PHYSICAL REVIEW B VOLUME 16, NUMBER 8 15 OCTOBER 1977

# Temperature dependence of dynamic conductivity of electrons in the surface inversion layer of semiconducting silicon

A. K. Ganguly
*Naval Research Laboratory, Washington, D.C. 20375*

C. S. Ting*
*Physics Department, University of Houston, Houston, Texas 77004*
(Received 25 April 1977)

The cyclotron resonance of conduction electrons in a semiconducting silicon (100) surface inversion layer is studied by using the memory-function approach. The effects due to electron-impurity and electron-electron interactions are included. The cyclotron-resonance mass shift and the transport lifetime are calculated as functions of temperature, electron concentration, and frequency in the absence of a magnetic field. The obtained mass shift as a function of temperature is compared with the measurement of Kennedy *et al.*, and the agreement is only qualitative.

## I. INTRODUCTION

The cyclotron-resonance experiments of several groups[1-4] have shown that the effective mass of the electrons on the silicon (100) surface inversion layer depends on a number of experimental parameters. The variation of the cyclotron mass with frequency and carrier concentration was observed by Kennedy *et al.*[3] The frequency and temperature dependence of the cyclotron mass has been experimentally studied by Kuhlbeck and Kotthaus[4] and also by Kennedy *et al.*[5] The theoretical aspect of this problem was investigated independently by Ting *et al.*,[6] Tzoar *et al.*,[7] and Ando.[8] The authors of Ref. 7 have calculated the zero-temperature ac conductivity for a two-dimensional interacting electron gas in the absence of a magnetic field and they also discussed the effects at high temperatures where the dielectric function is classical. However the thickness of the surface inversion layer and the valley degeneracy have not been considered in their work. Ting *et al.*[9] have numerically calculated the ac conductivity for a silicon-surface inversion layer in the presence of a strong magnetic field. They find that the line shape of the resonance is sensitive to the single-particle lifetime $\tau$. Since $\tau$ is affected not only by the electron-impurity interaction but also by electron-electron scattering, $\tau$ was not evaluated from first principles but chosen empirically by fitting one of the cyclotron resonance line shapes at each concentration. Although the calculated line shapes agree reasonably well with experiment, the results for cyclotron mass shift are too small to account for the measurements of Ref. 3. Moreover, the electron concentration and the temperature dependence of $\tau$ are not known. It is therefore inconvenient to use the method outlined in Ref. 9 to calculate the variation of the cyclotron mass shift with electron concentration and temperature.

In the present paper, we calculate the ac conductivity of surface inversion layers by using the memory function $M(\omega)$ of Götze and Wölfle,[10] and taking into account the thickness of the surface inversion layer and the valley degeneracy. In this approach, the single-particle lifetime $\tau$ need not be introduced. Therefore the cyclotron mass shift $\Delta m/m$ and the transport lifetime $\tau_{tr}$ can be numerically calculated as functions of concentration, frequency, and temperatures. We neglect the magnetic-field dependence of $M(\omega)$. The effect of the magnetic field $H$ might cause $\Delta m/m$ and $\tau_{tr}$ to oscillate as the frequency (or $H$) or the carrier concentration varies.[9] Since the amplitudes of the oscillations in $\Delta m/m$ and $\tau_{tr}$ are expected to be small, the results with $H=0$ should still yield valuable information about the understanding of the cyclotron resonance in the silicon-surface inversion layer.

In Sec. II, we evaluate the memory function $M(\omega)$, including the electron-electron and electron-impurity interaction. The impurity potential is obtained by solving Poisson's equation in the semiconductor, insulator, and metal with appropriate boundary conditions at the interfaces.[11] $\Delta m/m$ and $\tau_{tr}$ are expressed in terms of $M(\omega)$ and the variations of these quantities with temperature, electron concentration, and frequency are obtained. In Sec. III, the numerical results are presented and compared with experimental data. The final section contains a summary and discussion of our results.

