

Critical temperature and interface transparency of N/S/N triple layers: theory and experiment

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Abstract. The influence of the finite transparency, \mathcal{T} , of superconductor/normal metal (S/N) interface on the critical temperature of proximity coupled layered structures is investigated in the dirty limit on the basis of the microscopic equations solved exactly by a matrix method. The calculated theoretical curves satisfactorily reproduce the experimental dependencies of the critical temperature on the thickness of the superconducting layers in N/S/N trilayers. The relation between the transparency coefficient and the normal metal coherence length is also discussed.

PACS. 74.45.+c Proximity effects; Andreev effect; SN and SNS junctions – 74.78.Fk Multilayers, superlattices, heterostructures

Introduction

In recent years the interest in superconducting layered structures has grown up because of their possible applications in nanoelectronics and spintronics. In particular, in the last case one should deal with artificially fabricated layered ferromagnet/superconductor (F/S) systems (for a review see Ref. [1]) and in many applications of these structures a high transparency \mathcal{T} of the F/S interface is necessary. For this reason many papers were recently devoted to the study of the interface transparency both in normal metal/superconductor (N/S) and F/S hybrids [2–8].

The mechanism responsible for the existence of the superconducting state in these systems is the proximity effect [9–12], i.e. the diffusive penetration of the Cooper pairs into the normal metal. The basis of the theory of N/S structures were developed by de Gennes and Werthamer (dGW) in the framework of the microscopic BCS theory [11, 13]. The behavior of the order parameter inside S and N layers and the dependence of the critical temperature T_c on the geometrical and material parameters of N/S and N/S/N structures have been calculated in the dirty limit of this theory [14]. The dGW theory was generalized by Takahashi and Tachiki (TT) to calculate the upper critical fields H_{c2} of multilayers [15], theory which was then developed in [16–22]. In all the above mentioned papers

calculations have been performed assuming a total transparency of the N/S interface. In this case the $T_c(d_S)$ (d_S is the S-layer thickness), $H_{c2||}(T)$ and $H_{c2\perp}(T)$ dependencies could be satisfactorily fitted but only if considered separately. However, in [21] it was shown that, to determine all the thermodynamic characteristics in a self consistent way, the processes of quantum scattering of the electrons due to potential barriers at the N/S interfaces (related, for example, to different values of the Fermi velocities in S and N metals [5]) must be taken into account. These processes determine the appearance of a finite transparency coefficient. As it was shown in reference [6], when considering the finite transparency of the N/S boundary in the framework of the TT formalism, a satisfactory description of the thermodynamic characteristics of infinite N/S structures can be obtained. Using the same approach a more general model for the T_c determination in bilayers, consisting of two different superconductors with no restriction on the film thickness and on the resistivity of the interface between two metals, was derived in [23].

In [7, 8] we performed detailed experimental studies of the interface transparency in Cu/Nb/Cu and Pd/Nb/Pd trilayers. The interpretation of the experimental data was done on the basis of the formulas obtained as a limiting case of the one mode approximation of the microscopic theory [24]. In this work we analyze the $T_c(d_S)$ dependence in S/N structures as a function of the sample parameters using the multimode solution of the microscopic equations written as a system of linear ordinary differential

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equations, as proposed in [20]. In this way we have interpreted the experimental data for Cu/Nb/Cu and Pd/Nb/Pd trilayers of references [7] and [8] and we have compared the results with the ones obtained using the Werthamer's one mode approximation. A good agreement between the theory and the data was achieved using reasonable values for the sample parameters. Moreover, the functional relation between \mathcal{T} and the normal metal coherence length was obtained.

