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Theory of Scattering of Electrons in a Nondegenerate-Semiconductor-Surface Inversion Layer by Surface-Oxide Charges*

T. H. Ning† and C. T. Sah

Department of Electrical Engineering and Materials Research Laboratory,
University of Illinois, Urbana, Illinois 61801

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We present a systematic study of the effects of (i) the screening by mobile carriers, (ii) the correlation of the oxide charges, (iii) the distribution of the surface-oxide charges in the oxide, and (iv) the distribution of the electrons in the surface channel on the electron mobility in a nondegenerate-semiconductor-surface inversion layer covered with an insulator or oxide. It is found that the Debye–Huckel screening parameter for a two-dimensional classical electron gas is not valid for most ranges of temperature and electron concentration of practical interest. In these temperature and electron concentration ranges, the formula overestimates the screening effect. The effect of position correlation of the surface-oxide charges on the surface mobility is discussed in detail in the hard-sphere model. Correlation effect is important, especially at low temperatures where the mean electron wavelength is greater than the mean separation among the surface-oxide charges. Both the distribution of the surface-oxide charges in the oxide layer and the distribution of the electrons in the surface channel have similar effects in reducing scattering. Evaluation of experimental surface-conductivity mobility of electrons in a nondegenerate Si-SiO$_2$ surface channel due to scattering by surface-oxide charges is made.

I. INTRODUCTION

The influence of the built-in surface-oxide charges on the electron transport in n-type inversion channels on oxide-covered silicon surfaces has been demonstrated in the past few years.[1–4] Recently we reported a more quantitative study of the electron-conductivity mobility in weakly inverted and nondegenerate silicon surface channels as a function of temperature and the surface-oxide charge density.[5] At low temperatures and high surface-oxide charge densities, where scattering by lattice vibrations is unimportant, the observed mobility varied as T/N_I, where T is the temperature and N_I is the average density of the surface-oxide charges. Such temperature and oxide charge concentration dependence was predicted by a simple two-dimensional model of scattering by surface-oxide charges randomly distributed at the oxide-semiconductor interface.[5] The mobility, assuming that both the scattering ions and the electrons are confined in a sheet, is[5]

$$\mu_0 = \frac{e}{m_\mu}\left(\frac{\bar{\epsilon}}{e^2}\right)^2 \frac{2\hbar k_B T}{\pi^2 N_I}, \qquad (1.1)$$

where $\bar{\epsilon} = \frac{1}{2}(\epsilon_{\mathrm{Si}} + \epsilon_{\mathrm{ox}})$ and m_μ is the mobility effective mass. The observed mobility, however, is about 20 times larger than the value predicted by this simple two-dimensional model, if bulk values of $\bar{\epsilon}$ and m_μ are used.[5]

The simple two-dimensional model, which leads to the electron mobility given by Eq. (1.1), is very idealized. Several factors have been neglected which may be responsible for the discrepancy between theory and experiment. These are (i) the screening by mobile electrons in the surface channel, (ii) the finite distribution of the surface-oxide charges into the oxide layer, (iii) the correlation effect of the surface-oxide charge distribution, and (iv) the electron distribution into the semiconductor layer.

In this paper, we present a systematic study of the effects of these factors on the scattering of electrons in a nondegenerate surface channel, and determine the relative importance of these factors. We shall limit ourselves to nondegenerate surface channels where classical statistics apply since, through the temperature dependence of the mobility, they provide more information on the scattering mechanism than degenerate surface channels. The effect of screening on the mobility is studied first in Sec. II. The validity of screening for a two-dimensional classical election gas is also discussed. In Sec. III the effect of correlation of the surface-oxide charges is studied. Detailed discussion is given in the hard-sphere model for a δ-function distribution at the oxide-semiconductor interface. The results are then extended in Sec. IV to include the effect of finite distribution of the surface-oxide charges into the oxide layer. Finally, in Sec. V we study the effect of the finite electron distribution in the surface channel on the surface mobility.

Although we refer to the metal-Si-SiO$_2$ structure as our physical system, the results and discussions presented here should also apply to electronic transport in the surface channels of other systems.

II. CLASSICAL SCREENING EFFECTS FOR TWO-DIMENSIONAL ELECTRON GAS

A. Screening Parameter and Its Validity

The wave-vector-dependent static dielectric function for a two-dimensional electron gas has been obtained by Stern[6] as

$$\epsilon(\vec{q}) = \epsilon_b + 2\pi q \chi(\vec{q}) , \tag{2.1}$$

where ϵ_b is the dielectric constant of the surrounding medium and $\chi(\vec{q})$ is the polarizability of the electron gas:

$$\chi(\vec{q}) = \frac{e^2}{q^2 A} \sum_{\vec{k}} \frac{f_0(E_{\vec{k}}) - f_0(E_{\vec{k}+\vec{q}})}{E_{\vec{k}+\vec{q}} - E_{\vec{k}}} . \tag{2.2}$$