## II. FORMULATION AND CALCULATION

Using the holomorphic memory function approach of Götze and Wölfle,[10] we can express the dynamic conductivity in the presence of a mag-

netic field as[6]

$$\sigma_{\pm}(\omega)=\frac{ine^2/m}{\omega\mp\omega_c+M(\omega)}, \tag{1}$$

where $n$ is the total number of carriers per unit area with charge $e$ and bare band mass $m$, and $\omega_c$ is the frequency of the cyclotron resonance. The memory function $M(\omega)$ as a function of the far-infrared electric field frequency $\omega$ has the form[6]

$$M(\omega)=-\frac{n_i}{Nm\omega}\sum_q |u(q)|^2 q_x^2[s(q,\omega)-s(q,0)]$$

and (2)

$$s(q,\omega)=-i\int_{-\infty}^{\infty} dt\, e^{i\omega t}\Theta(t)\langle[\hat{\rho}_q(t),\hat{\rho}_{-q}(0)]\rangle,$$

where $u(q)$ is the electron-impurity interaction in $q$ space and $n_i$ is the number of impurities per unit area. $\Theta(t)=1$ if $t>0$ and $\Theta(t)=0$ if $t<0$. $\hat{\rho}_{-q}$ is the density operator and $s(q,\omega)$ is the density-density correlation function. The conductivity can be expressed in a more familiar form by introducing a frequency-dependent mass and relaxation time defined by

$$\begin{aligned} m^*(\omega)&=m[1+M_1(\omega)/\omega],\\ \tau_{tr}(\omega)&=M_2^{-1}(\omega)[1+M_1(\omega)/\omega]. \end{aligned} \tag{3}$$

Here $M_1(\omega)$ and $M_2(\omega)$ are, respectively, the real and imaginary parts of $M(\omega)$. From Eqs. (1) and (3) $\sigma_{\pm}(\omega)$ may be written in the Drude form

$$\sigma_{\pm}(\omega)=\frac{ine^2m^*(\omega)}{[\omega\mp eH/m^*(\omega)c]+i\tau_{tr}^{-1}(\omega)}. \tag{4}$$

The fundamental resonance occurs at the frequency $\omega=eH/m^*(\omega)c$. This is renormalized from the bare resonance by a factor $[1+M_1(\omega)/\omega]$. In general, the memory function $M(\omega)$ depends on $\omega$ and $H$. As explained in the introduction, we ignore the dependence of $M(\omega)$ on the magnetic field $H$ and evaluate $M(\omega)$ for $H=0$. Before calculating $M(\omega)$, let us discuss briefly the form of the electron-impurity interaction potential $u(q)$ to be used. If one of the charged impurities is located at the point $(\vec{r}', z')$ in the semiconductor and sets up a potential $\phi(\vec{r}-\vec{r}'; z, z')$ at the point $(\vec{r}, z)$ in the semiconductor, then the Fourier transform of $\phi$, with respect to $\vec{r}-\vec{r}'$ is given by[11]

$$\phi(q,z,z)=\frac{2\pi e}{\epsilon_s q}\left(e^{-q|z-z'|}+\frac{\epsilon_s-\epsilon_0\coth(qD)}{\epsilon_s+\epsilon_0\coth(qD)}\,e^{-q(z+z')}\right). \tag{5}$$

Here we have assumed that the charge carried by the impurity is $+e$. $\epsilon_s$ and $\epsilon_0$ are, respectively, the dielectric constant of the semiconductor and the insulator (oxide). $D$ is the oxide layer thickness. Equation (5) is obtained from classical electrostatics by solving Poisson's equation in the semiconductor, the insulator, and the metal, and imposing the appropriate boundary conditions at the interfaces. The effective unscreened interaction $u(q)$ between an electron and an impurity is taken to be

$$u(q)=-e^2\int_0^{\infty} dz\int_{-\infty}^{\infty} dz'\,|\psi_e(z)|^2 \times|\psi_i(z')|^2\phi(q,z,z'). \tag{6}$$

