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MECHANISMS OF SUPERCONDUCTIVITY AT SEMICONDUCTOR INTERFACES

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We solve the superconducting gap equation for electrons in a MOS inversion layer at the Si(111)/ SiO_2 interface so as to compare the efficiency of (a) plasmons, (b) electron-hole excitations and (c) phonons in promoting pairing. This last mechanism, enhanced by the proximity of the interface, is dominant in producing measurable T_C's at experimentally accessible electron densities.

I. Introduction and Formulation

In recent years there has been considerable interest in the mechanisms of superconductivity at surfaces and interfaces with a search for elementary excitations which would complement the role of bulk phonons in the pairing of quasiparticles. The Si/SiO_2 interface in metal-oxide-semiconductor (MOS) devices seems particularly attractive to study since (i) a wealth of information [1] confirms that the system is well-controlled and theoretically simply treated in an "effective mass" model [2,3], in contrast to the complexity of metal-semiconductor systems, (ii) the quasi-two-dimensional (2-d) nature of the electron gas produces unusual features including a plasmon mode [4] with a $\omega_p \sim q^{\frac{1}{2}}$ dispersion for small wavevector q, and inter-subband electron-hole excitations (resulting from space quantisation normal to the interface) of the order of, or smaller than, the Debye frequency, and (iii) the electron density can be varied over two orders of magnitude.

We have constructed and solved the superconducting gap equation in weak coupling for the Si(111)/SiO_2 MOS device as a function of electron density. The novel objects of our investigation include in particular the role of intervalley phonons in inducing inversion layer superconductivity, the finite thickness effects and the proximity of the interface. The principal result is that at high densities ($\sim 10^{13}$ electrons/cm^2), intervalley phonon exchange allows for T_C's of order 10mK. Other results follow from the rich variety of many-body effects which play unusual roles as the electron density is varied. For example, the dynamically screened Coulomb interaction can itself induce superconductivity, although this would occur at extremely low densities where other effects, such as surface roughness and impurity scattering would be important. We make simple estimates of (vertex) corrections which tend to revise downward the estimates of T_C.

The superconducting gap equation in weak coupling [5] can be written as

$$\Delta(\omega) = -\int_{-E_F}^{\infty} \frac{d\omega'}{2\omega'} \tanh\left(\frac{\hbar\omega'}{2k_B T_C}\right) \Delta(\omega')\, K(\omega,\omega') , \qquad (1)$$

for the frequency-dependent gap function $\Delta(\omega)$, and with the kernel K given by

$$K(\omega,\omega') = \frac{A}{4\pi^2}\frac{2m^*}{\hbar^2}\int_{|k-k'|}^{|k+k'|} \frac{q\,dq}{kk'\mathrm{Sin}\theta}\left[V^0(q) + \frac{2}{\pi}\int_0^{\infty} d\Omega \frac{\mathrm{Im}V^R(q,\Omega)}{\Omega+|\omega|+|\omega'|}\right] , \qquad (2)$$

where the device area is A, the electrons are assumed to have an isotropic two-dimensional mass m*, and the relationship between $\underset{\sim}{k}$ (a two-dimensional wavevector) and the frequency variable ω is given by $k=|\underset{\sim}{k}|=\{2m^*(\hbar\omega+E_F)/h^2\}^{\frac{1}{2}}$ and $q=|\underset{\sim}{k}'-\underset{\sim}{k}|=(k^2+k'^2-2kk'\mathrm{Cos}\theta)^{\frac{1}{2}}$. Takada [6] has used equations (1-2) in a study of the role of the $q^{\frac{1}{2}}$ plasmon dispersion in the superconductivity of a 2-d system. For us, $V^0(q)$ is the matrix element of the 2-d Fourier transform of the Coulomb interaction $v(q,z,z')$ including the image potential [7], and is calculated using simple effective-mass wavefunctions [1,2]

$$\psi(\vec{r}) = F_n(z)\phi_B(\vec{r})e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}} \equiv \text{(for n=0)} \quad 2\lambda^{3/2} A^{-\frac{1}{2}} ze^{-\lambda z}\phi_B(\vec{r})e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}, \qquad (3)$$

where $\phi_B(\vec{r})$ is a conduction band minimum Bloch function ($\vec{r}$ is 3-d) and $F_n(z)$ the variational form of an effective-mass Schrödinger equation [8], with the inverse inversion layer thickness λ related to the electron density ρ by $\lambda=(15\pi\rho/(8a^*))^{1/3}$ with effective Bohr radius $a^*=\varepsilon_{Si}\hbar^2/(m_{zz}e^2)$ and m_{zz} the effective mass normal to the interface. For Si(111)/SiO_2 the electrons occupy six equivalent valleys and the elliptical dispersion is replaced by a circular equivalent. The density can vary from 10^{11} to 10^{13} cm^{-2}. V^R is the irreducible electron-electron interaction as mediated by phonons, plasmons etc.

The direct Coulomb interaction is easily calculated for the lowest and first excited subbands with the inversion layer wavefunctions given in equation (3), and the contributions with $q=q_{intervalley}$ can be shown to be negligible. The same holds for the screened interaction which is a matrix (in m and n)

$$V^R_{\text{Intra-Coul}}(q,\Omega) = \int F_n(z_1)F_m(z_1)v(q,z_1,z_3)v(q,z_3,z_4) \times \chi_\Omega(q,z_4,z_2)F_n(z_2)F_m(z_2)dz_1..dz_4. \qquad (3)$$

With the wavefunctions of equation (3) the interacting susceptibility χ is easily obtained since the non-interacting polarisation χ^0_Ω is separable in z and z' [7] and the integral equation for χ solved. The intrasubband contribution (m=n=0) contains the plasmon contribution whereas the intersubband transitions correspond to electron-hole excitations [7].

