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Temperature dependence of many-body effects in inversion layers

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The temperature-dependent self-energies of the lowest three subbands in a Si(100) surface inversion layer are evaluated in the plasmon-pole approximation for the screened interaction. The magnitudes of the self-energies decrease with increasing temperature. For the excited subbands the self-energies show very similar dependence on temperature. At low concentration the quasiparticle energy differences are independent of temperature, but at higher concentrations these subband separations increase slightly with temperature.

The large electric field of a surface inversion layer causes quantization of the motion of electrons normal to the surface. Because the electrons are free to move parallel to the surface, each quantized level of the surface potential gives rise to a two-dimensional band of free carriers, which is referred to as an electric subband. Intersubband spectroscopy has shown that many-body effects play a significant role in determining the subband separations.[1] In contrast to other "metallic" systems, inversion layers have Fermi temperatures that fall within an easily accessible range. Recently, Kneschaurek and Koch[2] investigated the temperature dependence of intersubband transitions by means of infrared absorption. Despite the known importance of many-body effects at very low temperatures, previous theoretical work on subband separations at finite temperature has been limited to the Hartree approximation.[3] In this paper we investigate the exchange and correlation contributions to the subband energies of a Si(100)-SiO_2 system as a function of temperature.

Our starting point is the Hartree approximation.[3] The Hartree potential depends upon the solution of Poisson's equation

$$\frac{d^2\Phi(z)}{dz^2} = \frac{4\pi e}{\kappa_s}\left((N_A - N_D)\Theta(d-z) + \sum_{j,\vec{k}} n(E_j(\vec{k}))\,|\xi_j(z)|^2\right). \tag{1}$$

The first term is the potential of the depletion layer, which contains $N_A - N_D$ fixed negative charges per unit volume and has a width d. The second term is the potential of the inversion layer carriers. E_j and $\xi_j(z)$ are the eigenvalues and eigenfunctions of the Hartree Hamiltonian; n is the Fermi distribution function and κ_s the dielectric constant of Si. The Hartree wave functions of the lowest three subbands are obtained variationally. We parametrize $\xi_j(z)$ and use the following two conditions to obtain the values of the parameters; (i) the energy of each subband must be a minimum with respect to the variations in the parameters, and (ii) the wave functions corresponding to 0, 1 must be orthonormal. The variational energy for the zeroth subband agrees very well with the numerical Hartree value[4] at all temperatures. The agreement for the excited subbands is also quite good; the discrepancy is always less than 10%.

At finite temperature it is customary to define a self-energy function $M(\vec{R},\vec{R}'; i\omega_n)$ over a discrete set of imaginary frequencies.[5] The subband self-energies are defined by expanding $M(\vec{R},\vec{R}'; i\omega_n)$ in the complete set of Hartree eigenfunctions $\xi_j(z)$.[6] To lowest order in the effective interaction the i-j element of M is given by[5]

$$M_{ij}(\vec{k}, i\omega_n) = -\beta^{-1}\sum_{l}\sum_{\omega_m} e^{i\omega_m\eta}\int\frac{d^2p}{(2\pi)^2}\,U_{illj}(\vec{k}-\vec{p}, i\omega_n - i\omega_m)G^0_{ll}(\vec{p}, i\omega_m), \tag{2}$$

where the sum over l runs over all subbands, and $\beta = (k_BT)^{-1}$. Here G^0_{ll} is the noninteracting Green's function for the lth subband. Throughout this paper we choose $\hbar = 1$.

From the Dyson equation for the effective interaction U we can obtain the relation[5]

$$U_{ijlm}(\vec{k}, z) = V_{ijlm}(\vec{k}) + \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\frac{f_{ijlm}(\vec{k};\omega')}{z-\omega'}, \tag{3}$$

where z is a complex frequency and $f_{ijlm}(\vec{k},\omega')$ is simply related to the imaginary part of $U_{ijlm}(\vec{k}; z = \omega' + i\eta)$. The unscreened interaction $V_{ijlm}(\vec{k})$ between electrons in the inversion layer arises from the direct Coulomb interaction and the image effect.[6] Substituting Eq. (3) in Eq. (2) and performing the sum over ω_m, we find the M is a sum of exchange and correlation terms.[5] The exchange part of self-energy M^x_{ij} is given by