Basic equations

We chose the coordinate system with the OZ axis directed perpendicular to the surface of a layered structure. The coordinates $z = 0$ and $z = L$ correspond to the left and to the right boundaries of the sample respectively. The order parameter, which describes the critical state of the superconducting condensate in the N/S structure in absence of the external magnetic field, is determined by the linearised integral Gorkov self-consistent condition [25] in the form [11]

$$\Delta(z) = k_B T \cdot V(z) \sum_{\omega} \int dz' Q_{\omega}(z, z') \Delta(z'). \quad (1)$$

The functions $Q_{\omega}(z, z')$, which determine the kernel of the integral equation (1), in the dirty limit satisfy the differential equation

$$\left(2|\omega| - D(z) \frac{d^2}{dz^2} \right) Q_{\omega}(z, z') = \frac{2\pi}{\hbar} N(z) \delta(z - z'). \quad (2)$$

Here the Matsubara frequency ω is defined by $\hbar\omega = \pi k_B T (2m + 1)$ ($m = 0, \pm 1, \pm 2, \dots, \pm m_D$) with the frequency cutoff $|\omega| \leq \omega_D$, where ω_D is the Debye frequency,

$$m_D \equiv \left[\frac{\omega_D}{2\pi k_B T_S} - \frac{1}{2} \right]$$

(square brackets here denote the integer part), and T_S is the critical temperature of bulk sample.

$$D(z) = \begin{cases} D_s, & z \in I_s \\ D_n, & z \in I_n \end{cases},$$

I_s and I_n are the regions of z values which correspond to the S and N layers respectively; D_s, D_n are the diffusion constants of S and N layers respectively. Functions $N(z)$ and $V(z)$ are determined analogously (via the density of states at the Fermi level, N_s and N_n , and via the electron-phonon interaction constants, V_s and V_n).

As it was noticed in [20], the definition

$$\Delta_{\omega}(z) \equiv \int dz' Q_{\omega}(z, z') \Delta(z') \quad (3)$$

reduces the system of integro-differential equations (1, 2) to the homogeneous system of linear ordinary differential

equations

$$\left(2\hbar|\omega| - \hbar D(z) \frac{d^2}{dz^2} \right) \Delta_{\omega}(z) = 2\pi k_B T N(z) V(z) \sum_{\omega'} \Delta_{\omega'}(z), \quad (4)$$

which coincides with the linearised Usadel equations [26].

The order parameter of the superconducting state is then expressed as

$$\Delta(z) = k_B T \cdot V(z) \sum_{\omega} \Delta_{\omega}(z). \quad (5)$$

The boundary conditions at the external surfaces and at the N/S interfaces for the functions $\Delta_{\omega}(z)$ can be written as [27]

$$\frac{d\Delta_{\omega}(0)}{dz} = \frac{d\Delta_{\omega}(L)}{dz} = 0 \quad (6)$$

$$D(z_i + 0) \frac{d\Delta_{\omega}(z_i + 0)}{dz} = D(z_i - 0) \frac{d\Delta_{\omega}(z_i - 0)}{dz} \quad (7.1)$$

$$D(z_i - 0) \frac{d\Delta_{\omega}(z_i - 0)}{dz} = \frac{v_{F,n} t_n N_n}{2} \times \left(\frac{\Delta_{\omega}(z_i + 0)}{N(z_i + 0)} - \frac{\Delta_{\omega}(z_i - 0)}{N(z_i - 0)} \right). \quad (7.2)$$

In equations (6) and (7) z_i is Z-coordinate of the N/S interfaces (index i corresponds to the i th interface, in a trilayered structure $i = 1, 2$), $v_{F,n}$ is Fermi velocity for N metal, t_n is the transparency parameter of the N/S interface. t_n is related to the quantum transparency coefficient \mathcal{T} by the expression: $\mathcal{T} = t_n / (1 + t_n)$.