$\psi_e(z)$ is the wave function of the electron associated with lowest subband of the inversion layer potential well, and it is given by[12]

$$\psi(z)=(\tfrac{1}{2}b^3)^{1/2}ze^{-bz/2}, \tag{7}$$

where $b=3/\langle z\rangle$, and $\langle z\rangle$ measures the thickness of the inversion layer. $\psi_i(z)$ is the wave function describing the motion of the impurity. If we assume that the impurities are located at the interface between the insulator and the semiconductor, i.e., at $z'=0$, then we have

$$|\psi_i(z')|^2=\delta(z'). \tag{8}$$

Substituting Eqs. (7) and (8) into Eq. (6), we get

$$u(q)=(-2\pi e^2/\epsilon_s q)I_i(q/b), \tag{9}$$

where

$$I_i(x)=2(1+x)^{-3}\epsilon_s(\epsilon_s+\epsilon_0\coth Dq)^{-1}.$$

The density-density correlation function $s(q,\omega)$, in the absence of a magnetic field is given by

$$s(q,\omega)=\Pi(q,\omega)/[1-v(q)\Pi(q,\omega)], \tag{10}$$

where $\Pi(q,\omega)$ is the density-density correlation function without the contribution from electron-electron interaction $v(q)$. $\Pi(q,\omega)$ is the form

$$\Pi(q,\omega)=4\sum_{\vec{k}}\frac{n(\vec{k})-n(\vec{k}+\vec{q})}{\omega-\epsilon(\vec{k}+\vec{q})+\epsilon(\vec{k})+i\delta}. \tag{11}$$

Here $n(k)$ is the finite-temperature Fermi function

$$n(k)=(\exp\{[\epsilon(k)-E_F]/k_BT\}+1)^{-1},$$

$k_B$ is the Boltzmann constant, $\epsilon(k)=k^2/2m$ and $E_F$ is the Fermi energy. The factor 4 in front of the summation sign in Eq. (11) is due to spin and valley degeneracies. The effective electron-electron interaction $v(q)$ can be obtained from Eq. (6) by replacing $\psi_i(z')$ with $\psi_e(z')$; the result is[13]

$$v(q)=(2\pi e/\epsilon_s q)I_e(q/b), \tag{12}$$

with

$$I_e(x)=(1+x)^{-6}[\tfrac{1}{8}\times(33+54x+44x^2+18x^3+3x^4)+2\epsilon_s(\epsilon_s+\epsilon_0\coth qD)^{-1}].$$

The final expression for $M(\omega)/\omega$ can be shown to

have the form

$$\frac{M(\omega)}{\omega}=\frac{2me^4}{\epsilon_s^2}\frac{E_F}{\omega^2}\frac{n_i}{N}\int_0^\infty d\eta I_i^2\left(\frac{k_F\eta^{1/2}}{b}\right)\times[Q(\eta,\alpha)-Q(\eta,0)], \quad (13)$$

where

$\eta=q^2/k_F^2$ and $\alpha=\omega/E_F$,

$$Q(\eta,\omega)=\frac{F_1(\eta,\alpha)+F_2(\eta,\alpha)}{1+4me^2/(\epsilon_s\eta^{1/2}k_F)I_e(k_F\eta^{1/2}/b)[F_1(\eta,\alpha)+F_2(\eta,\alpha)]}, \quad (14)$$

$$F_1=\int_0^1\frac{d\xi}{(1-\xi)^{1/2}}\frac{1}{4\eta}[\phi(B,\xi,\eta)-\phi(A,\xi,\eta)], \quad (15)$$

$$F_2=\frac{1}{2(\eta\xi_F)^{1/2}}\int_0^1\frac{d\xi}{(-\ln\xi)^{1/2}}[\psi(A,\xi,\eta)-\psi(B,\xi,\eta)], \quad (16)$$

with

$$\phi(x,\xi,\eta)=x\left\{\exp\left[\left(\frac{x^2\xi}{4\eta}-1\right)\xi_F\right]+1\right\}^{-1}, \quad (17)$$

$$\psi(x,\xi,\eta)=\left\{\exp\left[\left(\frac{x^2\xi}{4\eta}-1\right)\xi_F\right]+\xi\right\}^{-1}. \quad (18)$$