Here the sum is taken over all one-electron states, $E_{\vec{k}} = \hbar^2 k^2/2m^*$ is their energy, A is the normalization area, and f_0 is the Fermi–Dirac occupation function. For a classical electron gas, we have

$$f_0(E_{\vec{k}}) = e^{(E_F - E_{\vec{k}})/k_B T} , \tag{2.3}$$

where E_F is the Fermi energy. Substituting (2.3) into (2.2) and converting the summation into a sum over spin states and an integral over $\vec{k}$ space, we find

$$\chi(\vec{q}) = (e^2 m^* n_v / q^2 \pi \hbar^2)\, e^{E_F/k_B T} F(q) , \tag{2.4}$$

where n_v is the valley-degeneracy factor, and $F(q)$ is given by

$$F(q) = \tfrac{1}{2} \int_0^1 e^{-bx}/(1-x)^{1/2}\, dx , \tag{2.5a}$$

with

$$b = \hbar^2 q^2 / 8 m^* k_B T . \tag{2.5b}$$

The screening parameter s is defined by

$$\epsilon(\vec{q}) = \epsilon_b (1 + s/q) . \tag{2.6}$$

Using (2.1) and (2.4), we obtain

$$s = (2e^2 m^* n_v / \epsilon_b \hbar^2) e^{E_F/k_B T} F(q) \tag{2.7a}$$

$$= (2\pi e^2 N / \epsilon_b k_B T) F(q), \tag{2.7b}$$

where

$$N = (1/A) \textstyle\sum_{\vec{k}} f_0(E_{\vec{k}})$$

$$= (m^* n_v k_B T / \pi \hbar^2) e^{E_F/k_B T} \tag{2.8}$$

is the number of electrons per unit area. Equation (2.7b) shows that the screening parameter for a two-dimensional nondegenerate electron gas is proportional to the electron density, in contrast with the degenerate electron gas for which the screening parameter is independent of the electron density at 0 °K.[6–8]

As defined by Eq. (2.6), s is a function of the wave vector $\vec{q}$ through the function $F(q)$. If we consider the elastic scattering of an electron of energy $E_k = \hbar^2 k^2/2m^* = k_B T$ from state $|\vec{k}\rangle$ into state $|\vec{k}'\rangle$, then the appropriate value of q is $q = 2k \sin\frac{1}{2}\theta$, where θ is the angle between $\vec{k}$ and $\vec{k}'$. That is, $q_{\max} = 2k$ and $q_{\min} = 0$. Using (2.5a), we find $F(q_{\min}) = 1.0$ and $F(q_{\max}) = 0.536$. Therefore, to within a factor of order unity the screening parameter may be written as

$$s = 2\pi e^2 N / \epsilon_b k_B T . \tag{2.9}$$

Since $F(q) \leq 1$, Eq. (2.9) overestimates the true value of s by a factor of order unity.

It is well known in plasma[9] and solid-state[10] physics that there are two validity criteria for the screening of a potential center by mobile carriers: (i) There must be a considerable cloud of screening electrons within a screening length of each potential center, and (ii) the mean wavelength of the electrons must be smaller than the screening length. It turns out that for bulk semiconductors the usual Debye–Huckel and Thomas–Fermi screening-length formulas do not satisfy these validity criteria over most of the ranges of temperatures and carrier concentrations of interest.[10]

We can apply the same criteria to test the range of validity of the two-dimensional screening parameter given by Eq. (2.9). Let $\pi r_0^2 = N^{-1}$ be the mean area per electron and $\lambda_{\text{th}} = 2\pi\hbar/(2m^* k_B T)^{1/2}$ be the wavelength of an electron of thermal energy. The two validity criteria then read

$$s r_0 = 2e^2 (\pi N)^{1/2} / k_B T \epsilon_b \ll 1 \tag{2.10a}$$

and

$$s \lambda_{\text{th}} = 4\pi^2 e^2 N \hbar / k_B T \epsilon_b (2m^* k_B T)^{1/2} \ll 1 . \tag{2.10b}$$

In Fig. 1, we plot $s r_0$ and $s\lambda_{\text{th}}$ as a function of T and N, using $\epsilon_b = 12$ and $m^* = 0.323 m_0$ for Si. It shows that for $N = 10^{10}$ cm^{-2} the screening parameter given by Eq. (2.9) is not valid for T less than about 50 °K, and for $N = 10^{11}$ cm^{-2} it is not valid for T less than about 200 °K. At the temperatures for which the validity criteria are not satisfied, the use of Eq. (2.7) or (2.9) leads to overestimating the screening effects. The same "overscreening" effect also shows up at low temperatures in the the three-dimensional scattering by ionized impurities when the usual Brooks–Herring formula is used, causing the calculated mobility to rise rapidly at low temperatures.[11]

B. Screening Effects of Electron Mobility

In two-dimensions, the momentum relaxation time for scattering of an electron from state $|\vec{k}\rangle$ into state $|\vec{k}'\rangle$ by N_I unscreened surface-oxide charges per unit area randomly distributed at the oxide-semiconductor interface is given by[5]

$$1/\tau_0(E) = \pi^2 e^4 N_I / \hbar \bar{\epsilon}^2 E , \tag{2.11}$$

where $E = E_k = \hbar^2 k^2 / 2m^*$. When screening effect is included, the relaxation time is given by

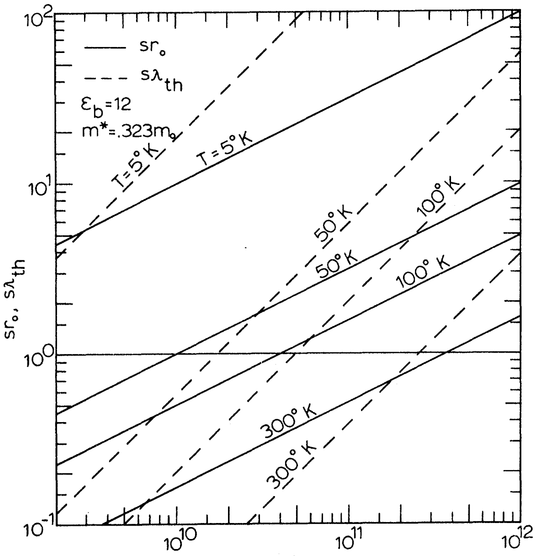

FIG. 1. sr_0 and $s\lambda_{\text{th}}$ as a function of electron concentration. The screening parameter formula is expected to be valid only when both sr_0 and $s\lambda_{\text{th}}$ are less than 1.

