Electron Exchange Energy in Si Inversion Layers

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The exchange energy is found for electrons in a two-dimensional system and in Si inversion layers which are dynamically two dimensional. We find that exchange lowers the energy of the lowest sub-band in Si inversion layers significantly, but affects the energies of higher sub-bands and the spatial extent of the wave functions in the direction perpendicular to the surface only slightly.

An inversion layer is formed in a semiconductor when the energy bands at a semiconductor-insulator interface are bent so strongly that the carriers near the interface are electrons although the carriers in the bulk are holes, or vice versa. The energy levels in an inversion layer form a series of sub-bands, each of which is a two-dimensional (2D) continuum of levels which are associated with the two degrees of freedom parallel to the interface.

Calculations of the energy levels and wave functions of electrons in inversion layers have heretofore ignored the contribution of exchange and correlation effects.[1-5] We find that the exchange term lowers the energy of the lowest sub-band in Si inversion layers significantly, but has little effect on the energies of higher sub-bands or on the wave functions. We give an analytic result for the exchange energy in the extreme 2D limit of zero inversion-layer thickness.

The exchange energy[6] of an inversion-layer electron with 2D wave vector $\vec{k}$ in sub-band i is[7]

$$v_{xi\vec{k}} = \sum_{j\vec{k}'}{}' \iint \psi_{j\vec{k}'}{}^*(\vec{r})\psi_{i\vec{k}}{}^*(\vec{r}\,')V(\vec{r},\vec{r}\,')\psi_{j\vec{k}'}(\vec{r}\,')\psi_{i\vec{k}}(\vec{r})\,d^3r\,d^3r', \tag{1a}$$

$$V(\vec{r},\vec{r}\,') = -\frac{e^2}{4\pi\kappa_{sc}\epsilon_0}\left[\frac{1}{(|\vec{R}-\vec{R}'|^2+|z-z'|^2)^{1/2}}+\frac{s}{(|\vec{R}-\vec{R}'|^2+|z+z'|^2)^{1/2}}\right], \tag{1b}$$

$$s = (\kappa_{sc}-\kappa_{ins})/(\kappa_{sc}+\kappa_{ins}), \tag{1c}$$

where $\vec{R}$ is the 2D radius vector and z is the distance from the semiconductor-insulator interface. The primed sum in (1a) is over all occupied states with parallel spin. The Coulomb interaction (1b) between inversion-layer electrons has been divided by the static dielectric constant κ_{sc} of the semiconductor and includes a term for the image potential[8] which results from the interface with the insulator, whose dielectric constant is κ_{ins}.

For the n-type inversion layers we consider, the effective-mass-approximation envelope wave function of the state with wave vector $\vec{k}$ in sub-band i is[2]

$$\psi_{i\vec{k},\mathrm{env}}(\vec{r}) = \zeta_i(z)\exp(i\vec{k}\cdot\vec{R}); \tag{2}$$

it is multiplied by the Bloch function for the conduction-band valley from which the state arises. Because of this factor, exchange integrals connecting sub-bands from different valleys are much smaller than those which connect sub-bands from the same valley, and are neglected here.

The exchange energies take a particularly simple form when the inversion-layer thickness goes to zero, i.e., $\zeta_0(z) = \delta(z)$. In this case the effective dielectric constant is $\bar{\kappa} = \frac{1}{2}(\kappa_{sc}+\kappa_{ins})$. There are no excited sub-bands, so we drop the sub-band index i. The exchange energy of an electron with wave vector $\vec{k}$ in this extreme 2D limit is found to be

