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Calculation of T_C in a normal-superconductor bilayer using the microscopic-based Usadel theory☆

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Abstract

The Usadel equations give a theory of superconductivity, valid in the diffusive limit, that is a generalization of the microscopic equations of the BCS theory. Because the theory is expressed in a tractable and physical form, even experimentalists can analytically and numerically calculate detailed properties of superconductors in physically relevant geometries. Here, we describe the Usadel equations and review their solution in the case of predicting the transition temperature T_C of a thin normal-superconductor bilayer. We also extend this calculation for thicker bilayers to show the dependence on the resistivity of the films. These results, which show a dependence on both the interface resistance and heat capacity of the films, provide important guidance on fabricating bilayers with reproducible transition temperatures. Published by Elsevier Science B.V.

Microcalorimeters and microbolometers based on transition-edge sensors (TES) [1] show great potential for improving the detection of X-ray, optical, and infrared photons in scientific and commercial instruments [2]. Presently, TES microcalorimeters have the best X-ray energy resolutions, achieving a resolution of 2 eV at 1.5 keV [3] and 4.5 eV at 6 keV [4].

When designing detectors based on transition-edge sensors, it is important to be able to reproducibly control and adjust the transition temperature T_C. Bilayers are practical choices for the TES because the T_C can be simply adjusted by changing the relative thickness of the normal and superconducting layers. Because the TES should have low resistance so that heat diffuses rapidly throughout the sensor [5], the bilayer is also an ideal sensor because it enables the use of high-conductivity normal metals such as Cu, Ag, or Au.

Although the T_C can be parametrized for bilayers by making a series of samples with differing thickness, it is very useful to be able to predict T_C from more fundamental physical parameters. It is also convenient to predict T_C even for relatively large thickness changes. Predictions based on simple physical parameters guide the experimentalist as to what physical parameters need to be controlled in order to make sensors reproducibly. Several previous papers have presented theories on predicting the T_C for bilayers [6]. We believe the predictions given in this paper based on the Usadel equations [7] give simpler and more physical predictions for T_C and also more clearly indicate the crucial importance of the interface resistance between the two bilayer films.

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The Usadel theory is based on the assumption that electrons travel diffusively through the metal. This is an excellent assumption for most thin-film superconductors because electrons either have short mean-free paths in the metals or scatter diffusively from the boundaries.

We refer the reader to Ref. [8,9] for a derivation of the Usadel equations as well as a more detailed description of its physical significance. Because the Usadel theory is a microscopic theory, the states of the electrons must be described. In the BCS theory, which assumes no impurity scattering, k-vectors can be used to describe the superconducting state. For a diffusive conductor, k-vectors are no longer eigenstates, and thus the electron states must be described through an energy variable E.

The superconducting state is described by a function $\theta(x,E)$, where x is a position coordinate (we consider here only one dimension for simplicity). The variable θ is complex and ranges in magnitude from 0 to $\pi/2$, where $\theta=0$ corresponds to the normal state.

The Usadel equations used to solve for $\theta(x,E)$ are

$$\frac{\hbar D_s}{2}\frac{\partial^2\theta}{\partial x^2}+iE\sin\theta - \left[\frac{\hbar}{\tau_{sf}}+\frac{\hbar D_s}{2}\left(\frac{\partial\varphi}{\partial x}+\frac{2e}{\hbar}A_x\right)^2\right]\cos\theta\sin\theta + \Delta(x)\cos\theta=0 \quad (1)$$

and

$$\Delta(x)=n_s V_{eff}\int_0^{\hbar\omega_D} dE\,\tanh(E/2k_BT)\,\mathrm{Im}[\sin\theta] \quad (2)$$

where $D_s=\sigma_s/n_s e^2$ is the diffusivity constant, n_s is the density of states, σ_s is the normal state conductivity, V_{eff} is the BCS-like interaction potential, τ_{sf} is the spin-flip time, φ is the usual superconducting phase, A_x is the vector potential, Δ is the superconducting order parameter, $\hbar\omega_D$ is the Debye energy, and T is the temperature. Because the superconducting state is formed from a pairing of two electron states, the pairing is described by a spinor term which has only three possible components. These components correspond in Eq. (1) to an excitation-energy term iE which tends to make $\theta=0$ (normal state), a term which describes pair breaking through spin-flip scattering, current, or magnetic fields, and a superconducting pairing term. At an interface, conservation of spectral current requires that

$$\sigma_l\frac{\partial\theta_l}{\partial x}=\sigma_r\frac{\partial\theta_r}{\partial x}=\frac{G_{int}}{A}\sin(\theta_l-\theta_r) \quad (3)$$

where r and l index the right and left side of the interface, and G_{int}/A is the electrical conductance of the interface per unit area.