Here $\xi=k^2/k_F^2$, $\xi_F=\xi_F/k_BT$, $A=\alpha-\eta$, and $B=\alpha+\eta$. The Fermi energy $E_F$ is a temperature-dependent quantity and has to be determined self-consistently from the equation of charge conservation

$$4\int\int\frac{d^2k}{(2\pi)^2}n(k)=n, \quad (19)$$

where $n$ is the number of electrons per unit area. Performing the integration in Eq. (19) it is found that

$$E_F=k_BT\ln[\exp(n\pi/2mk_BT)-1]. \quad (20)$$

## III. RESULTS

$M(\omega)$ is obtained numerically from Eqs. (13)–(18). $\Delta m/m=(m^*-m)/m$ and $\tau_{tr}(\omega)$ may then be calculated from Eq. (3) as functions of temperature and electron concentration. The impurity concentration $n_i$ is calculated from

$$\frac{1}{\tau_{tr}}=\frac{mn_i}{2\pi}\int_0^{2\pi}\left|\frac{u(q)}{\epsilon(q,0)}\right|^2(1-\cos\phi)\,d\phi, \quad (21)$$

where $q=2k_F(1-\cos\phi)^{1/2}$, and $\epsilon(q,0)=1-v(q)\pi(q,0)$. $\epsilon(q,0)$ can be obtained from Eq. (11). The static transport lifetime $\tau_{tr}$ is realted to the mobility by

$$\mu=(e/m)\tau_{tr}. \quad (22)$$

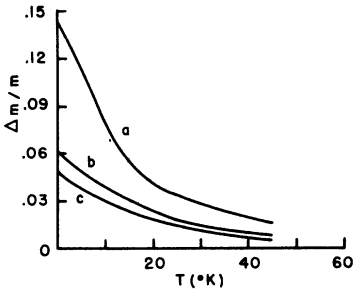


FIG. 1. Cyclotron resonance mass shift ($\Delta m$) as a function of temperature for three different electron concentrations ($n$): (a) $n=3.2\times10^{11}$ cm$^{-2}$, (b) $n=6.4\times10^{11}$ cm$^{-2}$, and (c) $n=7.7\times10^{11}$ cm$^{-2}$. Other parameters used are $n_i=7.5\times10^{10}$ cm$^{-2}$ and $\omega=25.4$ cm$^{-1}$.

By knowing the mobility $\mu$ at a particular carrier density $n$, one is able to obtain $n_i$ from Eqs. (21) and (22).[14] For[5] $\mu=13\,000$ cm$^2$/V s and $n=7.7\times10^{11}$/cm$^2$, it is found that $n_i=7.5\times10^{10}$/cm$^2$. We use $\epsilon_s=11.8$ and $\epsilon_0=3.8$ for the dielectric constants of silicon, and oxide layer thickness $D$ is taken to be 1000 Å. The thickness of the inversion layer is take as $\langle z\rangle\simeq20\,[3\times10^{12}/n]^{1/3}$ Å.

The results of numerical calculation are shown in Figs. 1–4 for frequency 25.4 cm$^{-1}$. $\Delta m/m$ and $\tau_{tr}$ are plotted in Figs. 1 and 2, respectively, as functions of temperature for three different electron concentrations. $\Delta m/m$ and $\tau_{tr}(\omega)$ decrease with temperature. While $\Delta m/m$ decreases with electron concentration, $\tau_{tr}(\omega)$ increases with $n$. In Fig. 3, theoretical and experimental[5] values of $m^*$ are compared as functions of temperature for three different electron concentrations. The band mass is taken to be $0.195m_0$. The experimental values of $m^*$ at $n=3.2\times10^{11}$ cm$^{-2}$ and $n=6.4\times10^{11}$ cm$^{-2}$ for $T\leq30$ °K are in general decreasing much faster than the calculated values. The experimental value of $m^*$ at $n=3.2\times10^{11}$ cm$^{-2}$ and $T\simeq35$°K indicates that the electron-phonon interaction might play an important role at higher temperatures. Within the experimental uncertainties, the measured values of $m^*$ at $n=1.6\times10^{12}$ cm$^{-2}$