$$v_{xk} = -(2\bar{U}/\pi)E(k^2/k_F{}^2), \tag{3}$$

$$\bar{U} = e^2k_F/4\pi\bar{\kappa}\epsilon_0. \tag{4}$$

$E(x)$ is the complete elliptic integral of the second kind,[9] and $k_F = (2\pi n/n_v)^{1/2}$ is the Fermi wave vector, where n is the electron density per unit area, and where n_v is the multiplicity of the valleys from which the lowest sub-band arises. We assume the 2D effective mass to be isotropic. The exchange energies v_{x0} and v_{xF} at $k=0$ and at $k=k_F$, respectively, and $v_{x\,\mathrm{av}}$, the average over all occupied states, are listed in Table I both for the extreme 2D limit and for the 3D cases.[6,10-12] In the 3D case, $\bar{\kappa}$ is the semiconductor dielectric constant and $k_F = (3\pi^2n/n_v)^{1/3}$.

The total exchange energy per electron is ϵ_x

TABLE I. Comparison of 2D and 3D results for the exchange energies of states with wave vector 0 and k_F, for an average over all occupied states, and for the quantities ϵ_x and μ_x defined in the text and in Ref. 6. The unit of energy is $\bar{U}=e^2k_F/4\pi\bar{\kappa}\epsilon_0$, where k_F is the Fermi wave vector and $\bar{\kappa}$ is the effective static dielectric constant. The carrier concentration is n and the valley multiplicity is n_v. The 2D results are for the δ-function limit $\zeta(z)=\delta(z)$.

	k_F	v_{x0}	v_{xF}	$v_{x\,\mathrm{av}}$	ϵ_x	μ_x
2D	$(2\pi n/n_v)^{1/2}$	$-\bar{U}$	$-2\bar{U}/\pi$	$-8\bar{U}/3\pi$	$-4\bar{U}/3\pi$	$-2\bar{U}/\pi$
3D	$(3\pi^2 n/n_v)^{1/3}$	$-2\bar{U}/\pi$	$-\bar{U}/\pi$	$-3\bar{U}/2\pi$	$-3\bar{U}/4\pi$	$-\bar{U}/\pi$

$=\frac{1}{2}v_{x\,\mathrm{av}}$; the factor $\frac{1}{2}$ compensates for the double counting of the interactions. The effective exchange potential[6] is

$$\mu_x=(d/dn)[n\epsilon_x(n)]. \tag{5}$$

In the extreme 2D limit considered here, $\mu_x=\frac{3}{2}\epsilon_x$, and $\mu_x=v_{xF}$ as in the 3D case. The 2D and 3D values of ϵ_x and μ_x are given in Table I.

We have also calculated the exchange energy for the lowest sub-band using the variational wave function

$$\zeta_0(z)=(\tfrac{1}{2}b^3)^{1/2}z\exp(-\tfrac{1}{2}bz) \tag{6}$$

instead of making the simplifying assumption $\zeta_0(z)=\delta(z)$. In addition, we have used numerical self-consistent[4] wave functions to obtain exchange energies for the lowest sub-band and for higher sub-bands. Details of the calculations will be submitted for publication elsewhere.

To illustrate the results, we consider a (100) Si surface at low temperature, with only the lowest sub-band occupied. This sub-band has $n_v=2$ and an isotropic effective mass.[2] We consider a sample with a bulk acceptor concentration $N_A=4\times10^{20}$ m^{-3}, for which the density of depletion-layer charges is $N_{\mathrm{depl}}=7.6\times10^{14}$ m^{-2}, and with an inversion-layer electron concentration $N_{\mathrm{inv}}=n=5\times10^{15}$ m^{-2}. We use $\kappa_{\mathrm{sc}}=11.7$ and $\kappa_{\mathrm{ins}}=3.9$. Then $k_F=1.25\times10^8$ m^{-1}, $\bar{U}=23.1$ meV, and the parameter b in the variational wave function (6) is 8.2×10^8 m^{-1}. The exchange energy per electron in the lowest sub-band is $\epsilon_x=-4\bar{U}/3\pi=-9.8$ meV in the δ-function limit. It is -7.7 meV if we use the variational wave function, and is -7.9 meV if we use a numerical self-consistent wave function. The exchange energy at the Fermi level obtained using the latter wave function is $v_{xF}=-11.1$ meV.