Physical quantitites can be computed once $\theta(x,E)$ is known. For example, the quasiparticle density of states is given by $n_{qp}=n_s\,\mathrm{Re}[\cos\theta]$. The supercurrent density is given by

$$j_s=(\sigma_s/e)[\partial\varphi/\partial x+(2e/\hbar)A_x]\times\int_{-\infty}^{+\infty}dE\,\tanh(E/2k_BT)\,\mathrm{Im}[\sin^2\theta].$$

An interesting limit of the Usadel equations is the case of a uniform superconductor, where there is no spatial dependence and no pair breaking from magnetic impurities, fields, or currents. The first and third terms of Eq. (1) are then zero, and θ is easily solved to be $\theta_{BCS}(E)=\arctan(i\Delta/E)$, or equivalently $\cos\theta_{BCS}=|E|/(E^2-\Delta^2)^{1/2}$ and $\sin\theta_{BCS}=\Delta/(\Delta^2-E^2)^{1/2}$. Substituting θ_{BCS} into Eq. (2), the usual BCS form for the pair potential is obtained.

The transition temperature of a superconductor can be calculated [8] by first noting that just above T_C, superconductivity is very weak and $\theta\ll1$. If pair breaking is neglected, Eq. (1) can be linearized to yield

$$\frac{\hbar D_s}{2}\frac{\partial^2\theta}{\partial x^2}+iE\theta+\Delta=0. \quad (4)$$

This equation can be solved analytically if one considers a bilayer film that is thin enough so θ is approximately constant across the film, and small changes in θ can be accounted for by a polynomial expansion (see Fig. 1). If derivatives of order higher than two can be neglected, a parabolic form of θ need only be considered in the normal and superconductor region. In the superconducting region Δ is taken to be constant, and Eq. (4) yields a constant second derivative $\theta_s''=-(iE\theta_s+\Delta)(2/\hbar D_s)$

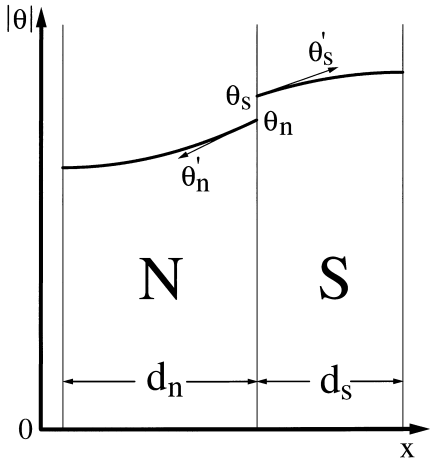

Fig. 1. Plot of the magnitude of θ versus x for a NS bilayer.

and $\theta_n'' = -(iE\theta_n)(2/\hbar D_n)$, where θ_s and θ_n are the values of θ at the interface. Because the conductivity is zero outside the bilayer, Eq. (3) implies $\partial\theta/\partial x = 0$ at the outside interfaces of both metals. Combining the outside boundary conditions with θ'', we find at the interface $\theta_s' = \partial\theta_s/\partial x = -d_s\theta_s''$ and $\theta_n' = \partial\theta_n/\partial x = d_n\theta_n''$, where d_n and d_s are the thickness of the normal and superconducting films. At the bilayer interface, the two constraints of Eq. (3) then allow θ_s to be determined as

$$\theta_s = \frac{i\Delta}{E}\left[1 - \frac{d_n n_n}{d_n n_n + d_s n_s}\frac{1}{1 - iE/\tau}\right] \tag{5}$$

where n_n and n_s are the density of electronic states in the normal and superconducting films and $\tau = [(G_{int}/A)/(4\pi G_K)][1/d_n n_n + 1/d_s n_s]$, where $G_K = e^2/h$ is the conductance quantum.

Taking the imaginary part of θ_s and inserting into the gap (2) yields

$$\frac{1}{n_s V_{eff}} = \int_0^{\hbar\omega_D} \frac{dE}{E}\left[1 - \frac{d_n n_n}{d_n n_n + d_s n_s}\frac{1}{1 + E^2/\tau^2}\right] \times \tanh\frac{E}{2k_B T_C}. \tag{6}$$

The first term in the bracket gives the integral that appears in the BCS gap equation that determines T_{C0}, the transition temperature of the bare superconductor. Eq. (6) can thus be rewritten as a suppression of the T_C due to the normal metal

$$\ln\frac{T_C}{T_{C0}} = -\int_0^{\hbar\omega_D} \frac{dE}{E}\left[\frac{d_n n_n}{d_n n_n + d_s n_s}\frac{1}{1 + E^2/\tau^2}\right] \times \tanh\frac{E}{2k_B T_C}. \tag{7}$$

This integral result can be well approximated by the expression

$$\frac{T_C}{T_{C0}} = \left[\left(\frac{k_B T_{C0}}{1.13\hbar\omega_D}\right)^2 + \left(\frac{k_B T_{C0}}{1.13\tau}\right)^2\right]^{d_n n_n/2d_s n_s} \tag{8}$$

as long as the pre-exponential (quantity in brackets) is less than approximately 0.8. For most bilayers the films are thick enough so that in Eq. (8) the first term in the bracket can be neglected.