$$\frac{1}{\tau_I(E)}=\frac{1}{2\pi\tau_0(E)}\int_0^{2\pi}\left(1+\frac{s}{q}\right)^{-2}d\theta\ , \tag{2.12}$$

where s is the screening parameter given by (2.7), θ is the angle between $\vec{k}$ and $\vec{k}'$, and $\vec{q}=\vec{k}-\vec{k}'$. The electron mobility is given by

$$\mu_I=\frac{e}{m_\mu}\ \frac{\langle E\tau_I\rangle}{\langle E\rangle}\ , \tag{2.13}$$

where m_μ is the mobility effective mass and

$$\langle A\rangle=\int_0^\infty A\,e^{-E/k_BT}dE \tag{2.14}$$

is the average value of A for a two-dimensional classical gas.

Figure 2 shows the mobility as a function of temperature and carrier concentration. Here the mobility has been normalized to the mobility without screening μ_0 given by Eq. (1.1). The apparent large screening effect at low temperatures is actually due to the breakdown of the screening parameter formula used. For, as shown in Fig. 1, the screening parameter formula at $N=5\times10^{10}$ cm^{-2} is invalid for $T\leq100$ °K and at $N=2\times10^{11}$ cm^{-2} is invalid for $T\leq250$ °K. Such overscreening effect at low temperatures also occurs in the three-dimensional bulk case when the usual Brooks–Herring formula is used.[11]

In the temperature ranges where the screening parameter formula is valid, Fig. 2 shows that inclusion of screening increases the calculated mobility by about 5–20%. For a given electron concentration, the effect of screening increases slowly as the temperature decreases.

III. EFFECTS OF CORRELATION OF SURFACE-OXIDE CHARGES ON ELECTRON SURFACE MOBILITY

The effective-mass Hamiltonian of an electron in the surface channel may be written in the form[5]

$$H=H^0+H'\ , \tag{3.1a}$$

where

$$H^0=-(\hbar^2/2m^*)\nabla^2-e\phi^0(z) \tag{3.1b}$$

and

$$H'=-e\delta\phi(\vec{r}). \tag{3.1c}$$

Here $\phi^0(z)$ is the electrostatic potential due to the charge density averaged over the xy plane (the oxide-semiconductor interface is assumed to lie in the $z=0$ plane), i.e.,

$$\rho^0(z)=\langle\rho(\vec{r})\rangle_{\text{av}}\ , \tag{3.2a}$$

and $\delta\phi(\vec{r})$ is the electrostatic potential due to the spatial charge-density variation in the xy plane, i.e.,

$$\delta\rho(\vec{r})=\rho(\vec{r})-\rho^0(z)\ . \tag{3.2b}$$

In energy-level calculations[7,12,13] it is usually assumed that ρ and ϕ are functions only of z and uniform in the xy plane, so that $\delta\rho=\delta\phi=0$. Spatial variations of ρ and ϕ in the xy plane due to atomic irregularities at the interface and surface region were neglected. Such spatial variations of ρ and ϕ are very important in surface transport phenomena, for although H^0 determines the average properties of the electronic states, it is H' that scatters the electrons in the surface channel.[5,14]

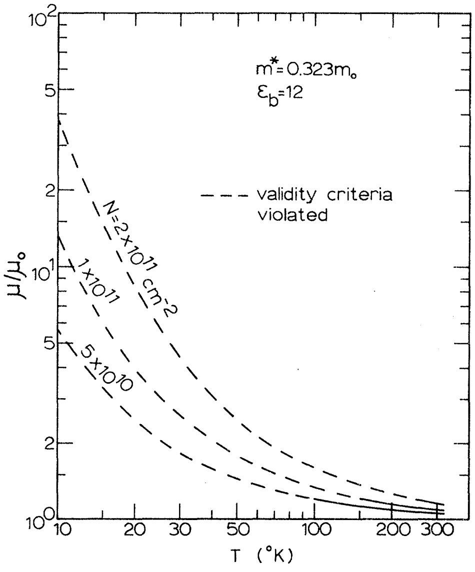

FIG. 2. Surface mobility due to scattering by surface-oxide charges as a function of the mobile carrier concentration.

In this section, we assume that the only important contribution to $\delta\phi$ is from the surface-oxide charges, and that these charges are located in the oxide at the oxide-semiconductor interface. Furthermore, in order to study the effects of the correlation of the surface-oxide charges alone on the electron surface mobility, we shall not include the effects of screening by mobile carriers here. The matrix element between two-dimensional states $|\vec{k}\rangle$ and $|\vec{k}'\rangle$ is then[5]

$$\langle \vec{k}' \,|\, H' \,|\vec{k}\rangle = -(2\pi e^2/Aq\bar{\epsilon}) \int [\, n_I(\vec{x}) - N_I] e^{i\vec{q}\cdot\vec{x}} d^2x \,, \tag{3.3}$$

where $\bar{\epsilon}$ is the average dielectric constant, A is the normalization area, $\vec{q}=\vec{k}'-\vec{k}$, and $en_I(\vec{x})$ and eN_I are the areal local and average surface-oxide charge densities, respectively. We define the surface-oxide charge-density fluctuation $\tilde{n}_I(\vec{x})$ by[15]

$$\tilde{n}_I(\vec{x}) = n_I(\vec{x}) - N_I \tag{3.4a}$$

and its Fourier transform $\tilde{n}_I(\vec{q})$ by

$$\tilde{n}_I(\vec{q}) = (1/A) \int \tilde{n}_I(\vec{x})\, e^{-i\vec{q}\cdot\vec{x}} d^2x \,. \tag{3.4b}$$

