Localized superconductivity at a twin plane

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The modification of the electron spectrum caused by twinning of a metal crystal is discussed. A mechanism for the occurrence of a localized superconductivity at a twin plane is proposed. © *1995 American Institute of Physics.*

In 1981, Khaĭkin and Khlyustikov[1] observed a surface superconductivity at a twin plane in several metal crystals, with transition temperatures above the bulk values. In an effort to describe the superconductivity phenomena in the presence of twin planes, Buzdin and Bulaevskiĭ[2] proposed a modification of the Ginzburg–Landau equations, assuming that the electron–interaction constant increases at the twin boundary. However, it was later shown that this constant would have to increase by a factor of 30 in order to explain the observed increase in transition temperature.[3] On the other hand, it had been suggested in the paper by Khaĭkin and Khlyustikov[1] that surface (Tamm) states might play an important role in the onset of a localized superconductivity. This idea was utilized in Ref. 4, but no microscopic derivation or further development was offered. The temperature dependence of the critical supercooling field indicates that a modification of the electron spectrum in the twins plays an important role.[5] In this letter we wish to show just which change in the electron spectrum associated with twinning leads to the localized superconductivity.

The superconducting transition temperature in an electron system with an interaction constant λ is the maximum temperature at which a nontrivial solution of the linearized integral equation for the order parameter $\Delta(\mathbf{r})$ arises:

$$\Delta(\mathbf{r})=\lambda\int K(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r}')dr'. \tag{1}$$

The kernel here is

$$K(\mathbf{r},\mathbf{r}')=T\sum_{\omega}\sum_{\alpha,\beta}\frac{\psi_\alpha(\mathbf{r})\psi_\beta(\mathbf{r})\psi_\alpha^*(\mathbf{r}')\psi_\beta^*(\mathbf{r}')}{(\xi_\alpha+i\omega)(\xi_\beta-i\omega)}. \tag{2}$$

Here $\psi_\alpha(\mathbf{r})$ is the wave function of an electron in state α with energy ξ_α, reckoned from the Fermi level; the summation is over all states; and $\omega=\pi T(2n+1)$, where n are integers.

If the twin plane coincides with the $x=0$ plane, then a solution which depends on x alone satisfies the equation

$$\Delta(x)-\lambda\int_{-\infty}^{+\infty}K_0(x-x')\Delta(x')dx'=\lambda\int_{-\infty}^{+\infty}K_1(x,x')\Delta(x')dx', \tag{3}$$

where $K_0(x-x')$ is the kernel in the absence of twinning. This kernel is significantly different from zero only at $|x-x'|<\xi_0$, where the right side is the coherence length. In the isotropic model, this length is 0.18 v/T, and the quantity $K_1(x,x')=K(x,x')-K_0(x-x')$ is significantly different from zero at $|x|$, $|x'|<\xi_0$. In contrast, near the transition temperature the order parameter $\Delta(x)$ varies significantly only over large distances, on the order of $\xi(T)=\eta\xi_0(1-T/T_c)^{-1/2}$, where we have $\eta=0.74$ in the isotropic model. Integral equation (3) can thus be transformed into a differential equation:

$$\left(\tau-\eta^2\xi_0^2\frac{d^2}{dx^2}\right)\Delta(x)=\frac{1}{\nu}\Delta(0)\int_{-\infty}^{+\infty}K_1(x,x')dx'. \tag{4}$$

Here $\tau=\ln(T/T_c)\approx(T-T_c)/T_c$, and ν is the density of states at the Fermi surface. For the isotropic model, it is $mp_0/2\pi^2$, where p_0 is the Fermi momentum. We thus find the following result for the transition temperature:

$$\sqrt{\tau}=\frac{1}{2\eta\nu\xi_0}K_1, \quad K_1=\int_{-}^{+}\int_{\infty}^{\infty}K_1(x,x')dxdx'. \tag{5}$$

Let us consider a free-electron model in which the twin surface can be described by a δ-function potential well or barrier in the $x=0$ plane:

$$\hat{H}=-\frac{1}{2m}\nabla^2-\frac{\kappa}{m}\delta(x). \tag{6}$$

For $\kappa>0$, the free states, described by the wave functions $\sqrt{2}\sin p_x x$ and $\sqrt{2}\cos[p_x|x|+\gamma(p_x)]$, where $\gamma=\arctan(\kappa/p_x)$, are joined by a bound state with a wave function $\sqrt{\kappa}\exp(-\kappa|x|)$ and an energy $(p^2-\kappa^2)/2m$, where p is the momentum in the (p_y,p_z) plane.

We can thus find the values of K_1 and the transition temperature:

$$K_1=\frac{m}{(2\pi)^2}\ln\frac{1.14\omega_0}{T}\arctan\frac{\kappa}{p_0}, \quad \sqrt{\tau}=\frac{1}{2.96\xi_0 p_0}\ln\frac{1.14\omega_0}{T}\arctan\kappa p_0, \tag{7}$$

where ω_0 is the Debye frequency, which determines the usual cutoff of the summation over frequency in (2). For $\kappa<0$, i.e., for a potential barrier, we would have $K_1<0$, and the superconductivity at the surface would be suppressed.