For the phonon-mediated electron-electron interaction, arguments based on a continuum expansion [9] show that intravalley phonons provide a weak attraction giving $K(\omega=0,\omega'=0)=-0.01D^2r_s^{-2/3}$ where r_s is the electron spacing parameter in units of **a*** $(0.7<r_s<7)$. As with bulk calculations [10], we find a large attractive contribution from intervalley phonons: hence our choice of the Si(111) interface. With j denoting both branches and q_z values, we calculate the electron phonon matrix-element $g_j(\underset{\sim}{q})$ coupling valleys a and b

$$g_j(\underset{\sim}{q}_{ab}) = \int\psi_b^*(\vec{r})\left[\int\varepsilon^{-1}(\vec{r},\vec{r}')\sum_R \delta\vec{R}_j\cdot\nabla V_{\mathrm{Ion}}(\vec{r}-\vec{R})d\vec{r}'\right]\psi_a(\vec{r})d\vec{r} , \qquad (4)$$

where $\delta\vec{R}_j$ is the displacement of the ion at site $\vec{R}$ from the phonon j. We have calculated this quantity, and the corresponding phonon kernel

$$V^R_{Ph}(\underset{\sim}{q},\omega) = -\sum_j \frac{2\hbar\omega_j(\underset{\sim}{q})|g_j(\underset{\sim}{q})|^2}{(\hbar\omega_j(\underset{\sim}{q}))^2-(\hbar\omega)^2} , \qquad (5)$$

on a 24-layer slab of silicon bounded by (111) surfaces to which free and periodic boundary conditions are applied normal to the surface, using the following ingredients (i) a simple two-parameter force-constant model for the phonons, (ii) a tight-binding expansion over antibonding orbitals for the Bloch functions, (iii) a microscopic formulation for the surface screening function [11], and (iv) a simple parameterisation of the Si pseudopotential V_{Ion}. Results with free boundary conditions are enhanced over those with periodic boundary conditions by 30% since the relaxation of selection rules near a surface allows more phonons to couple the electron states and more than compensate for the loss of phase coherence that the bulk selection rules guaranteed. Using the enhanced value to simulate the proximity of the interface, we obtain from the intervalley contribution $K(\omega=0,\omega'=0)=-0.22r_s^{-2/3}$, and since the deformation potentials D for the intravalley contributions are less than 1Ryd, we see the dominating effect of intervalley phonons.

II. Results and Discussion

The results for the transition temperature T_c as a function of the density parameter r_s are displayed in Figure 1. The gap equation has been solved numerically [6], for three kernels (a) including only the intra-subband contribution of equation (4), (b) including the electron-hole excitations to the first excited subband as well, and (c) including the phonon kernel in addition. We comment on each result in turn. We note a threshold for pairing mediated by intra-subband excitations only at $r_s=3$, and a maximum for T_c occurs at higher values of r_s, since T_c depends on the Fermi energy ($\sim r_s^{-2}$) and on the exponential factor involving the interaction which increases with r_s. This result corresponds to some extent to that of Takada [6], but we have retained the thickness of the inversion layer. In (b) we include the e-h excitations to the first excited subband, and we see that the T_c's are further enhanced by this extra mechanism, which is analogous to the exciton mechanism of superconductivity. Finally, in (c) we have also included the phonon-mediated contribution, as enhanced by the proximity to the surface. This provides an upper estimate of T_c, as there are two surfaces in the calculation of the kernel. The use of the kernel derived from the use of periodic boundary conditions gives T_c values about a factor of 20 lower, and we see that the surface enhancement is important in producing T_c's that are experimentally accessible. The more widely studied $Si(100)/SiO_2$ system is not considered as good a candidate for superconductivity as only intravalley phonons contribute to the kernel. Under stress four valleys can be occupied [13] and stress-induced superconductivity is an intriguing possibility there. The phonon mechanism is the one that produces measureable T_c's, and other materials might be used to replace silicon, and so exploit the greater bulk electron-phonon coupling, e.g. InAs, PbTe or even $SrTiO_3$ (which exhibits bulk superconductivity in doped samples).

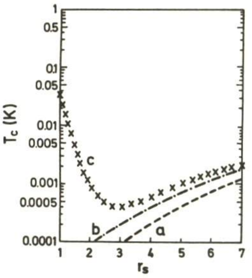

Figure 1 T_c versus r_s for three cases as described in the text

Our results must be considered as order-of-magnitude estimates because of the approximations that have gone into the kernel, and because of the higher-order corrections that need to be added to our mean-field theory. While we have omitted the excited subbands above the first, which, when included, would further raise T_c, most corrections, such as electron-hole ladder diagrams in the screening of the e-e interaction, strong coupling corrections, and the paramagnon effect all reduce T_c by factors of order two each. Fluctuation effects can be discussed along the lines of Aslamov and Larkin[14]. The novel feature of this system, however, is the fact that the electron density also controls the inversion layer thickness, and the "excess superconductivity" resulting from pairing due to thermal effects in the normal phase could be monitored as the third dimension is squeezed out as a function of density. Other considerations that will be discussed in subsequent publications include the effects of interface roughness and disorder on both kernels, as well as the competition of other broken symmetries (such as the Wigner crystallisation at low densities).

In summary, we have demonstrated the possibility of superconductivity in MOS system, highlighting the density dependence of the various coupling mechanisms. The Si(111)/SiO_2 system is the most favourable of the current generation of MOS devices, but the use of other materials, with higher bulk electron-phonon matrix-elements could further enhance the range of variables over which superconducting phenomena would be observed.

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