The exchange energy for the excited sub-bands is not strongly dependent on wave vector. It is equal to -0.4 meV for the first excited sub-band of the valleys with $n_v=2$ in the case considered here, with decreasing magnitudes for higher sub-bands. The excited sub-bands associated with the other conduction-band valleys, with $n_v=4$, will be lowered even less, as discussed above.

If we take the exchange energy for $k=k_F$ as a measure of the lowering of each sub-band, ignoring higher-order many-body corrections[13,14] as well as the k dependence of the exchange energy, we find that the calculated splitting between the lowest and the first excited sub-bands is increased from 12.4 to 23.1 meV for the case considered here. The calculated splitting between the lowest sub-band and the third excited sub-band is increased from 21.4 to 32.4 meV, in better agreement with the measurements of Wheeler and Ralston,[15] who report this splitting to be 44.3 meV when $N_{\mathrm{inv}}=5.3\times10^{15}$ m^{-2}. Inclusion of higher-order many-body effects should further reduce the discrepancy; in 3D multivalley semiconductors,[10-12] the correlation energy is approximately as large as the exchange energy.

We have also considered the effect of exchange on the wave function of the lowest sub-band. This can be done in a variational calculation by including the exchange energy in the total energy of the system and finding the value of the variational parameter b which minimizes the total energy. For the numerical example given above, we find that the resulting shrinkage of the wave function is less than 2%. We conclude that the exchange effect on the spatial extent of the wave functions is relatively small.

Further experiments on sub-band splittings and additional theoretical work to evaluate the higher-order many-body effects should be of considerable interest, because the inversion layer, with its continuously variable carrier concentration, promises to be a valuable system for studying many-body Coulomb interactions.[14,16]

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X-Ray Photoemission from Aluminum

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An x-ray photoemission study of evaporated Al films has been performed in ultrahigh vacuum. The striking similarity of the valence-band spectrum with computed density of states allows a straightforward interpretation of the results. Core level spectra reveal structures which can be attributed to either inelastically scattered electrons or to satellites due to hole-plasmon coupling.

The nearly free-electron band structure of aluminum is rather well known from theoretical calculations. At the present moment no experimental technique yields an accurate and direct picture of the energy density of states, but valuable contributions have been brought by soft-x-ray spectroscopy and photoemission spectroscopy. We present in this Letter a study of aluminum by x-ray photoemission spectroscopy (XPS). The characteristic x-ray emission lines $K\alpha_{1,2}$ of Mg were used, and the kinetic energy of the photoemitted electrons was analyzed in a hemispherical electrostatic analyzer.[1] The total instrumental resolution including the x-ray linewidth is slightly better than 1.0 eV. The complete system is bakable and ultrahigh vacuum is obtained by conventional ion and titanium sublimation pumps. The major difficulty encountered in the study of Al by an emission technique is the preparation of a clean metallic surface. We have evaporated Al films *in situ* on optically flat quartz substrates. The filament of W supporting a twisted Al wire was carefully outgassed for several hours. During the 1 min of rapid evaporation, the pressure rose to 1×10^{-9} Torr. 10 min after completion of the evaporation, the base pressure of 2×10^{-11} Torr was reached. In spite of this careful preparation very weak O 1*s* and C 1*s* signals were present in the spectra. The intensity of these two lines was less than 1% of the intensity of the Al 2*s* line, and no increase was observed during the few days necessary for the measurements. Because of the low photoelectric cross section for the nearly free electrons of the Al band, very long integration times are required for recording the spectrum. The energy selected by the spectrometer was varied in steps of 0.1 eV. The counts at each energy were accumulated for 1 sec and stored in a multichannel analyzer. The scan over the band region was repeated 1700 times in order to improve the statistics and to eliminate intensity fluctuations of the x-ray tube. Figure 1