The exact solutions of the equations system (4) are easy to construct by joining the exact solutions for each layer via the interface conditions (7). Then we build the matrizant $\hat{\mathbf{R}}(z)$ of (4) [28], and get by (6) the system of linear algebraic equations which connects vectors $\Delta(z) \equiv (\Delta_0(z), \Delta_1(z), \dots, \Delta_{m_D}(z), \Delta'_0(z), \Delta'_1(z), \dots, \Delta'_{m_D}(z))^T$ at the edges of the structure:

$$\begin{pmatrix} \Delta(L) \\ \mathbf{0} \end{pmatrix} = \hat{\mathbf{R}}(L) \begin{pmatrix} \Delta(0) \\ \mathbf{0} \end{pmatrix}. \quad (8)$$

The expression for the matrix $\hat{\mathbf{R}}(L)$ via the matrizants $\hat{\mathbf{S}}(z)$ and $\hat{\mathbf{M}}(z)$, which correspond to S and N layers respectively and via matrices $\hat{\mathbf{P}}_{ns}, \hat{\mathbf{P}}_{sn}$ of joining conditions (7) is

$$\hat{\mathbf{R}}(L) = \hat{\mathbf{M}}(d_n) \left[\hat{\mathbf{P}}_{ns} \hat{\mathbf{S}}(d_s) \hat{\mathbf{P}}_{sn} \hat{\mathbf{M}}(d_n) \right]^{Nbl}. \quad (9)$$

In equation (9) Nbl is the number of bilayers and d_n is the thickness of N layer. It is known the expression for matrix $\hat{\mathbf{M}}(d_n)$ [28]:

$$\hat{\mathbf{M}}(d_n) = \begin{pmatrix} \text{diag} \left[ch \left(\frac{d_n}{\xi_n^{(m)}} \right) \right] & \text{diag} \left[\xi_n^{(m)} sh \left(\frac{d_n}{\xi_n^{(m)}} \right) \right] \\ \text{diag} \left[\frac{1}{\xi_n^{(m)}} sh \left(\frac{d_n}{\xi_n^{(m)}} \right) \right] & \text{diag} \left[ch \left(\frac{d_n}{\xi_n^{(m)}} \right) \right] \end{pmatrix}, \quad (10)$$

$$\hat{\mathbf{S}}(d_s) = \begin{pmatrix} \hat{\mathbf{C}} \text{diag} \left[ch \left(\frac{d_s}{\xi_S^{(m)}} \right) \right] \hat{\mathbf{C}}^T & \hat{\mathbf{C}} \text{diag} \left[\xi_S^{(m)} sh \left(\frac{d_s}{\xi_S^{(m)}} \right) \right] \hat{\mathbf{C}}^T \\ \hat{\mathbf{C}} \text{diag} \left[\frac{1}{\xi_S^{(m)}} sh \left(\frac{d_s}{\xi_S^{(m)}} \right) \right] \hat{\mathbf{C}}^T & \hat{\mathbf{C}} \text{diag} \left[ch \left(\frac{d_s}{\xi_S^{(m)}} \right) \right] \hat{\mathbf{C}}^T \end{pmatrix} \quad (11)$$

and it is easy to obtain the following expression for the matrix $\hat{\mathbf{S}}(d_s)$:

See equation (11) above.

In equations (10) and (11) the following definitions are used:

$$\xi_n^{(m)} = \xi_n^{(m)}(T) = \xi_n \sqrt{\frac{T_S}{(2m+1)T}}, \quad \xi_n = \sqrt{\frac{\hbar D_n}{2\pi k_B T_S}}, \quad (12.n)$$

$$\xi_S^{(m)} = \xi_S^{(m)}(T) = \xi_S \sqrt{-\frac{T_S}{2T\mu^{(m)}(T)}}, \quad \xi_S = \sqrt{\frac{\hbar D_S}{2\pi k_B T_S}}. \quad (12.s)$$