$$M^x_{ij}(\vec{k}) = -\sum_l \int \frac{d^2p}{(2\pi)^2} V_{illj}(\vec{p}) n_l(\vec{k}-\vec{p}), \tag{4}$$

and the correlation part by

$$M^c_{ij}(\vec{k}, i\omega_n) = -\sum_l \int \frac{d^2p}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} [i\omega_n - \omega' - E_l - \tfrac{1}{2} m_l^{-1}(\vec{k}-\vec{p})^2 + \mu]^{-1} \times f_{illj}(\vec{p}, \omega')[n_l(\vec{k}-\vec{p}) + (e^{-\beta\omega'} - 1)^{-1}]. \tag{5}$$

Here $n_l(\vec{k})$ is the Fermi function for an electron of energy $E_l + k^2/2m_l$, and μ is the chemical potential of the system.

Explicit calculations for the bare interaction reveal that V_{ijlm} has a significant contribution only if $i=j$ and $l=m$. Under these conditions, the self-energy M becomes diagonal.[6] For convenience, we denote M_{ii} by M_i, V_{iijj} by V_{ij}, and f_{iijj} by f_{ij}.

The calculation of exchange energy is straightforward. For the evaluation of $M^c_i(\vec{k}; i\omega_n)$ we need the imaginary part of the retarded effective interaction, f_{ii}. The latter is calculated in the plasmon pole (PP) approximation. Vinter has demonstrated the validity of the PP approximation in the calculation of subband separations in metal-oxide-semiconductor (MOS) systems at zero temperature.[6] The appropriateness of plasmon pole approximation has been discussed by Lundqvist[7] and by Overhauser.[8] We start with the ansatz that for $\omega > 0$

$$\mathrm{Im}\,\epsilon^{-1}_{ij}(\vec{k}, \omega) = C_{ij}(\vec{k}) \delta(\omega - \omega_k), \tag{6}$$

where ϵ_{ij} is an element of the dielectric matrix ϵ defined by $\epsilon \cdot U = V$. Substituting $U = \epsilon^{-1} \cdot V$ in Eq. (3) and letting $z = \omega + i\eta$ we obtain the Kramers-Kronig relations between the real and imaginary parts of ϵ^{-1}. Taking the random-phase-approximation (RPA) expression for the real part of ϵ^{-1}, we determine $C_{ij}(\vec{k})$ and ω_k from the static limit of Kramers-Kronig relations and the f-sum rule.[6,7] From the knowledge of C_{ij} and ω_k we obtain $\mathrm{Im}\,\epsilon^{-1}_{ij}$ and subsequently f_{ii}.

The quasiparticle energies are the solutions of Dyson's equation. Rice has pointed out that if the self-energy is evaluated only to lowest order in effective interaction, it is inappropriate to solve the exact Dyson equation since it generates not only the lowest-order terms in effective interaction, but also selected higher-order terms that should not be included in the calculation.[9] Instead, the self-energy should be evaluated at a frequency corresponding to the noninteracting quasiparticle energy, that is,

$$\omega_i(\vec{k}) \approx E_i + \tfrac{1}{2} m_i^{-1} k^2 - \mu + \mathrm{Re} M_i(\vec{k}; E_i + \tfrac{1}{2} m_i^{-1} k^2 - \mu). \tag{7}$$

The quasiparticle energies $E^*_i(\vec{k})$ are then given by $\omega_i(\vec{k}) + \mu$.

We have evaluated the exchange and correlation parts of the self-energy as a function of temperature at several values of the inversion layer concentration for the three subband model. According to the self-consistent Hartree calculation[4] most of the electrons reside in 0, 1, and 0′ subbands and, therefore, the three subband model is expected to be a reasonable approximation. Figure 1 illustrates the variation of self-energies 0, 1, and 0′ subbands with temperature. At low and intermediate temperatures the main contribution to the self-energy of the zeroth subband comes from exchange. The small size of M^c_0 results from the large cancellation between the first and second terms in the parentheses of Eq. (5). As the temperature increases, the population in the zeroth subband decreases; this results in a decrease in the exchange energy and an increase in the correlation contribution to the self-energy. At extremely high temperature, the

