Calculated Temperature Dependence of Mobility in Silicon Inversion Layers

Frank Stern
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598
(Received 3 March 1980)

Calculations of the temperature dependence of mobility have been carried out for silicon (001) inversion layers in which Coulomb scattering and surface roughness scattering, but not phonon scattering, are included. The wave-vector and temperature dependence of screening contribute to a temperature-dependent part of the scattering rate that increases approximately linearly with temperature from 0 to 40 K. The results are supported by recent experiments of Cham and Wheeler.

PACS numbers: 73.25.+i, 73.40.Lq

Phonon scattering in inversion layers has been of interest for many years, but has been a puzzle because the temperature-dependent part of the resistivity is much larger than predicted from phonon scattering alone.[1] Recent data[2-4] on the temperature dependence of mobility at low temperatures have generated new interest in this problem, because the theory should be directly applicable when only one subband is occupied and when intervalley phonon processes are weak.

I present results of calculations for the temperature dependence of mobility showing that a substantial temperature dependence arises from Coulomb scattering and surface roughness scattering, without phonon scattering. The magnitude, sample mobility dependence, and carrier concentration dependence of the calculated effects are in good agreement with new results of Cham and Wheeler[5] when Coulomb scattering is dominant. Thus a significant part of the observed temperature dependence appears to arise from sources other than phonon scattering, and the long-standing puzzle about its magnitude may have a very simple explanation.

The models used in the present calculation are familiar and will not be described here. The two principal scattering mechanisms, Coulomb scattering[6] from charges near the semiconductor-insulator interface (also called oxide charge scattering) and surface roughness scattering,[7] are both screened. A generalization that allows for numerical self-consistent wave functions rather than variational wave functions has already been described.[8] Numerical self-consistent wave functions that vanish at the semiconductor-insulator interface are used in the present calculation.

A key element in the calculation is the use of the full dependence of the screening parameter q_s on temperature T and on wave vector q. Its wave-vector dependence at $T=0$ and temperature dependence at $q=0$ have already been given.[6,9] Maldague[10] showed how the polarizability, which is proportional to the screening parameter, could be calculated for arbitrary q and T. Results for q_s for a silicon (001) inversion layer with 2×10^{12} electrons/cm^2 are shown in Fig. 1.

Figure 2 shows how the wave-vector dependence of q_s influences the scattering rate

$$\tau^{-1}(E)=\int_{-\pi}^{\pi}\tau^{-1}(\kappa,\theta)(1-\cos\theta)\,d\theta. \quad (1)$$

Here $E=\hbar^2\kappa^2/2m^*$, where m^* is the effective mass for motion parallel to the surface, and $\tau(\kappa,\theta)$ is the rate for scattering into a unit angular interval at scattering angle θ. Figure 2 shows that inclusion of the full wave-vector dependence of screening increases the scattering rate significantly.

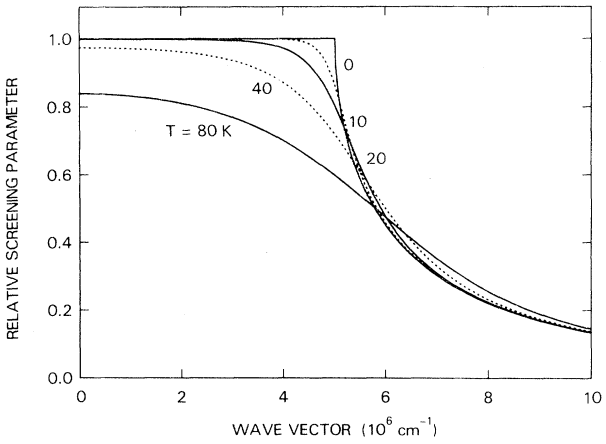

FIG. 1. Relative screening parameter $q_s(q,T)/q_s(0,0)$ as a function of wave vector q at $T=0$, 10, 20, 40, and 80 K for a (001) Si inversion layer with 2×10^{12} electrons/cm^2, for which the Fermi-circle diameter is $2k_F=5.013\times10^6$ cm^{-1}. The magnitude of the screening parameter at long wavelengths and low temperatures is $q_s(0,0)=1.23\times10^7$ cm^{-1} if the silicon dielectric constant is taken to be 11.7.