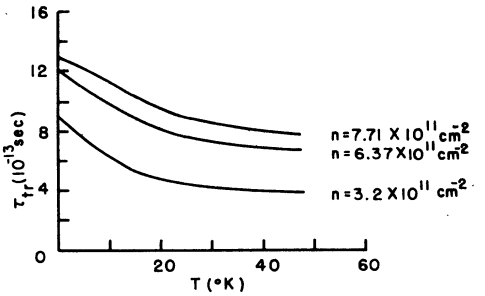


FIG. 2. Transport lifetime $\tau_{tr}$ vs temperature for the same parameters as in Fig. 1.

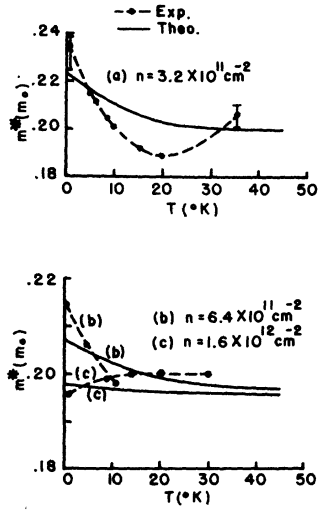


FIG. 3. Comparison between theoretical and experimental values (see Ref. 5) of $\Delta m$ as function of temperature for three different values of electron concentration ($n$): (a) $n=3.2\times10^{11}$ cm$^{-2}$, (b) $n=6.7\times10^{11}$ cm$^{-2}$, and (c) $n=1.6\times10^{12}$ cm$^{-2}$. The solid and the dashed lines denote theoretical and experimental values, respectively. $n_i=7.5\times10^{10}$ cm$^{-2}$, $\omega=25.4$ cm$^{-1}$ and $m=0.195\,m_0$.

are almost independent of temperature, and this is in agreement with our calculation. Figure 4 shows the variation of $\Delta m/m$ with electron concentration at two different temperatures. Initially, $\Delta m/m$ decreases rapidly with electron concentration and then tails off. This feature agrees qualitatively with the measurements of Kuhbeck and Kotthaus.[4] In Fig. 5, $\Delta m/m$ at $T=0$ is plotted as a function of frequency $\omega$ for two different samples. One of them with $\mu=6500$ cm$^2$/V s at $n=1.5\times10^{12}$/cm$^2$ has been studied by Kennedy *et al.*[3]; the other with $\mu=7000$ cm$^2$/V s at $n=2.6\times10^{12}$/cm$^2$ has been studied by Abstreiter *et al.*[2] Our results which have shown a 3% effect are within the experimental error bars of Abstreiter *et al.* Although the calculated $\Delta m/m$ as function of $\omega$ qualitatively agrees with the measurements of Kennedy *et al.*,[3] it is still not big enough to account for the

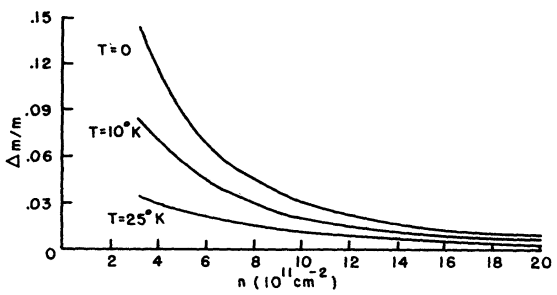


FIG. 4. $\Delta m/m$ as a function of electron concentration for three different values of temperature $T=0$, 10, and 25 °K at $\omega=25.4$ cm$^{-1}$ and $n_i=7.5\times10^{10}$ cm$^{-2}$.