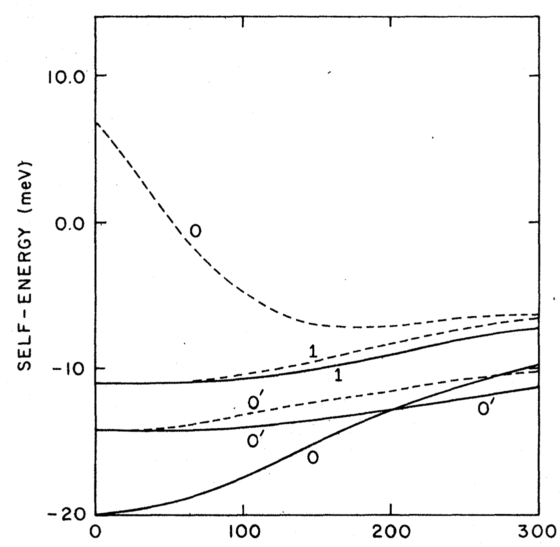

FIG. 1. Temperature dependence of the correlation and the total self-energies of 0, 1, and 0′ subbands in Si(100)-SiO_2 inversion layer. The inversion and depletion layer densities are $10^{12}/cm^2$ and $3.2 \times 10^{11}/cm^2$, respectively. Solid curves—total self-energies; dashed curves—correlation contribution to self-energies.

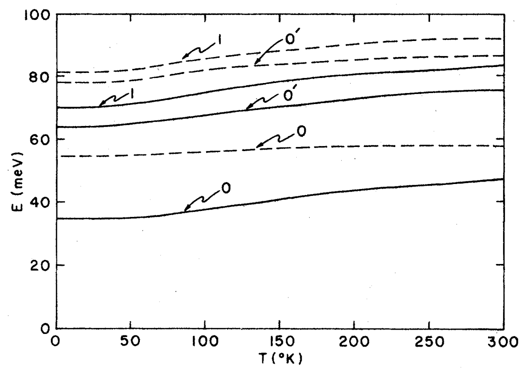

FIG. 2. Temperature dependence of the quasiparticle energies in the inversion layer of Si(100)-SiO_2 system. $N_{inv}=10^{12}/cm^2$ and $N_{dep}=3.2\times10^{11}/cm^2$. Here, the quasiparticle energies of 0, 1, and 0′ subbands are given by $\omega_i(\vec{k}=0)+\mu$, where ω_i is obtained from Eq. (7). Dashed curves—Hartree energies; solid curves—Hartree and exchange correlation.

self-energy becomes very small, indicating that the system approaches the classical limit.

The exchange energy for the excited subbands is very small at low and intermediate temperatures; the main contribution comes from the correlation part. For these subbands almost no cancellation occurs between the two terms in the parentheses of Eq. (5), because the first term has a negligible value at low and intermediate temperatures. With increase in temperature, the exchange contribution grows and the correlation part diminishes. Finally, at very high temperatures, the total self-energies for the 0′ and 1 subbands become very small. It should be observed that the self-energies for the 0′ and 1 subbands show a remarkably similar dependence on temperature.

In Fig. 2 we display the quasiparticle energies at the subband minima as a function of temperature for $N_{inv}=10^{12}/cm^2$. For very low concentrations ($N_{inv}\simeq10^{11}/cm^2$) the subband separations turn out to be almost independent of temperature. At higher concentrations they increase slightly with increasing temperature. The exchange-correlation energies are quite insensitive to the value of the wave vector $\vec{k}$ parallel to the surface, so that the self-energy effects produce only a rigid shift in the subbands.

At $T=200$ and 300 °K Nakamura *et al.*[10] have used the static approximation for U to calculate the quasiparticle energies at the subband minima. The static approximation for effective interaction is expected to be reasonable at high temperatures. Our results for the quasiparticle energies are in good agreement with their calculation.

For a quantitative comparison with experiment considerably more numerical work remains. We have evaluated E_{10} and $E_{0'0}$ only for a few values of N_{inv} and $N_{dep}=(N_A-N_D)d$. Furthermore the depolarization shift[11] and the effect of final state interactions[1,6] must be included in a comparison of theory with infrared absorption. At zero temperature these two effects tend to cancel,[1] but even at zero temperature the degree of cancellation is not accurately known. At finite temperature these effects will be even more difficult to calculate. One experiment which would be extremely useful for comparison with theory is surface-channel tunneling.[12] Surface-channel tunneling experiments are in progress[13] and should yield the subband separations directly.

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