Let us plug in some numbers. We set $\xi_0\sim10^{-5}$ cm and $p_0\sim10^8$ cm^{-1}; κ/p_0 could hardly be greater than 0.1; and the logarithm is at best less than 5. The relative increase in the transition temperature is therefore negligible, on the order of 10^{-8}. The reason is that the coordinate-dependent density of states at the Fermi surface increases only negligibly near the twin plane, since the contribution from bound states is cancelled almost entirely by the decrease in the contribution of free states.

We have considered several anisotropic lattice models in the approximation of tightly bound electrons. The results basically reduce to an insignificant renormalization

(on the order of unity) of the quantities in (5) and (8). Even if the Fermi surface passes near singular points, so a logarithmic singularity arises in the 2D density of states of the localized electrons, and even if the Fermi level passes through it (this situation is exceedingly unlikely), then a factor on the order of ln [(the Fermi energy)/T_c]<10 would arise in (7). Our basic parameter is $\kappa=a^{-1}\ln(\epsilon'/\epsilon)$, where a is on the order of the lattice constant, and ϵ and ϵ' are the overlap integrals of the atoms in the interior and near the twin plane, respectively. However, the primary result of our analysis of lattice models is the formation of bound states whose energies are not only smaller than but also greater than those of the free states. There are even energies above the top of the band. This circumstance is the key to an explanation of the mechanism for localized superconductivity.

Let us assume that the top of the filled lower band or the bottom of the empty upper band lies near the Fermi level. If the extreme energy of the bound states of the second band, reckoned from the bottom (the top), which is equal to $\mp\kappa_2^2/2m_2$ (the subscript 2 means the second band, not the conduction band), is greater than the distance between the bottom (the top) and the chemical potential, then bound electrons of the second band lying at the Fermi level also participate in creating the superconducting state. A term with a kernel formed from the wave functions of the bound states of the second band then appears in Eq. (3):

$$K_2(x,x')=\frac{m_2\kappa_2^2}{2\pi}\ln\frac{1.14\omega_0}{T}\exp[-2\kappa_2(|x|+|x'|)]. \tag{8}$$

This expression is also valid for lattice models, since the bound states lie near the bottom or top of the second band, and the anisotropy can be eliminated through a coordinate transformation.

Making use of the degeneracy of kernel (8), we write the order parameter as the sum $\Delta(x)=\Delta_1(x)+\Delta_2\exp(-2\kappa_2|x|)$. Making use of the slow variation of $\Delta_1(x)$ over distances on the order of ξ_0 and $1/\kappa_2$, and also using the condition $1/\kappa\ll\xi_0$, we find

$$\Delta_2=2\frac{\ln(1.14\omega_0/T)}{\ln(T/T_2)}\,,\quad T_2=1.14\omega_0\exp(-1/\lambda\nu_2),$$
$$\left(\tau-\eta^2\xi_0^2\frac{d^2}{dx^2}\right)\Delta_1(x)=\frac{1}{\kappa_2\nu_1}\Delta_2K(x,0). \tag{9}$$

Here we have ignored the surface contribution, which is inconsequential, as was shown above. The quantity T_2 is the transition temperature in the isolated system of bound electrons of the second band. This temperature is determined by the effective density of states of these electrons (which is independent of the position of the Fermi level, provided that the latter is above the bottom or below the top of the 2D band): $\nu_2=m_2\kappa_2/4\pi$. Comparing with the density of states of the conduction band (which is $mp_0/2\pi^2$ in the isotropic case), we find that T_2 is probably smaller than the bulk value of T_c, but it may also be greater, if the effective mass of the electrons of the second band is sufficiently large.

From (9) we finally find

$$\sqrt{\tau}=\sqrt{\ln(T/T_c)}=\frac{\ln^2(1.14\omega_0/T)}{\kappa_2\xi_0\ln(T/T_2)}\,. \tag{10}$$

If the interactions of the electrons of the different bands are not the same, then the quantity λ_{22} appears in the expression for T_2, a coefficient of $\lambda_{12}/\lambda_{22}$ arises on the right side of (10), and λ_{11} remains in the expression for the bulk value of T_c.

The equivalent thickness of the superconducting layer of a twin plane in tin was estimated as a function of the temperature on the basis of Meissner effect in Ref. 1. The minimum value of this thickness at the temperature of the local transition was about $10a$, where a is the lattice constant. This thickness can be identified with $1/\kappa$, which is the effective thickness of the $\Delta_2(x)$ layer. Using $\xi_0\sim 10^3 a$, and $\omega_0/T_c\sim 100$ for tin, we find $\sqrt{\tau}\approx 0.3/\ln(T/T_2)$ from (10). This result agrees with the observed value $\sqrt{\tau}\approx 0.1$ for tin.

The results derived here indicate that the formation of a "2D metal" at a twin plane in a semiconductor crystal is a realistic possibility, if the energy shift of the bound states is greater than the half-width of the band gap. This metallic state might be manifested in a variety of effects, but it would be most prominent in the 2D superconductivity. The transition temperature would then be given by (9).

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