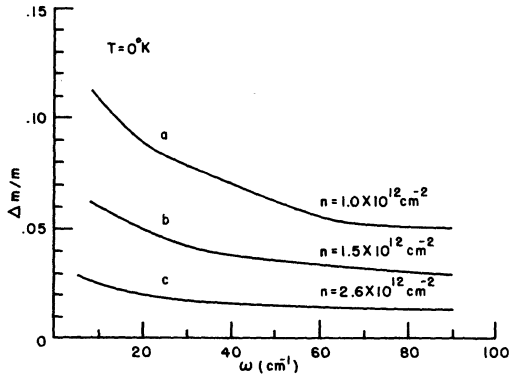


FIG. 5. $\Delta m/m$ as a function of frequency at $T=0$. Curves (a) and (b) are for the sample of Ref. 3 with $\mu=6500$ cm$^2$/V s at $n=1.5\times10^{12}$ cm$^{-2}$ and curve (c) is for the sample of Ref. 4 with $\mu=7000$ cm$^2$/V s at $n=2.6\times10^{12}$ cm$^{-2}$.

experimental 10% effect on $\Delta m/m$ at $\omega=10$ cm$^{-1}$ for $n=1.5\times10^{12}$ cm$^{-2}$. In the last two figures, we have not attempted to make a quantitative comparison with experimental measurements.

## IV. DISCUSSION

In this paper, we have studied the dependence of the cyclotron resonance mass on temperature, frequency, and density from the memory-function approach. The effects of electron-impurity and electron-electron interactions are included and the contribution from electron-phonon interaction is neglected.[4] The frequency-dependent effective mass and the transport lifetime are related to the memory function $M(\omega)$ through Eq. (3). $M(\omega)$ is calculated only in the absence of a magnetic field. The theoretically obtained cyclotron resonance mass shift $\Delta m$ as functions of electron density and frequency agrees qualitatively with experimental results,[3,4] but not quantitatively. The temperature dependence of $\Delta m$ was measured by Kuhlbeck and Kotthaus[4] from $n\simeq2\times10^{11}$ cm$^{-2}$ to $n=1.5\times10^{12}$ cm$^{-2}$. They observed that the effective cyclotron mass $m^*$ always increases with temperature $T$; our calculated result for $m^*$ however shows that $m^*$ decreases with temperature. A most recent experiment by Kennedy *et al.*,[5] who have used a high mobility sample ($\mu=13\,000$ cm$^2$/V s at $n=7.7\times10^{11}$ cm$^{-2}$), shows that $m^*$ is almost independent of $T$ at $n=1.6\times10^{12}$ cm$^{-2}$ and $m^*$ decreases with $T$ at $n=6.37\times10^{11}$ cm$^{-2}$ and $n=3.2\times10^{11}$ cm$^{-2}$. Their measurements[5] agree qualitatively with our calculation. The discrepancy between the results of these two experiments[4,5] at low density ($n<10^{12}$ cm$^{-2}$) is not clear to us at this moment. One possible explanation is that the electrons in the sample of Ref. 4, in which $n_i=2.1\times10^{11}$ cm$^{-2}$,[15] see more scattering centers and then form Mott-An-

derson[16] localized states more easily than the electrons in the sample of Ref. 5, in which $n_i = 0.75 \times 10^{11}$ cm$^{-2}$. It is possible that the conductivity of the first sample[4] becomes thermally activated for $n \leq 1.0 \times 10^{12}$ cm$^{-2}$ while the conductivity of the second sample[5] remains metallic until $n \leq 3 \times 10^{11}$ cm$^{-2}$. Since our calculation is valid only in the metallic region, the qualitative agreement with the measurements of Ref. 5. is not unexpected. Our calculated values of $\Delta m/m$ as functions of electron concentration and frequency agree qualitatively, but not quantitatively, with the results in Refs. 2, 3, and 4. Finally, we wish to compare our calculations with the results of Tzoar *et al.*[7] Our calculated values of $\Delta m/m$ as functions of frequency and concentration are larger but behave very similarly to theirs. For example, our $\Delta m/m$ for $n = 1.0 \times 10^{12}$ cm$^{-2}$ and $\omega = 20$ cm$^{-1}$ at $T = 0$°K is almost one-third larger than the value obtained[7] by them. This discrepancy is primarily due to the fact that the valley degeneracy has not been considered in their work. They also discussed very qualitatively the effects at high temperatures where the dielectric functions is classical,[7] and found that $\Delta m/m$ becomes very small, and that the resistivity (or $1/\tau_{tr}$) is roughly a factor of 2 smaller than at zero temperature. Our numerical results for the temperature dependence of $\Delta m/m$ agree qualitatively with their prediction. However, our calculation shows that $1/\tau_{tr}$ (or the resistivity[17]) increases and then seems to level off as the temperature is raised. This is completely contradictory to their prediction.[7] We have checked our calculation very carefully and we are not able to reproduce their high-temperature resistivity result.[7]