Substituting (3.4) into (3.3), we obtain

$$\langle \vec{k}' \,| H' \,| \vec{k}\rangle = -(2\pi e^2/q\bar{\epsilon})\tilde{n}_I^*(\vec{q}) \,. \tag{3.5}$$

The transition rate is given by the Golden rule as

$$\begin{aligned}\Gamma_{\vec{k}\to\vec{k}'} &= (2\pi/\hbar)\langle |\, \langle \vec{k}' \,| H' \,| \vec{k}\rangle \,|^2\rangle_{\text{av}}\, \delta(E_{\vec{k}} - E_{\vec{k}'}) \\ &= (2\pi/\hbar)(2\pi e^2/q\bar{\epsilon})^2 \langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}}\delta(E_{\vec{k}} - E_{\vec{k}'}) \,. \end{aligned} \tag{3.6}$$

$\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}}$ is the density correlation function of the surface-oxide charges. The three-dimensional analog of $\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}}$ in a bulk semiconductor has been calculated for certain model-correlated impurity distributions and applied to the scattering of electrons[16] and to the scattering of light.[17] Here we shall derive an expression for $\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}}$ in terms of two-dimensional distribution functions and evaluate it for three interesting distributions: the completely random, the superlattice, and the hard-sphere distributions. Detailed discussion of the effects of correlation of the surface-oxide charge distribution on the electron surface mobility will be given in the hard-sphere model.

Let $N=N_IA$ be the total number of surface-oxide charge particles, and $P(\vec{x}_1, \ldots, \vec{x}_N)d^2x_1 \cdots d^2x_N$ be the probability that particle 1 is located in d^2x_1, particle 2 in d^2x_2, and so on.[18] The normalization condition is

$$\int P(\vec{x}_1, \ldots, \vec{x}_N) d^2x_1 \cdots d^2x_N = 1 \,. \tag{3.7}$$

We define a two-particle correlation function $W(\vec{x}_i, \vec{x}_j)$ by

$$W(\vec{x}_i, \vec{x}_j) = \int P(\vec{x}_1, \ldots, \vec{x}_N) d^2x_1 \cdots d^2x_N / d^2x_i d^2x_j \,, \tag{3.8}$$

where the integration is over all particle coordinates except those of the ith and jth particles. $W(\vec{x}_i, \vec{x}_j)d^2x_i d^2x_j$ is just the joint probability of finding particle i in d^2x_i and particle j in d^2x_j, regardless of the positions of the other $N-2$ particles. We also define the pair-distribution function $D(\vec{x})$ (sometimes also called the pair-correlation function) by

$$\begin{aligned} D(\vec{x}) &= \sum_{i,j} \int \delta(\vec{x} - \vec{x}_i + \vec{x}_j) P(\vec{x}_1, \ldots, \vec{x}_N) d^2x_1 \cdots d^2x_N \\ &= N_I A\delta(\vec{x}) + {\sum_{i,j}}' \int \delta(\vec{x} - \vec{x}_i + \vec{x}_j) \\ &\qquad \times W(\vec{x}_i, \vec{x}_j) d^2x_i d^2x_j \,, \end{aligned} \tag{3.9}$$

where the primed sum means that the $i=j$ term is to be excluded. $D(\vec{x})d^2x$ is the probability that there is a particle in d^2x at $\vec{x}$, when there is one at $\vec{x}=0$. Writing the particle density as

$$n_I(\vec{x}) = \sum_{i=1}^{N} \delta(\vec{x} - \vec{x}_i) \,, \tag{3.10a}$$

we obtain, from (3.4b),

$$\tilde{n}_I(\vec{q}) = (1/A) \textstyle\sum_j e^{-i\vec{q}\cdot\vec{x}_j} - N_I \delta_{\vec{q},\vec{0}} \,. \tag{3.10b}$$

By definition,

$$\begin{aligned}\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}} &= \int P(\vec{x}_1, \ldots, \vec{x}_N)\tilde{n}_I(\vec{q}) \\ &\qquad \times \tilde{n}_I^*(\vec{q}) d^2x_1 \cdots d^2x_N \,. \end{aligned} \tag{3.11}$$

It can be shown by using (3.9) that

$$\begin{aligned}\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}} &= (1/A)D(\vec{q}) - N_I^2 \delta_{\vec{q},\vec{0}} \\ &= \frac{N_I}{A} + \left\{ \frac{1}{A^2} {\sum_{i,j}}' \int W(\vec{x}_i, \vec{x}_j) \right. \\ &\qquad \left. \times e^{-i\vec{q}\cdot(\vec{x}_i - \vec{x}_j)} d^2x_i d^2x_j - N_I^2 \,\delta_{\vec{q},\vec{0}} \right\} \,, \end{aligned} \tag{3.12}$$

where $D(\vec{q})$ is the Fourier transform of $D(\vec{x})$ defined by

$$D(\vec{q}) = (1/A) \int D(\vec{x}) e^{-i\vec{q}\cdot\vec{x}} d^2x \,. \tag{3.13}$$

Thus, for a given two-particle correlation function, the density correlation function could be evaluated by using (3.12).