It is more convenient and physical to express the interface conductivity in terms of a transmission coefficient t of the Landauer conductance formula $G_{int} = 2tN_{ch}G_K$, where $N_{ch} = A/(\lambda_f/2)^2$ is the number of conductance channels, and λ_f is the Fermi wavelength. Although t is considered an adjustable parameter that depends on the details of the interface layer, in practice for most clean metals and interfaces it will have a value of order one.

In summary, the transition temperature can be written as

$$T_C = T_{C0}\left[\frac{d_s}{d_0}\frac{1}{1.13(1 + 1/\alpha)}\frac{1}{t}\right]^{\alpha}$$

$$1/d_0 = (\pi/2)k_B T_{C0}\lambda_f^2 n_s$$

$$\alpha = d_n n_n/d_s n_s. \tag{9}$$

For a MoCu bilayer, presently our preferred TES material [4], we calculate $d_0 = 1.18\,\mu m$ and $n_n/n_s = 0.431$, where we have used $n_n = 0.125\times10^{23}$ states/eVcm^3, $n_s = 0.29\times10^{23}$ states/eVcm^3, $T_{C0} = 1.01$ K, and $\lambda_f = 0.462$ nm. The nominal value of λ_f for Cu is used since Cu is better described as a Fermi metal. We find that our experimental data is well described by this formula with a transmission factor $t = 0.21$. We also note

that d_0 is approximately equal to the coherence length.

The above calculation is valid in the limit of thin bilayers where θ does not vary greatly across the film. We have also calculated T_C for thick films. In the case where only the normal film is thick, the differential equation of Eq. (4) can be solved exactly, giving the form $\theta_n(x) = \theta_0 \cosh(kx)$, where $k^2 = -2iE/\hbar D_n$. This result changes the relationship between θ_n and θ'_n at the internal interface. Modifying our previous calculation with this new θ_n relationship and expanding to lowest order in d_n, we find a similar formula for T_C as that given in Eq. (9) but with the replacement

$$\frac{1}{t} \rightarrow \frac{1}{t} + \frac{1}{3}\frac{d_n}{\sigma_n}\frac{2G_K}{(\lambda_f/2)^2}. \quad (10)$$

This formula corresponds physically to summing the interface resistance with the resistance of the normal metal over a depth $\frac{1}{3}$ the thickness of the normal film.

We have also numerically solved Eq. (4) for T_C in the case of arbitrary thickness and stacking of metals. For the case of a thick superconducting MoCu bilayer, we find that the numerical solutions to T_C correspond to Eqs. (9) and (10) but with an additional correction in $1/t$ due to the resistance of the Mo film with, again, a depth of $\frac{1}{3}$ the film thickness.

The formula for T_C is dependent on both the ratio of the heat capacity of the two metals (through $d_s n_s$ and $d_n n_n$) as well as the resistance between the two metals. The heat capacity controls how much the pairing interaction $n_s V_{eff}$ is reduced because electrons spend part of their time in the normal metal where there is no pairing interaction ($V_{eff} = 0$). The resistance controls how well the electron states in the superconductor are coupled with the normal metal. All of the interface resistance but only a fraction of the total resistance perpendicular to the film affect the coupling because the electron states are distributed throughout the films.

A useful formula for the T_C of MoCu bilayers that takes the film resistance into account uses Eq. (9) with the substitution

$$\frac{1}{t} \rightarrow \frac{1}{t} + \frac{1}{3}\left(\frac{d_s}{0.0130\ \mu m}\frac{\sigma_{s0}}{\sigma_s} + \frac{d_n}{0.0405\ \mu m}\frac{\sigma_{n0}}{\sigma_n}\right) \quad (11)$$

where $\sigma_{s0} = 1.89 \times 10^5/\Omega\,cm$ and $\sigma_{n0} = 5.88 \times 10^5/\Omega\,cm$ are the nominal room temperature conductivity of the metals.

These calculations have important implications when fabricating TES bilayers since the resistance of the films, perpendicular to the plane of the films, enter into the suppression of T_C. While it is normally straightforward to make the resistivity of bulk films reproducible, the interface conductance is of greater concern due to the possibility of surface contamination. In the fabrication of both our AlAg and MoCu bilayers, we purposely chose to deposit the entire bilayer in a single step under clean conditions in order to improve reproducibility. In contrast, when we attempted to make a MoCu bilayer in two deposition steps (in order to pattern the Mo layer separately from the Cu), even with a light Ar-ion surface clean of the Mo we found that T_C was irreproducible, with corresponding run-to-run transmission-factor variations of 0.05–0.15. We caution that materials which oxidize rapidly, such as Al or Ti, may be particularly sensitive to deposition conditions. We have also found that MoCu is more stable than AlAg with respect to thermal annealing, presumably because Mo and Cu have negligible interdiffusion at the interface.

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