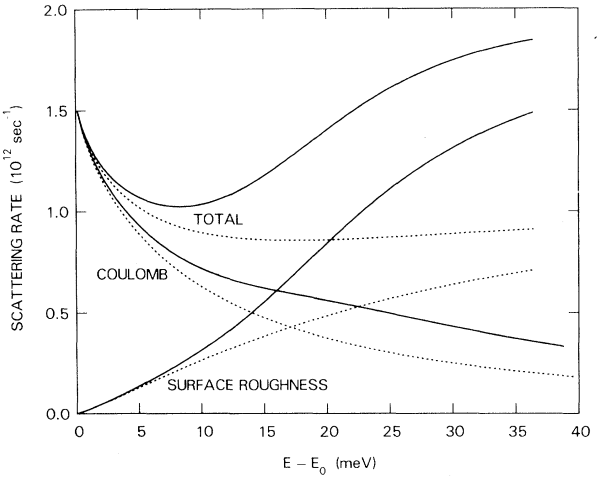

FIG. 2. Dependence of the scattering rate $\tau(E)$, which enters in Eq. (2), for Coulomb scattering, surface roughness scattering, and for the sum of the two, on the energy above E_0, the bottom of the lowest subband. The dashed curves use the long-wavelength limit for the screening parameter and the full curves include the wave-vector dependence. All curves are for a (001) Si inversion layer at 40 K with 2×10^{12} electrons per square centimeter on a substrate with 8.9×10^{15} bulk acceptors per cubic centimeter, 10^{11} Coulomb scatterers per square centimeter at the Si-SiO_2 interface, and surface roughness with an rms height of 0.6 nm and a lateral correlation length of 1.3 nm. The Fermi level in this example lies at $E_F - E_0 = 12.5$ MeV, and $k_BT = 3.4$ MeV.

Figure 3 gives the temperature dependence of the scattering rate for Coulomb and roughness scattering separately and for the combined scattering, where

$$\tau = \frac{\int_0^\infty \tau(E)E(-df_0/dE)\,dE}{\int_0^\infty E(-df_0/dE)\,dE} \tag{2}$$

and f_0 is the Fermi-Dirac distribution. The mobility is $\mu = e\tau/m^*$. As is well known,[11-13] the energy-averaged scattering rates do not add in general, i.e.,

$$1/\tau \geq 1/\tau_{ox} + 1/\tau_{s.r.}, \tag{3}$$

because the averaging in Eq. (2) is for τ rather than for $1/\tau$. Equation (3) becomes an equality in some special cases, notably at absolute zero where there is no averaging over a range of energies. Thus Matthiessen's rule[13] on the additivity of resistivities for different scattering mechanisms will not hold in most cases at temperatures above absolute zero. The present calculations show that the left side of Eq. (3) can exceed the right side by as much as 15% at 40 K when $N_s = 2\times10^{12}$ cm^{-2}, with the largest errors found when the component scattering mechanisms are of about the same strength. The differences are smaller for higher electron concentrations and for lower temperatures. The deviations from Matthiessen's rule are illustrated in Fig. 3. A model calculation for a series of samples with fixed roughness scattering and with oxide charge density varying from 0 to 10^{12} cm^{-2} shows that the slope of the curve of reciprocal mobility versus oxide charge gives the oxide charge scattering quite accurately while the intercept at zero oxide charge overestimates the other contributions to the scattering by an amount of order 30% at 40 K

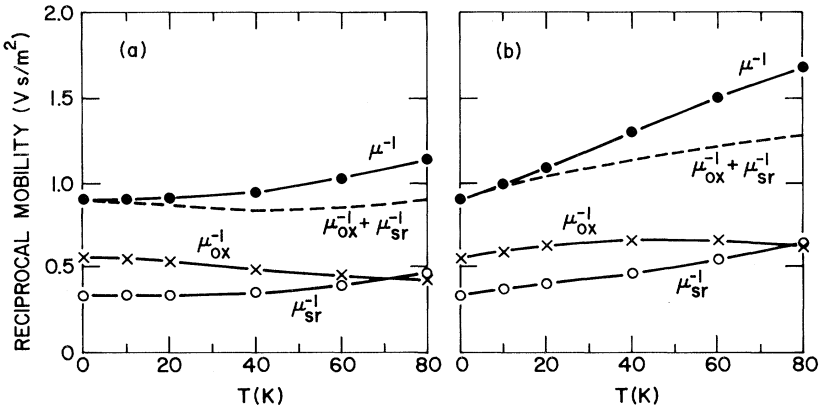

FIG. 3. Temperature dependence of reciprocal mobility for a silicon inversion layer, with all electrons assumed to be in the lowest subband, with (a) the long-wavelength limit for the temperature-dependent screening parameter and (b) the full wave-vector dependence. Results are shown for oxide charge scattering alone, surface roughness scattering alone, and for the sum of the two mechanisms. The difference between the upper full curve and the dashed curve shows the departure from Matthiessen's rule. All parameters as in Fig. 2.

for $N_s = 2\times10^{12}$ cm^{-2}, with smaller errors at lower temperatures or higher values of N_s.