Here the temperature functions $\mu^{(m)}(T)$ represent the roots of the characteristic equation

$$\psi \left(\frac{\omega_D}{2\pi k_B T} + 1 + \mu^{(m)}(T) \right) - \psi \left(\frac{1}{2} + \mu^{(m)}(T) \right) = \psi \left(\frac{\omega_D}{2\pi k_B T_S} + 1 \right) - \psi \left(\frac{1}{2} \right), \quad (13)$$

where $\psi(x)$ is the real part of digamma function. Matrices $\hat{\mathbf{C}}$ in equation (11) are determined by the expressions

$$C_j^{(m)} = \frac{s^{(m)}}{j + \frac{1}{2} + \mu^{(m)}(T)}, \quad s^{(m)} = \left[\sum_{j=0}^{mD} \left(j + \frac{1}{2} + \mu^{(m)}(T) \right)^{-2} \right]^{-1/2} \quad (14)$$

and are orthogonal: $\hat{\mathbf{C}}^T \hat{\mathbf{C}} = \hat{\mathbf{C}} \hat{\mathbf{C}}^T = \hat{\mathbf{1}}$.

The joining matrices are determined by the formulas:

$$\hat{\mathbf{P}}_{sn} = \begin{pmatrix} \hat{\mathbf{1}} & \gamma_b \xi_n \hat{\mathbf{1}} \\ \hat{\mathbf{0}} & p \hat{\mathbf{1}} \end{pmatrix}, \quad \hat{\mathbf{P}}_{ns} = \begin{pmatrix} \hat{\mathbf{1}} & \gamma_b \xi_n p^{-1} \hat{\mathbf{1}} \\ \hat{\mathbf{0}} & p^{-1} \hat{\mathbf{1}} \end{pmatrix}. \quad (15)$$

In equation (15) the following parameters are used:

$$p = \frac{\rho_S}{\rho_n}, \quad \gamma_b = \frac{l_n}{3\xi_n t_n}, \quad (16)$$

where ρ_S and ρ_n are the resistivities of superconducting and normal materials respectively, l_n is the electron mean free path in normal metal.

For N/S/N 3-layers, considered in this article, equation (8) reduces to:

$$\left[\hat{\mathbf{S}}_t(d_S/2) + p \hat{\mathbf{M}}_t(d_n) \hat{\mathbf{M}}_b^{-1}(d_n) \right] \times \hat{\mathbf{M}}_b(d_n) \hat{\mathbf{M}}_{I,I}(d_n) \mathbf{\Delta}(0) = \mathbf{0} \quad (17)$$

where:

$$\hat{\mathbf{M}}_b = \hat{\mathbf{1}} + \gamma_b \xi_n \hat{\mathbf{M}}_t, \quad \hat{\mathbf{S}}_t = \hat{\mathbf{S}}_{I,I}^{-1} \hat{\mathbf{S}}_{II,I}, \quad \hat{\mathbf{M}}_t = \hat{\mathbf{M}}_{I,I}^{-1} \hat{\mathbf{M}}_{II,I}. \quad (18)$$

In equations (18) matrices with the Roman indexes mean the corresponding square blocks of the same matrices. During the deduction of the equation (17) we used the fact that the symmetrical solution of the system (8) corresponds to the critical temperature, so that $\mathbf{\Delta}(L) = \mathbf{\Delta}(0)$. So, the critical temperature corresponds to the zero (at the same time to the minimum) eigenvalue of the matrix

$$\hat{\mathbf{R}}_{L/2} \equiv \hat{\mathbf{S}}_t(d_S/2) + p \frac{\hat{\mathbf{M}}_t(d_n)}{\hat{\mathbf{1}} + \gamma_b \xi_n \hat{\mathbf{M}}_t(d_n)}. \quad (19)$$

