a temperature shift of ~ 20 K due to the imaging electric field is assumed, the conflict would almost disappear.[7]

In conclusion, whereas the comments be Seidman, Wilson, and Nielsen[1] brought up some difficulty with our proposal of free migration of interstitials at 15 K in W, the issue seems not yet decided, and their results could be reconciled with our proposed model.

In line with the greater importance that di-interstitials seem to play, we have revised our interpretation of the 27-K peak. In Ref. 2, the 27-K peak was considered to correspond with the peak by DiCarlo, Snead, and Goland[8] at 30 K. Good agreement in a peak height expected from the Frenkel-pair concentration between neutron and electron irradiations had led us to discard the possibility of di-interstitials as the defects responsible for the 27-K peak; these defects were considered to be the interstitials trapped by impurity atoms. However, close examination of the results, including those of impure specimens, indicates that the peak reported by DiCarlo, Snead, and Goland at 30 K does not correspond with the 27-K peak in the present experiment, but possibly with the 30-K peak, which appears half buried in the 27-K peak in the pure single-crystal specimen. Therefore, the defects responsible for 27-K peak are more likely to be di-interstitials. In the neutron irradiation, the high-energy primary knock-on atom produces a cascade where the local defect density is sufficiently high to give a large chance for the interstitials to form di-interstitials. Since the locally high defect density in the cascades remains almost the same as the irradiation dose increases, so long as overlap of the cascades does not occur, the number of di-interstitials and also the 27-K peak height increase linearly with irradiation dose. On the other hand, since DiCarlo, Snead, and Goland irradiated the specimen with electrons at 20 K where the free interstitials were mobile and the formation of di-interstitials was scarce, they could not observe the large 27-K peak. A detailed account will be published elsewhere.

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Correlation Energy and Effective Mass of Electrons in an Inversion Layer

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I have calculated the correlation energy and effective mass of electrons in a two-dimensional electron gas. The results on the effective mass show good agreement with experiments on Si. However, when the finite thickness of the inversion layer is taken into account the effective mass is reduced. The difference between our results and those recently published by Ting *et al.* is due to their use of an approximation to the Dyson equation. Dispersion in the insulator and a finite insulator thickness have been considered.

The possibility of studying many-body effects on an electron gas in the inversion layer of a metal-insulator-semiconductor structure has been recognized for some years. The g factor has been measured by Fang and Stiles[1] and the effective mass for motion parallel to the surface was measured by Smith and Stiles[2] as a function of carrier density. Some theoretical calculations on the electron-electron interaction in a two-dimensional electron gas have been published. Chaplik's[3] results on the mass are valid only in the high-density limit. Janak[4] and Suzuki and Kawamoto[5] used various static approximations to the screening and obtained some agreement with experiment for the g factor. However, the static approximations lead to a mass which is lower than the bulk value (at least for $N > 3\times 10^{12}$ cm^{-2}) in qualitative disagreement with experiment. Very recently Ting, Lee, and Quinn[6] have calculated the g factor and effective mass based on dynamic screening in the random-phase approximation (RPA) and the Hubbard approximation with greatly improved results.

I have performed calculations on the correlation energy and effective mass. The calculations employ dynamic screening in the approximation to the RPA screening suggested by Lundqvist[7] and by Overhauser.[8] For the effective mass we get results which differ from those of Ting, Lee, and Quinn.[6] The difference can be traced to their use of an approximation to the Dyson equation.

The self-energy[9] is given by ($\hbar = 1$)

$$\Sigma(k,E) = i\int \frac{d^2q\,d\omega}{(2\pi)^3}\frac{e^2}{2q\epsilon(q,\omega)}G(\vec{k}-\vec{q},E-\omega), \qquad (1)$$

where the bare Coulomb interaction is $e^2/2q\epsilon_\infty$. ϵ_∞ is the permittivity of the surrounding medium, in this case the average dielectric constant of oxide and semiconductor. $G(\vec{k},E)$ is the one-particle Green's function. The Lundqvist-Overhauser approximation represents the imaginary part of the propagator for density fluctuations by a δ function:

$$\mathrm{Im}\left(\frac{\epsilon_\infty}{\epsilon(q,\omega)}-1\right) = -\frac{\pi}{2}\frac{\omega_p^2(q)}{\omega_q}\delta(\omega-\omega_q). \qquad (2)$$

The strength and the effective plasma frequency ω_q are determined by the requirements that (2) fulfill the f sum rule[10] and the sum rule for $\omega^{-1}\times\mathrm{Im}[\epsilon_\infty/\epsilon(q,\omega)]$. Thus $\omega_p^2(q) = \frac{1}{2}qNe^2/\epsilon_\infty m$,[10] and

$$\omega_q^2 = -\frac{\omega_p^2(q)}{\epsilon_\infty/\epsilon(q,0)-1}, \qquad (3)$$

where m is the bulk mass for motion parallel to the surface. The RPA result of Stern[10] is used for $\epsilon(q,0)$:

$$\epsilon(q,0) = \epsilon_\infty + \epsilon_0 s(q)/q, \quad s(q) = (2n_v e^2 m/4\pi\epsilon_0)\{1-\theta(q-2k_F)[1-(2k_F/q)^2]^{1/2}\}. \qquad (4)$$