For a completely random distribution with no correlation, we have

$$W(\vec{x}_i, \vec{x}_j) = (1/A)^2 \tag{3.14}$$

and

$$\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q})\rangle_{\text{av}} = N_I(1 - \delta_{\vec{q},\vec{0}})/A \quad \text{(random)} \,. \tag{3.15}$$

The corresponding mobility for a nondegenerate surface channel has been evaluated to be[5]

$$\mu_I = \frac{e}{m_\mu}\left(\frac{\bar{\epsilon}}{e^2}\right)^2 \frac{2\hbar k_B T}{\pi^2 N_I} \quad \text{(random)} \,, \tag{3.16}$$

which is just Eq. (1.1).

If the surface-oxide charges form a two-dimensional superlattice, then

$$W(\vec{x}_i, \vec{x}_j) = \delta(\vec{x}_i - \vec{R}_i)\delta(\vec{x}_j - \vec{R}_j) , \tag{3.17}$$

where $\vec{R}_i$ and $\vec{R}_j$ are the lattice position vectors of particles i and j, respectively. For a superlattice, we have

$$(1/N) \sum_{j=1}^{N} e^{-i\vec{q}\cdot\vec{R}_j} = \delta_{\vec{q}, \vec{K}_h} , \tag{3.18}$$

where $\vec{K}_h$ is a reciprocal-lattice vector of the superlattice, so that

$$\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q}) \rangle_{\text{av}} = N_I^2(\delta_{\vec{q}, \vec{K}_h} - \delta_{\vec{q}, \vec{0}}) \quad \text{(superlattice)}. \tag{3.19}$$

Thus, scattering occurs for $\vec{q} = \vec{K}_h$ only. This is just the well-known result that a perfectly periodic potential does not cause momentum randomization.

The experimental evidence of scattering by surface-oxide charges[1–5] appears to demonstrate certain degree of randomness in the surface-oxide charge distribution. For surfaces with low charge densities, the distribution is probably completely random. For surfaces with high charge densities, the distribution is probably correlated because of the interaction among the charges.

Here we consider the simple model of hard-sphere distribution, which has often been used in the theory of liquid state to represent the short-range repulsion among the fluid particles.[19] That is, we assume that the distribution of the surface-oxide charges is random to the extent that no two particles can be found within a radius of R_0 from each other. In this case, we have

$$\begin{aligned} W(\vec{x}_i, \vec{x}_j) &= 0 , & |\vec{x}_i - \vec{x}_j| &< R_0 \\ &= 1/A(A - \pi R_0^2) , & |\vec{x}_i - \vec{x}_j| &> R_0 \cdot \end{aligned} \tag{3.20}$$

Using (3.12), we obtain

$$\langle \tilde{n}_I(\vec{q})\tilde{n}_I^*(\vec{q}) \rangle_{\text{av}} = \frac{N_I}{A} \left(1 - \frac{2CJ_1(qR_0)}{qR_0} \right) \quad \text{(hard sphere),} \tag{3.21}$$

where J_1 is the Bessel function of first order, and

$$C = \pi R_0^2 / N_I^{-1} \tag{3.22}$$

is the ratio of the minimum area πR_0^2 to the average area N_I^{-1} occupied by a charge particle. C is a measure of the degree of correlation. $C = 0$ corresponds to a completely random distribution; $C = 1$ corresponds to a uniform distribution.

From (3.6) and (3.21), the momentum relaxation time τ_I is given by

$$\begin{aligned} 1/\tau_I &= \sum_{\vec{k}'} \Gamma_{\vec{k}\to\vec{k}'}(1 - \cos\theta) \\ &= \frac{e^4 \pi N_I}{\hbar \bar{\epsilon}^2 E} \int_0^{\pi} \left(1 - \frac{2CJ_1(qR_0)}{qR_0} \right) d\theta , \end{aligned} \tag{3.23}$$

where θ is the angle between $\vec{k}$ and $\vec{k}'$, $E = \hbar^2 k^2 / 2m^*$ is the electron energy, and $q = 2k \sin\frac{1}{2}\theta$. The surface mobility for a nondegenerate surface channel can be obtained from Eq. (2.13).

We have evaluated the surface mobility as a function of the temperature, with C as a parameter. The results for $N_I = 9.0 \times 10^{11}$ cm^{-2} and $m^* = 0.323 m_0$ are shown in Fig. 3, where the mobility has been normalized to μ_0 given by (3.16). It shows that, in general, correlation of the surface-oxide charges has the effect of reducing scattering, and hence increasing the mobility. At high temperatures, the mobility is relatively insensitive to the degree of correlation. This is to be expected since at high temperatures the mean wavelength of the electrons, $\lambda_{\text{th}} = 2\pi\hbar / (2m^* k_B T)^{1/2}$, is comparable to the mean separation of the oxide charges, and the electron "sees" only one or two oxide charges at a time. Thus, the distribution appears fairly random to the electron being scattered, regardless of the value of C. However, at low temperatures where the mean wavelength of the electrons is many times the mean separation of the surface-oxide charges, the electron sees many surface-oxide charges at a time, and the mobility becomes very sensitive to the degree of correlation.