It is worth to note that equations (13) and (17) in the one mode approximation are reduced to the well known form

$$\psi \left(\frac{1}{2} + \mu(T) \right) - \psi \left(\frac{1}{2} \right) = \ln \left(\frac{T_S}{T} \right) \quad (20)$$

$$tg \left(\frac{d_S}{2\xi_S} \cdot \sqrt{\frac{2T\mu(T)}{T_S}} \right) = \frac{1}{\sqrt{2\mu(T)}} \frac{\gamma \cdot th \left(\frac{d_n}{\xi_n} \sqrt{\frac{T}{T_S}} \right)}{1 + \gamma_b \sqrt{\frac{T}{T_S}} th \left(\frac{d_n}{\xi_n} \sqrt{\frac{T}{T_S}} \right)} \quad (21)$$

where $\mu(T) \equiv \mu^{(0)}(T)$ is the largest root of equation (13), and

$$\gamma \equiv p \frac{\xi_S}{\xi_n} = \frac{\rho_S \xi_S}{\rho_n \xi_n} = \frac{N_n D_n \xi_S}{N_s D_s \xi_n}. \quad (22)$$

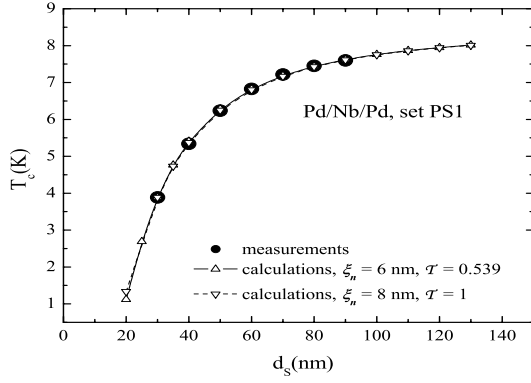
According to [24], the one-mode approximation will be self-consistent at low transparency of N/S interface, which for thick N layer means $\gamma_b \gg \sqrt{T_S/T}$. In this case instead of equation (21) we get

$$tg \left(\frac{d_S}{2\xi_S} \cdot \sqrt{\frac{2T\mu(T)}{T_S}} \right) \approx \frac{\gamma}{\gamma_b} \sqrt{\frac{T_S}{2T\mu(T)}}. \quad (23)$$

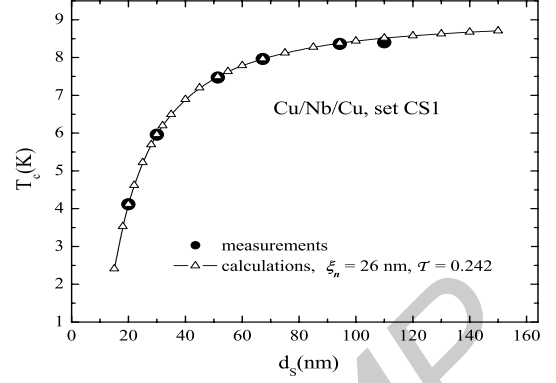
The last equation was used in [7, 8] for describing the experimental data.

Transparency coefficient and critical temperature of Pd/Nb/Pd and Cu/Nb/Cu 3-layers

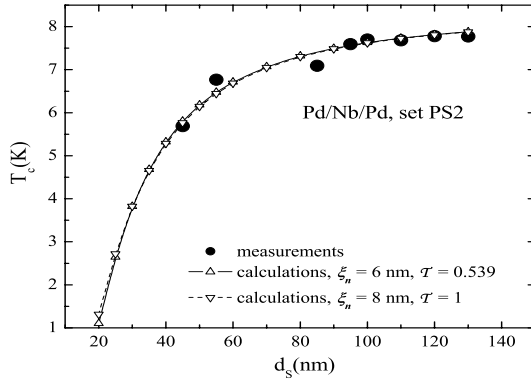
By solving the exact equations (13) and (17) it was possible to reproduce the experimental $T_c(d_S)$ dependencies for two sets of Pd/Nb/Pd samples [8] (sets PS1 and PS2) obtained by dc sputtering and for two sets (CS1 and CS2) of Cu/Nb/Cu samples, obtained by MBE. Data for CS2 were already published in [7]. The estimated values of the