Comparison of Figs. 3(a) and 3(b) shows that it is the wave-vector dependence of the screening which is principally responsible for the temperature dependence of the mobility at low temperatures. When the long-wavelength limit is used, the scattering has a very weak temperature dependence up to 20 K, at least for the parameters of this figure. At absolute zero, where the maximum wave-vector change on scattering is the Fermi-circle diameter, $2k_F$, the screening is constant, and use of the long-wavelength limit is correct. Because of intuition based on calculations at low temperatures, the importance of the wave-vector dependence has been largely overlooked in discussions of transport properties of inversion layers, although it is known to have a significant effect on electron mobility in bulk multivalley semiconductors such as GaSb (Ref. 14) and Ge (Ref. 15). An increase in the Coulomb scattering rate with increasing temperature, in qualitative agreement with the present results, was found by Ganguly and Ting[16] in connection with calculations of the temperature dependence of the cyclotron-resonance mass in silicon inversion layers but was not related to the apparent anomaly in the phonon scattering contribution to the resistivity.

The temperature-dependent part of the scattering rate, defined as

$$\frac{1}{\tau_T} \equiv \frac{1}{\tau(T)} - \frac{1}{\tau(0)}, \tag{4}$$

has been compared with experiment by Cham and Wheeler.[5] For a sample with 4×10^{14} bulk acceptors per cubic centimeter, with 10^{12} Coulomb scatterers per square centimeter at the semiconductor-insulator interface, and with no surface roughness scattering, the calculations give

$$\tau_T^{-1} \sim 0.14\times\left(\frac{N_s}{2\times10^{12}\ \mathrm{cm}^{-2}}\right)^{-(1.9\pm0.1)}\ \mathrm{ps}^{-1} \tag{5}$$

at 4.5 K, which is in satisfactory agreement with the experimental results. The calculated values increase approximately linearly with T to about 40 K. They are thought to have numerical precision of ~2% at $N_s = 10^{12}$ cm^{-2} and ~10% at $N_s = 5\times10^{12}$ cm^{-2}.

In higher-mobility samples, where Coulomb scattering is less important, the temperature dependence of resistivity found by Cham and Wheeler is weaker than the calculated result and is superlinear where the calculated result is approximately linear. The resistivities measured by Kawaguchi and Kawaji[2] also increase faster than linearly with increasing T at low temperatures. My calculations predict that for high-mobility samples at large N_s values, τ_T^{-1} will increase with increasing N_s, rather than decreasing as found for Coulomb scattering. There is no evidence for such an increase in the published data at present.

Hartstein, Fowler, and Albert[4] measured the mobility in (001) Si inversion layers at several temperatures from 4.2 to 80 K for samples with varying oxide charge density and determined the oxide charge scattering for several values of N_s. For $N_s = 3\times10^{12}$ cm^{-2} they found a 5% increase of oxide charge scattering between 4.2 and 32 K, somewhat less than the 7% increase given by the present calculations. At 7×10^{12} cm^{-2} the measured temperature dependence is weak, and at 1.2×10^{13} cm^{-2} the oxide charge scattering decreases with increasing temperature. At these higher values of N_s, carriers will be in more than one subband and the simple calculation presented here does not apply.

Scattering effects are likely to round the sharp corner in the screening parameter of Fig. 1 at very low temperatures, by analogy with corresponding effects in three dimensions,[17] and could therefore modify the temperature dependence calculated here.

I am indebted to K. M. Cham and R. G. Wheeler for many valuable discussions of their data and of the relation of the data to the present model, to A. B. Fowler and A. Hartstein for making unpublished data available and for valuable discussions, and to T. M. Rice for pointing out the effect of scattering on the screening.

[1]H. Ezawa, S. Kawaji, and K. Nakamura, Jpn. J. Appl. Phys. 13, 126 (1974).

[2]Y. Kawaguchi and S. Kawaji, in Proceedings of the Third International Conference on Electronic Properties of Two-Dimensional Systems, Lake Yamanaka, Japan, September, 1979 (to be published), and to be published.