Using the free-particle Green's function and carrying out the integration over ω, one obtains the self-energy

$$\Sigma(k,E) = \Sigma_x(k) + \Sigma_c(k,E), \qquad (5)$$

$$\Sigma_x(k) = \int \frac{d^2q}{(2\pi)^2}\frac{e^2}{2\epsilon_\infty q}\theta(k_F - |\vec{k}-\vec{q}|), \qquad (6)$$

$$\Sigma_c(k,E) = \int \frac{d^2q}{(2\pi)^2}\frac{e^2}{2\epsilon_\infty q}\frac{\omega_p^2(q)}{2\omega_q}\left[\frac{\theta(k_F-|\vec{k}-\vec{q}|)}{E-\xi(\vec{k}-\vec{q})+\omega_q}+\frac{\theta(|\vec{k}-\vec{q}|-k_F)}{E-\xi(\vec{k}-\vec{q})-\omega_q}\right], \qquad (7)$$

where $\xi(\vec{k}) = (k^2-k_F^2)/2m$. The exchange energy $\Sigma_x(k)$ has been calculated earlier by Chaplik[3] and by Stern.[11] In order to determine the energy of a quasiparticle with momentum k one must solve the Dyson equation[12]:

$$E + \mu = k^2/2m + \Sigma(k,E), \qquad (8)$$

where μ is the chemical potential of the interacting electron gas.

Figure 1 displays the results for the self-energy of particles at the Fermi level. The parameters used in the calculation are those of a Si(001)-SiO_2 interface: $\epsilon_\infty = 7.8\epsilon_0$, $m = 0.1905\,m_e$, number of equivalent valleys $n_v = 2$. It can be seen that the self-energy considerably lowers the chemical potential.

Solutions of (8) for k values below the Fermi level show that the band is still very nearly parabolic with a mean mass 14% above the bulk mass for $N = 10^{12}$ cm^{-2} and decreasing with increasing density. Thus, at the bottom of the band, the correlation energy compensates a major part of the exchange energy (if only exchange is considered, the mean mass is $\sim\frac{1}{3}$ the bulk mass for $N = 10^{12}$ cm^{-2} and always smaller).

The effective mass defined by $m^{*-1} = k^{-1}dE/dk$ is obtained upon differentiation of the Dyson equa-

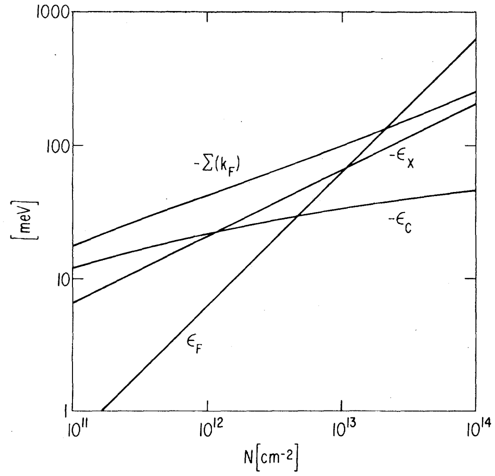

FIG. 1. Fermi energy ϵ_F, exchange energy ϵ_x, correlation energy ϵ_c, and self-energy Σ, all at the Fermi level, as a function of carrier concentration in the two-dimensional limit.

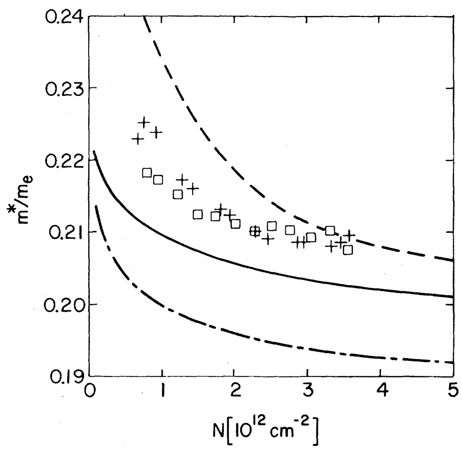

FIG. 2. Effective mass as a function of carrier concentration. Solid curve: present work. Magnetoconductivity measurements from Ref. 2: □ at $B = 1.56$ T, + at $B = 2.59$ T. Dashed curve: theoretical results from Ref. 6. Dash-dotted curve: present work, effect of finite inversion layer thickness included.

tion (8):

$$\frac{m^*}{m} = 1 - \frac{\partial\Sigma}{\partial E}\left(1 + \frac{m}{k}\frac{\partial\Sigma}{\partial k}\right)^{-1}. \tag{9}$$

Figure 2 shows the results for the effective mass as a function of carrier density. Also shown are the magnetoconductivity results of Smith and Stiles.[2] The theoretical results are seen to be $0.005 m_e$ below the experimental results over the whole range of the experiment. Since the theory is based on the limit of zero magnetic field, comparison should preferably be made with the lower-field results.