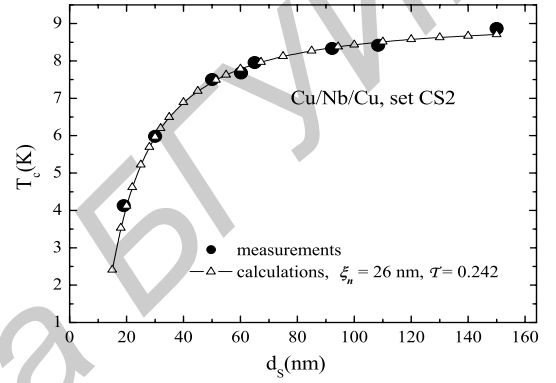
(a)



(a)



(b)



(b)

Fig. 1. (a) Critical temperature, T_c , versus Nb thickness, d_s , in Pd/Nb/Pd trilayers with constant Pd thickness, $d_n = 150$ nm (set PS1). The theoretical calculations refer to two different pairs of ξ_n and \mathcal{T} values (for details see text). (b) Critical temperature, T_c , versus Nb thickness, d_s , in Pd/Nb/Pd trilayers with constant Pd thickness, $d_n = 150$ nm (set PS2). The theoretical calculations refer to two different pairs of ξ_n and \mathcal{T} values (for details see text).

Fig. 2. (a) Critical temperature, T_c , versus Nb thickness, d_s , in Cu/Nb/Cu trilayers with constant Cu thickness, $d_n = 150$ nm (set CS1). The theoretical curve is obtained for $\xi_n = 26$ nm and $\mathcal{T} = 0.242$. (b) Critical temperature, T_c , versus Nb thickness, d_s , in Cu/Nb/Cu trilayers with constant Cu thickness, $d_n = 150$ nm (set CS2). The theoretical curve is obtained for the same ξ_n and \mathcal{T} values of (a).

material parameters are almost the same used in [7,8]. The critical temperature T_S of bulk Nb in Pd/Nb/Pd structures was chosen to be $T_S = 8.44$ K for PS1 and $T_S = 8.3$ K for PS2. For Cu/Nb/Cu structures we choose $T_S = 9.0$ K. These T_S values correspond to the critical temperatures of our thick Nb films. In all cases the superconducting coherence length was $\xi_S = \xi_{Nb} = 6.4$ nm. The Nb resistivity in Cu/Nb/Cu trilayers was measured as $\rho_{Nb,MBE} = 3.6 \mu\Omega\text{cm}$, while for Pd/Nb/Pd we used the value $\rho_{Nb,sputt} = 5.0 \mu\Omega\text{cm}$, typical for Nb sputtered films. In references [7] and [8] the ξ_n values (26 nm for Cu and 6 nm for Pd) were obtained from the empirical condition of the decay of the superconducting wave function in the normal layer of the Nb/Cu(Pd)/Nb structures [7, 8,29]. Since this method presents some degree of uncertainty, here the fitting procedure was performed for different values of ξ_n . The normal metal resistivity values were $\rho_{Cu} = 1.3 \mu\Omega\text{cm}$ and $\rho_{Pd} = 5.0 \mu\Omega\text{cm}$, resulting in an estimated electron mean free paths of $l_{n,Cu} = 10$ nm and $l_{n,Pd} = 6$ nm, respectively. Finally, the transparency parameter t_n was obtained as a fitting parameter.

The fitting procedure was organized as follows. We fixed a value for ξ_n and then the parameter t_n was obtained by imposing the equality between the theoretical and the experimental value of T_c at a certain d_s . We choose the point $T_c(d_s = 30$ nm) for the Pd/Nb/Pd structure, set PS1, and the point $T_c(d_s = 20$ nm) for the Cu/Nb/Cu structure, set CS1. Then the whole $T_c(d_s)$ curve was reconstructed. The pair (ξ_n, t_n) obtained for set PS1 was then used to fit the experimental data of set PS2. The results for both sets of Pd/Nb/Pd samples are shown in Figures 1a and 1b. The results for both sets of Cu/Nb/Cu are shown in Figures 2a and 2b. From Figures 1 and 2 follows that the theoretical curves reproduce with high accuracy the experimental $T_c(d_s)$ dependencies. The standard deviation between the theoretical and experimental data is 0.03 K for the series PS1 while it is 0.17 K for the series PS2. Analogous results were obtained for the sets CS1 and CS2. Moreover it is worth to notice that the theoretical curves $T_c(d_s)$ plotted for different $(\xi_n, \mathcal{T}(\xi_n))$ pairs overlap and, as it can be seen in Figures 1a and 1b, they are practically undistinguishable. In Figures 1a and 1b one curve corresponds to $\xi_n = 6$ nm,