Figure 4 shows the mobility as a function of N_I for $C = 1$ (uniform distribution). The vertical dotted bars in the figure indicate the temperatures above which the mean wavelength λ_{th} is less than $2/N_I^{1/2}$, where $1/N_I^{1/2}$ is the mean separation of the surface-oxide charges. When $\lambda_{\text{th}} < 2/N_I^{1/2}$, an electron sees only one surface-oxide charge at a time on the average, and Fig. 4 shows that the effect of correlation is small and increases slowly with decreasing temperature. When $\lambda_{\text{th}} > 2/N_I^{1/2}$, on the other hand, an electron sees more than one surface-oxide charge at a time on the average, and correlation effect becomes very important and a strong function of the temperature.

Most of the metal-Si-SiO$_2$ structures used to study transport phenomena in the surface inversion channel contain a total surface-oxide charge densi-

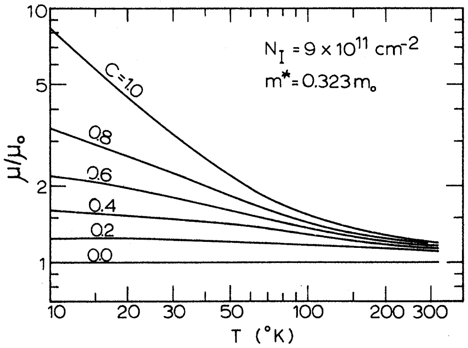

FIG. 3. Effect of correlation of the surface-oxide charges on the surface mobility in the hard-sphere model.

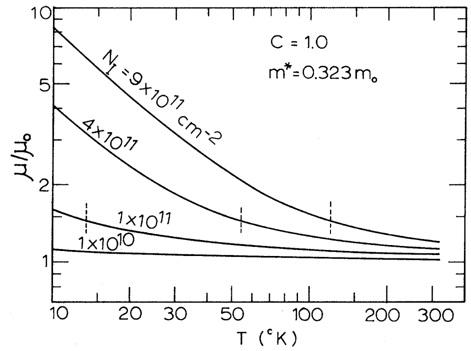

FIG. 4. Surface mobility with $C=1$ in the hard-sphere model. The dotted bars indicate the temperatures below which $\lambda_{\mathrm{th}} > 2/N_I^{1/2}$.

ty of between 5×10^{10} and 1×10^{13} cm^{-2}. Therefore, the correlation effect of the surface-oxide charges plays an important role in the interpretation of experimental data except for specially prepared samples with very low surface-oxide charge states at around room temperature. For such samples, the distribution of the surface-oxide charges is probably completely random anyway.

In the above discussion of the hard-sphere correlation model, we have implicitly assumed an ideal oxide layer for which there is but one hard-sphere radius R_0. In reality we expect the oxide layer to form patches, with a different average areal charge density and hard-sphere radius for each patch. Thus, in principle, we should also perform an average of the density correlation function over the distribution in R_0. The problem of describing such a patchy oxide charge distribution statistically is similar to that of describing statistically a crystal surface with smooth areas separated by growth steps and scratches and other irregularities.[20] There could be a probability distribution $P(R_0)$ for R_0, and we could define an average value of $\Gamma_{\vec{k}\to\vec{k}'}(R_0)$:

$$\bar{\Gamma}_{\vec{k}\to\vec{k}'} = \int P(R_0)\,\Gamma_{\vec{k}\to\vec{k}'}(R_0)\,dR_0 \;. \tag{3.24}$$

The distribution $P(R_0)$ is probably Gaussian, with a standard deviation σ_R. Lacking information on σ_R, we shall not pursue this problem any further here.

IV. EFFECTS OF DISTRIBUTION OF SURFACE-OXIDE CHARGES INTO OXIDE LAYER ON SURFACE MOBILITY

Thus far, we have assumed that the surface-oxide charges are located at the oxide-semiconductor interface. However, there is experimental evidence that oxide charges in Si-SiO$_2$ systems generated by oxygen heat treatment are spread out to as much as 20 Å or more from the Si-SiO$_2$ interface.[21–23] To incorporate this finite distribution into our model, we conceptually divide the oxide layer into two-dimensional sublayers parallel to the oxide-semiconductor interface. Let Δz_i be the thickness of the ith sublayer, and let $n_i(\vec{x})$ and N_i be its areal local and average oxide charge densities, respectively. The three-dimensional oxide charge density is then

$$n_I(\vec{x}, z) = \textstyle\sum_i n_i(\vec{x})\,\delta(z - z_i) \;. \tag{4.1}$$

Instead of (3.3), we now have[5]

$$\begin{aligned}\langle \vec{k}' \,|\, H' \,|\, \vec{k}\rangle &= -(2\pi e^2/Aq\bar{\epsilon})\textstyle\sum_i \int [n_i(\vec{x}) - N_i] \\ &\qquad\times e^{-q|z_i| + i\vec{q}\cdot\vec{x}}\,d^2x \\ &= -(2\pi e^2/q\bar{\epsilon})\textstyle\sum_i \tilde{n}_i^*(\vec{q})\,e^{-q|z_i|}\end{aligned} \tag{4.2}$$

where, by analogy with (3.4a) and (3.4b),

$$\tilde{n}_i(\vec{x}) = n_i(\vec{x}) - N_i \tag{4.3a}$$

and

$$\tilde{n}_i(\vec{q}) = (1/A)\int \tilde{n}_i(\vec{x})\,e^{-i\vec{q}\cdot\vec{x}}\,d^2x \;. \tag{4.3b}$$