Ting, Lee, and Quinn[6] used the full RPA expression for the dielectric function. They furthermore used an approximation to the Dyson equation (8) in which the energy variable in the self-energy is replaced by the noninteracting value $\xi(k)$. Thus by differentiation they obtain

$$\frac{m^*}{m} \simeq \left(1 + \frac{m}{k}\frac{\partial\Sigma}{\partial k} + \frac{\partial\Sigma}{\partial E}\right)^{-1}. \tag{10}$$

If one uses Eq. (10) instead of (9) results are obtained which closely resemble theirs, which are shown dashed in Fig. 2. This shows that the difference between the Lundqvist-Overhauser approximation and RPA is small. I find that $\delta\Sigma/\partial E$ varies from -2 to -0.5 in the density range 10^{11}–10^{13} cm^{-2}. Thus the difference in Fig. 2 between my results and theirs is almost entirely due to their using the approximation (10) rather than Eq. (9). This strongly suggests that RPA and Eq. (9) would give much lower values of the effective mass.

In the Lundqvist-Overhauser approximation it is simple to calculate the effect of the finite thickness of the inversion layer. As shown by Ando and Uemura[13] and Stern,[14] use of the variational wave function[15] in the z direction $\zeta(z) = (b^2/2)^{1/2} z \times \exp(-bz/2)$ leads to an effective dielectric function of the medium

$$\frac{1}{\epsilon_\infty(q)} = \frac{1}{\epsilon_{\rm Si}}\frac{8 + 9x + 3x^2}{8(1+x)^3} + \frac{1}{\epsilon_{\rm Si}}\frac{\epsilon_{\rm Si} - \epsilon_{\rm SiO_2}}{\epsilon_{\rm Si} + \epsilon_{\rm SiO_2}}\frac{1}{(1+x)^6}, \tag{11}$$

where $x = q/b$. All the previous expressions hold except for the fact that ϵ_∞ is now a function of q.

Lee, Ting, and Quinn[16] have shown that taking this effect into account has a strong influence on their RPA results. This is also the case in my calculations. I have used b values varying with density[17] from $b = 0.0978$ Å^{-1} at 10^{11} cm^{-2} to $b = 0.1761$ Å^{-1} at 10^{13} cm^{-2} corresponding to a bulk doping of 10^{16} cm^{-3}. The results are not very sensitive to the bulk doping.

The magnitude of the exchange part of the self-energy at the Fermi level is reduced by roughly 25% while the correlation part becomes very nearly a constant of -6 meV. The self-energy varies from -11 to -48 meV in the density range 10^{11} to 10^{13} cm^{-2} to be compared with -18 and -100 meV in the strictly two-dimensional case.

The results for the mass are shown by the dash-dotted curve in Fig. 2. It can be seen that the thickness of the inversion layer strongly reduces the enhancement of the mass. The agreement with experiment is now only qualitative. In view of the discussion of Eq. (10) it should be pointed out that the good agreement reported by Lee, Ting, and Quinn[16] is due to their use of Eq. (10) rather than Eq. (9).

Other contributions to the magnitude of the many-body effects have been studied. It is known that the dielectric constant of SiO_2 shows dispersion at an optical-phonon energy ω_0 of about 55 meV.[18] The oscillator strength S is about 0.8. The Lundqvist-Overhauser approximation for such a system is the usual oscillator model without losses. When the total dielectric function is formed by addition of the polarizability of the electron layer (in the same approximation) one is led to a mixed mode problem with two poles in the density fluctuation operator. Calculations show that the effect of the dispersion is to increase the magnitude of the self-energy at the Fermi level by 24%, 13%, and 8% for $N = 10^{11}$, 10^{12}, and 10^{13} cm^{-2}, respectively. The effect on the mass, however, is very marginal. The change is predicted to be an increase in the mass of at most 0.6%.

The effect of the finite thickness d of the oxide has also been studied. If the metal gate is considered perfectly conducting and one assumes $\omega \ll cq$, the effective dielectric function of the surrounding medium is easily shown to be[19]

$$\epsilon_\infty(q) = \tfrac{1}{2}[\epsilon_{Si} + \epsilon_{SiO_2} \coth(qd)]. \qquad (12)$$

The oxide layer has to be very thin in order to make any change. For $d = 100$ Å the magnitude of the self-energy at the Fermi surface is decreased by 16%, 7%, and 3% for $N = 10^{11}$, 10^{12}, and 10^{13} cm^{-2}, respectively. For the extreme value $d = 50$ Å the changes are 29%, 14%, and 6%, respectively. The effective mass is slightly enhanced by a finite thickness. For $d = 100$ Å the enhancement is 5%, 1.5%, and 0.3% for the same densities. It should be mentioned that strong cancelation occurs since the changes in the derivatives of the self-energy are much larger (about 25% at $N = 10^{12}$ cm^{-2}).

The contribution from the deformation potential electron-phonon interaction has been studied but the effect is very small.

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