---

*Research supported partly by Research Initial Grant, Office of Research at the University of Houston.

[1]G. Abstreiter, P. Kneschanrek, J. P. Kothaus, and F. J. Koch, Phys. Rev. Lett. 32, 104 (1974); J. S. Allen, D. C. Tsui, and J. V. Dalton, *ibid.* 32, 107 (1974).

[2](a) J. P. Kotthaus, G. Abstreiter, and J. F. Koch, Solid State Commun. 15, 517 (1974); (b) G. Abstreiter, J. F. Koch, P. Goy, and Y. Goulder, Phys. Rev. B 14, 2494 (1976).

[3]T. A. Kennedy, R. J. Wagner, B. D. McCombe, and D. C. Tsui, Phys. Rev. Lett. 35, 1031 (1975).

[4]H. Kuhlbeck and J. P. Kotthaus, Phys. Rev. Lett. 35, 1019 (1975).

[5]T. A. Kennedy, R. J. Wagner, B. D. McComb, and D. C. Tsui (unpublished); T. A. Kennedy, Bull. Am. Phys. Soc. 22, 304 (1977).

[6]C. S. Ting, S. C. Ying, and J. J. Quinn, Phys. Rev. Lett. 37, 215 (1976).

[7]N. Tzoar, D.M. Platzman, and A. Simons, Phys. Rev. Lett. 26, 1200 (1976).

[8]T. Ando, Phys. Rev. Lett. 36, 1383 (1976). There is no cyclotron mass shift from Ando's approach.

[9]C. S. Ting, S. C. Ying, and J. J. Quinn, Phys. Rev. B (to be published).

[10]W. Götze and P. Wölfle, Phys. Rev. B 6, 1226 (1972).

[11]A. V. Chaplik, Zh. Eksp. Teor. Fiz. 62, 746 (1972) [Sov. Phys.-JETP 35, 395 (1972).

[12]F. Stern and W. E. Howard, Phys. Rev. 163, 816 (1967).

[13]T. Ando and Y. Uemura, J. Phys. Soc. Jpn. 37, 1044 (1974); F. Stern, J. Appl. Phys. Jpn. Suppl. 2, 323 (1974).

[14]We have assumed here that the impurities are located at the interface between the oxide and the semiconductor, and they are charged. The effects due to the surface roughness have not been considered. Therefore, Eq. (21) is only an approximation.

[15]Sample used in Ref. 4 has $\mu = 7000$ cm$^2$/V s at $n = 2.6 \times 10^{12}$ cm$^{-2}$. Using Eq. (21) and (22) we obtain the number of impurities per unit area as $n_i = 2.1 \times 10^{11}$ cm$^{-2}$.

[16]N. F. Mott, Philos. Mag. 13, 689 (1966); P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[17]The resistivity is given by $\rho = (1/Ne^2)m^*/\tau_{tr}$. Here $\tau_{tr}$ and $m^*$ is obtained from Eq. (3) by letting $\omega \to 0$. For samples with $n = 1.0 \times 10^{12}$ cm$^{-2}$ to $n = 2.0 \times 10^{12}$ cm$^{-2}$ and $n_i \simeq 0.31 \times 10^{12}$ cm$^{-2}$, $m^*$ is weakly temperature dependent. The dominant temperature-dependent quantity comes from $\tau_{tr}$.