If we assume that there is no correlation among oxide charges of different sublayers, then

$$\left\langle \left| \textstyle\sum_i \tilde{n}_i(\vec{q})\,e^{-q|z_i|} \right|^2 \right\rangle_{\mathrm{av}} = \textstyle\sum_i \langle \tilde{n}_i(\vec{q})\tilde{n}_i^*(\vec{q})\rangle_{\mathrm{av}}\,e^{-2q|z_i|} \;, \tag{4.4}$$

so that (3.6) is replaced by

$$\begin{aligned}\Gamma_{\vec{k}\to\vec{k}'} = {}& \frac{2\pi}{\hbar}\left(\frac{2\pi e^2}{q\bar{\epsilon}}\right)^2 \delta(E_{\vec{k}} - E_{\vec{k}'}) \\ &\times \sum_i \langle \tilde{n}_i(\vec{q})\tilde{n}_i^*(\vec{q})\rangle_{\mathrm{av}}\,e^{-2q|z_i|} \;.\end{aligned} \tag{4.5}$$

In order to study the effect of the finite distribution of the surface-oxide charges into the oxide layer alone on the surface mobility, we shall assume the simple case where the distribution in each sublayer is random. For this simple case, we have

$$\begin{aligned}&\sum_i \langle \tilde{n}_i(\vec{q})\tilde{n}_i^*(\vec{q})\rangle_{\mathrm{av}}\,e^{-2q|z_i|} \\ &\qquad = \sum_i (N_i/A)\,e^{-2q|z_i|} \\ &\qquad = (1/A)\sum_i N_I(z_i)\,\Delta z_i\,e^{-2q|z_i|} \\ &\qquad = (1/A)\int N_I(z)\,e^{-2q|z|}\,dz \quad \text{(random)} \;,\end{aligned} \tag{4.6}$$

where $N_I(z_i)$ is defined by

$$N_I(z_i)\,\Delta z_i = N_i \;. \tag{4.7}$$

In our previous paper,[5] we evaluated the mobility for three interesting distributions: (i) $N_I(z) = N_I\delta(z)$, (ii) $N_I(z) = (N_I/\alpha)e^{(-z/\alpha)}$, and (iii) $N_I(z) = (N_I z/\beta^2) \times e^{(-z/\beta)}$. For convenience we have replotted the results in Fig. 5. The mobility for case (i) is simply μ_0 given by Eq. (1.1). It corresponds to the case where all of the surface-oxide charges are located in the oxide at the oxide-semiconductor interface. Figure 5 shows that the finite distribution of the charges into the oxide layer increases both the

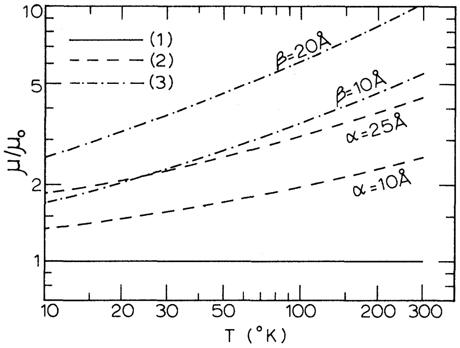

FIG. 5. Surface mobility for three different distributions of the surface-oxide charges: (1) $N_I(z) = N_I\delta(z)$; (2) $N_I(z) = (N_I/\alpha)e^{-z/\alpha}$; (3) $N_I(z) = (N_I z/\beta^2)e^{-z/\beta}$.

magnitude and the temperature dependence of the mobility.

V. EFFECT OF ELECTRON DISTRIBUTION ON SURFACE MOBILITY

Thus far, in our discussion of the surface mobility, we have assumed that the electrons in the channel have a δ-function distribution at the interface. This assumption is actually not valid, because for a nondegenerate-silicon-surface inversion channel with 10^{11}-cm^{-2} electrons the average distance of the electrons from the interface is about 100 Å.[12,13] To take into account the electron distribution exactly in the surface-mobility calculations would require analytic forms of the electron wave functions in the surface channel. Therefore, here we shall only give a semiquantitative discussion of the effect of the electron distribution on the surface mobility due to scattering by surface-oxide charges, assuming certain physically plausible distribution functions.

If the metal-oxide-semiconductor system is biased near flat-band condition, then the surface channel width would be semi-infinite. In this case, we have essentially a semi-infinite system, and the motion of the electrons perpendicular to the surface is no longer negligible. The method developed by Greene and O'Donnell[24,25] for the scattering by localized surface charges would be applicable.

If the system is biased so that a degenerate surface channel is formed, the behavior of the electrons in the channel is expected to be similar to those in thin metallic films. For a degenerate-semiconductor-surface inversion channel the surface mobility due to scattering by surface-oxide charges and by bulk ionized impurities has been formulated by Siggia and Kwok,[8] who take into account all of the electric subband energy levels. However, as far as we know, explicit evaluation of the mobility has not been performed, because it requires analytic forms of the electron wave functions which are not available. For thin metallic films, on the other hand, formulas for the relaxation time due to scattering by localized surface charges and by surface irregularities have been obtained.[26] This is possible because of the symmetry of the boundary conditions which gives simple analytic wave functions of the electrons.