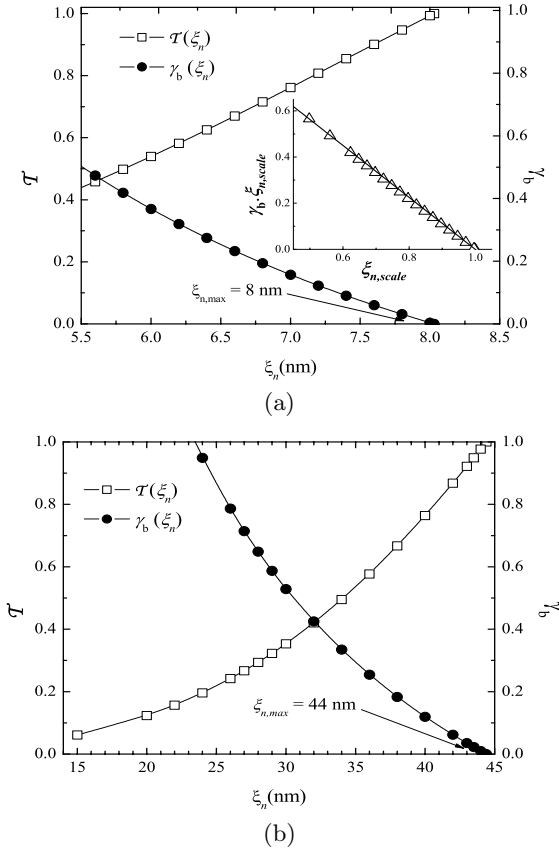


Fig. 3. (a) The calculated dependencies of \mathcal{T} and γ_b on the normal coherence length, ξ_n , for Pd/Nb/Pd samples. Inset: the dependencies $\gamma_b \xi_{n,\text{scale}}$ versus $\xi_{n,\text{scale}}$ obtained according to the exact solution, equations (13) and (17) (triangles), and to equation (24) (line). (b) The calculated dependencies of \mathcal{T} and γ_b on the normal coherence length, ξ_n , for Cu/Nb/Cu samples.

the value which was used in [8], and to a value of the interface transparency $\mathcal{T} = 0.539$, while the other corresponds to $\xi_n = 8$ nm and to a fully transparent S/N boundary. The same is valid for Cu/Nb/Cu samples. For this reason in Figures 2a and 2b only the theoretical curve corresponding to $\xi_n = 26$ nm, the value used in [7], is reported. In this case $\mathcal{T} = 0.242$, a smaller value compared to the one obtained in [20]. For $\xi_n = 30$ nm we obtained instead $\mathcal{T} = 0.353$. The functional relation between ξ_n and \mathcal{T} is plotted in Figures 3a and 3b for Pd/Nb/Pd and Cu/Nb/Cu systems, respectively. In the same figures we also show the dependence $\gamma_b(\xi_n)$. This dependence can be empirically expressed as:

$$\gamma_b(\xi_n) = \alpha \cdot \left(\frac{\xi_{n,\text{max}}}{\xi_n} - 1 \right) \quad (24)$$

where α is a coefficient and $\xi_{n,\text{max}}$ is the upper limit of the ξ_n values for which the solution of equations (13) and (17) exists. $\xi_{n,\text{max}}$ also corresponds to condition of a fully transparent interface, since when $\xi_n \rightarrow \xi_{n,\text{max}}$, then $\gamma_b \rightarrow 0$ resulting in $t_n \rightarrow \infty$ and $\mathcal{T} \rightarrow 1$. For the Pd/Nb/Pd structure we obtained $\alpha = 1.125$ and $\xi_{n,\text{max}} = 8$ nm; for