[3]K. M. Cham and R. G. Wheeler, in Proceedings of the Third International Conference on Electronic Properties of Two-Dimensional Systems (Yamada Conference II, Lake Yamanaka, Japan, September, 1979 (to be published).

[4]A. Hartstein, A. B. Fowler, and M. Albert, in Proceedings of the Third International Conference on Electronic Properties of Two-Dimensional Systems

(Yamada Conference II, Lake Yamanaka, Japan, September, 1979 (to be published).
[5]K. M. Cham and R. G. Wheeler, following Letter [Phys. Rev. Lett. 44, 1472 (1980)].
[6]F. Stern and W. E. Howard, Phys. Rev. 163, 816 (1967).
[7]Y. Matsumoto and Y. Uemura, Jpn. J. Appl. Phys. Suppl. 2, Pt. 2, 367 (1974).
[8]F. Stern, Surf. Sci. 73, 197 (1978).
[9]F. Stern, Phys. Rev. Lett. 18, 546 (1967).
[10]P. F. Maldague, Surf. Sci. 73, 296 (1978).
[11]See, for example, R. Mansfield, Proc. Phys. Soc. London, Sect. B 69, 76 (1956), and references therein to earlier work.
[12]P. K. Basu, Indian J. Pure Appl. Phys. 14, 769 (1976).
[13]See, for example, J. M. Ziman, *Electrons and Phonons* (Oxford Univ. Press, Oxford, England, 1960), pp. 286, 337, 434.
[14]J. E. Robinson and S. Rodriguez, Phys. Rev. 137, A663 (1965).
[15]J. B. Krieger and T. Meeks, Phys. Rev. B 8, 2780 (1973).
[16]A. K. Ganguly and C. S. Ting, Phys. Rev. B 16, 3541 (1977).
[17]P. G. de Gennes, J. Phys. Radium 23, 630 (1962).

Temperature-Dependent Resistivities in Silicon Inversion Layers at Low Temperatures

K. M. Cham and R. G. Wheeler
Department of Engineering and Applied Science, Yale University, New Haven, Connecticut 06520
(Received 3 March 1980)

The temperature dependence of the resistivities of n-type silicon inversion layers at liquid helium temperatures was studied in detail. The temperature dependence was found to be correlated to the mobility of the sample. Our results can be explained by Coulomb scattering, with possible contributions by surface-roughness scattering in high-mobility samples.

PACS numbers: 73.25.+i, 73.40.Lq

The electrons in a silicon inversion layer have the properties of a quasi two-dimensional system, with the advantage that the surface electron density (n_s) and the effective thickness ($\langle z \rangle$) of the layer can be varied continuously.[1] The temperature dependence of the resistivity at liquid helium temperatures had been studied recently by several authors[2,3] and was interpreted as due to electron-phonon scattering. We have made extensive studies of this temperature dependence as a function of n_s, $\langle z \rangle$, and the quality of the device, as given by the maximum effective mobility at 4.2 °K (μ_m) which ranged from 2400 to 22 000 $cm^2/V \cdot sec$.

In the metallic regime, where the conductivity shows no activated behavior, the mobility of the inversion layer at liquid helium temperatures is known to be limited by Coulomb scattering and surface-roughness scattering, and at higher temperatures also by electron-phonon scattering.[1,4] With use of Matthiessen's rule (which is an approximation in our case[5]), the resistivity is given by

$$\rho = \rho_C + \rho_{s.r.} + \rho_{e-ph} \quad (1)$$

with obvious abbreviations. ρ_C has been observed to be temperature dependent,[4] but detailed measurements have not been made at liquid helium temperatures. ρ_{e-ph} is obviously temperature dependent and is often considered to be the dominant temperature-dependent part of the total resistivity.

Resistivities ρ of n-channel metal-oxide-semiconductor field-effect transistors, fabricated on 30–40-ohm-cm [001] p-type substrates, were measured with both two-point and four-point probes with measuring fields $\lesssim 4$ mV/cm (as guided by hot-electron–effect measurements) to avoid heating effects.[2] The devices were drawn from an inventory accumulated over a two-year period of processing experimentation. The samples were immersed in liquid helium within a light-tight container mounted with a germanium thermometer. A light-emitting diode supplied radiation to the substrate in order to assist electrostatic equilibrium. The oxide fixed charge density, Q_{ss}, was estimated from flat-band shifts in C-V measurements for thick oxide devices ($\gtrsim 1000$ Å), and estimated from mobilities for thin oxide devices. Measurements of Shubnikov–de Haas extrema for $n_s > 10^{12}$ cm^{-2} as a function of temperature on three samples have assured