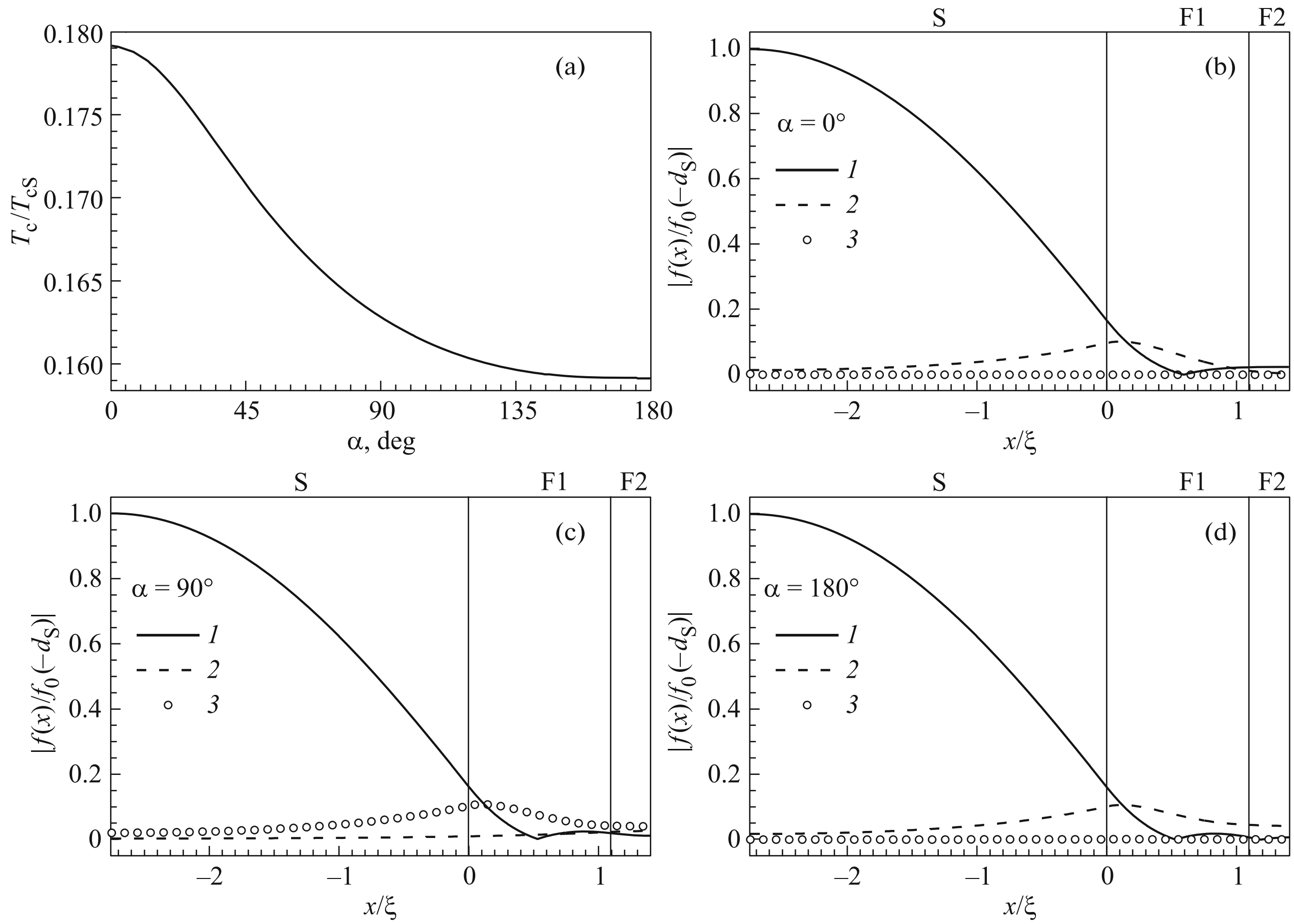

Fig. 4. (a) Superconducting transition temperature T_c as a function of angle α in the inverse regime. The spin singlet $|f_0(x)/f_0(-d_S)|$ (curve *1*) and the spin triplet $|f_3(x)/f_0(-d_S)|$ (curve *2*) and $|f_2(x)/f_0(-d_S)|$ (curve *3*) distributions of the superconducting pairing components in the inverse regime for (b) parallel, (c) orthogonal, and (d) antiparallel orientations of the magnetizations of ferromagnetic layers for $n = 2$.

through zero twice, which is not observed for parallel configuration (Fig. 4b).

The highest superconducting transition temperature T_c in each regime corresponds to the predominance of the singlet component over the triplet components (or they have the same order of magnitude) in the F2 layer accounts for. Conversely, the transition temperature has its minimum value when a triplet component dominates over the singlet component.

4. CONCLUSIONS

We have presented in this work the self-consistent calculations for the superconducting transition temperature of a finite-thickness spin valve SF1F2. Distributions of the spin-singlet and spin-triplet components of superconducting pairing over the heterostructure layers for direct, triplet, and inverse switching regimes have been obtained. The distribution of the spin-triplet component of pairing with a spin projection one, that carries the magnetic moment, is especially interesting, because this superconducting pairing component can be detected by using the technique of spin-polarized neutrons reflectometry (for example, in [7]). Since this technique is layer sensitive, it is important that we must know the layer or layers in which one should expect the peak of the triplet component of superconducting pairing with a spin projection one for a correct planning and interpretation of experimental data (for heterostructures with superconducting layers [8, 9]). This can considerably increase the reliability of the conclusions drawn from the results of reflectometry of spin-polarized neutrons.

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