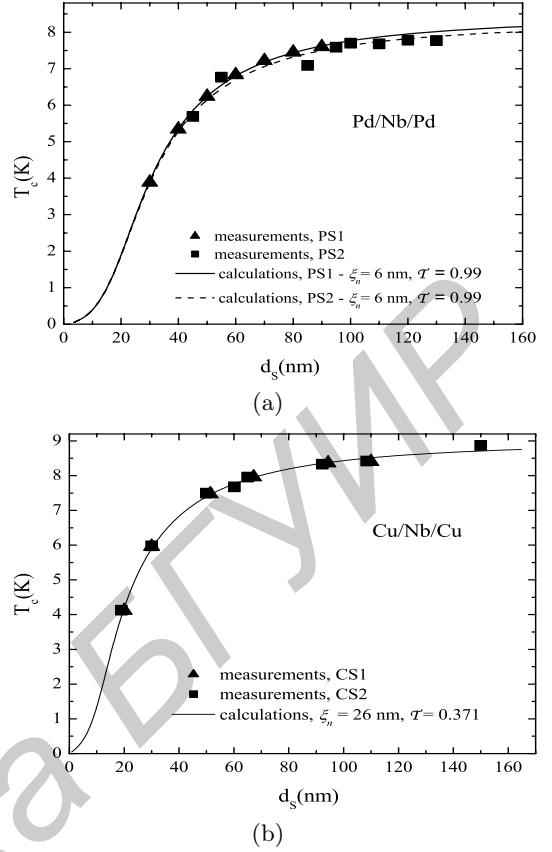


Fig. 4. (a) $T_c(d_S)$ dependencies of Pd/Nb/Pd trilayers. Different symbols refer to the different samples sets. Solid (dashed) line is the result of the theoretical calculation in the one mode approximation for set PS1 (PS2). (b) $T_c(d_S)$ dependencies in Cu/Nb/Cu trilayers. Different symbols refer to the different samples sets. The solid line is the result of the theoretical calculation in the one mode approximation.

the Cu/Nb/Cu structure $\alpha = 1.115$ and $\xi_{n,\text{max}} = 44$ nm. In the inset of Figure 3a we show the $\gamma_b \cdot \xi_{n,\text{scale}}$ versus $\xi_{n,\text{scale}}$ dependence, where $\xi_{n,\text{scale}} \equiv \xi_n / \xi_{n,\text{max}}$, obtained both from the solution of the exact equations (13) and (17) and from the empirical equation (24). The perfect agreement of the data obtained by the two methods proves the validity of equation (24).

Finally we compare the exact results with the ones obtained in the one mode approximation using the values of T_S and ρ_{Nb} reported here. Also in this case the theoretical curves satisfactorily describe the experimental results as presented in Figures 4a and 4b, but the obtained transparency coefficients are larger. For example, for the set PS1 the precise calculation gives $\mathcal{T} = 0.539$ for $\xi_n = 6$ nm, while from the one mode approximation the best fit to the data for the same ξ_n is obtained for $\mathcal{T} = 0.99$, an unrealistic value for the transparency of a real system [5].

Conclusions

The application of the microscopic equations, solved exactly by the matrix method, allows us to analyze the transparency of Pd/Nb/Pd and Cu/Nb/Cu systems. It was

shown that there is a set of ξ_n and $\mathcal{T}(\xi_n)$ values which gives identical results for the $T_c(d_S)$ dependencies. The functional relation between the values of ξ_n and $\mathcal{T}(\xi_n)$ has been established. The method could also be applied to the multilayered N/S structures with an arbitrary number of bilayers.

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