Here we are interested in nondegenerate surface inversion channels. The surface electric subbands of such a surface are broadened into a continuum, especially for samples with high surface-oxide charge states due to random surface band bending from randomly distributed ions,[27] so that we are dealing with essentially a classical surface channel instead of a quantum one. If the surface electric field is not too low ($E_S \gtrsim 1.5\times10^4$ V/cm for silicon), the channel width would be smaller than the mean wavelength of the electrons, so that the motion of the electrons perpendicular to the surface may be neglected. In this case, the electron wave function may be written in the form

$$\psi_{\vec{k}}(\vec{r}) = (1/\sqrt{A})e^{i\vec{k}\cdot\vec{\rho}}\zeta(z) , \tag{5.1}$$

where $\vec{k}$ is a wave vector in the xy plane, $\vec{\rho} = (x, y)$, $|\zeta(z)|^2$ gives the electron distribution in the surface channel, and A is the normalization area. The matrix element of H' between two-dimensional states $|\vec{k}\rangle$ and $|\vec{k}'\rangle$ is[7]

$$\langle\vec{k}'|H'|\vec{k}\rangle = (1/A)\int d^2\rho\, dz\, |\zeta(z)|^2 H' e^{i(\vec{k}-\vec{k}')\cdot\vec{\rho}} . \tag{5.2}$$

Suppose that H' is given by N_I surface-oxide charges randomly distributed in the oxide at the oxide-semiconductor interface; then we find

$$|\langle\vec{k}'|H'|\vec{k}\rangle|^2 = \left(\frac{2\pi e^2}{q\bar{\epsilon}}\right)^2 \frac{N_I}{A}\left|\int dz\, |\zeta(z)|^2 e^{-q|z|}\right|^2 , \tag{5.3}$$

where $\bar{\epsilon}$ is the average dielectric constant and $\vec{q} = \vec{k}' - \vec{k}$. The surface mobility may be evaluated as in the preceding sections.

We have calculated the surface mobility for three interesting electron distributions. They are (i) $|\zeta(z)|^2 = \delta(z)$, (ii) $|\zeta(z)|^2 = (1/\alpha)e^{(-z/\alpha)}$, and (iii) $|\zeta(z)|^2 = \frac{1}{2}b^3z^2e^{(-bz)}$. Case (i) corresponds to the simple two-dimensional model where the electrons are located in the semiconductor at the oxide-semiconductor interface. The surface mobility in this case is just μ_0 given by Eq. (1.1). Case (ii) is typical of the classical electron distribution of a semiconductor surface inversion channel, with no quantum boundary conditions imposed.[12,28] The distribution of case (iii) is typical for a semiconductor surface inversion channel with the quantum boundary condition $\psi(z=0)=0$ imposed on the electron wave function.[7,12,13] The results are shown in Fig. 6, where, again, the surface mobility has been normalized to μ_0. As expected, the effect of

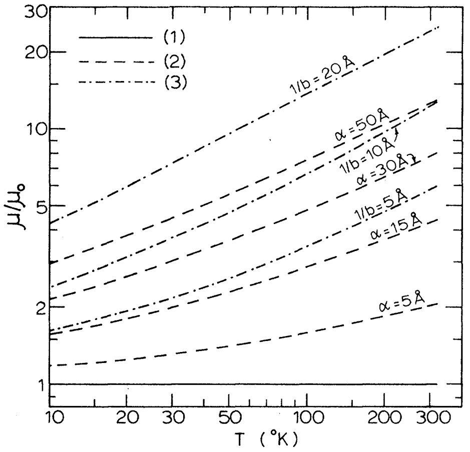

FIG. 6. Surface mobility for three different distributions of the electrons in the surface channel: (1) $|\zeta(z)|^2 = \delta(z)$; (2) $|\zeta(z)|^2 = (1/\alpha)e^{-z/\alpha}$; (3) $|\zeta(z)|^2 = \frac{1}{2}b^3 z^2 e^{-bz}$.

the distribution of the electrons in the surface channel on the surface mobility is very similar to that of the distribution of the surface-oxide charges into the oxide layer (see Fig. 5). As the mean separation between the electrons and the surface-oxide charges increases, the scattering decreases, and hence the mobility increases. The distribution of the surface-oxide charges is independent of temperature and the metal gate bias, but the distribution of the electrons in the surface channel is a function of temperature and the gate bias.

VI. DISCUSSION AND CONCLUSIONS

We have investigated individually the effects of screening, correlation and distribution of the surface-oxide charges, and distribution of the electrons on the mobility of electrons in a nondegenerate-semiconductor-surface channel. The results shown in Figs. 2–6 indicate that although some of the effects are more important than the others, none is completely negligible. Therefore, in principle, an exact calculation of the surface mobility should take into account all of these effects simultaneously. Such a calculation, however, would not be informative at the present because it involves too many yet unknown parameters. However, from the results of the preceding sections, we could draw the following conclusions: (i) Screening by mobile carriers is relatively unimportant for a nondegenerate-semiconductor-surface channel, provided that the screening parameter formula is not extended beyond its range of validity. A better theory is needed to describe the effects of the mobile carriers when the simple formulas for the screening parameter break down. (ii) The effect of correlation of the surface oxide charges on the surface mobility is important, especially at low temperatures where the mean electron wavelength is larger than the mean separation of the oxide charges. (iii) The surface mobility depends on the separation between the surface-oxide charges and the electrons in the surface channel. (iv) Both screening by mobile carriers and the correlation of the surface-oxide charges have the effect of increasing the magnitude but decreasing the temperature dependence of the surface mobility (recall that μ_0 is proportional to T), while both the distribution of the surface-oxide charges and the distribution of the electrons have the same effect of increasing the magnitude and the temperature dependence of the surface mobility.

As mentioned earlier in Sec. I, the observed electron conductivity mobility in a nondegenerate silicon surface due to scattering by surface-oxide charges shows a T/N_I dependence, as given by μ_0.[5] However, μ_0 is about 20 times too small. This discrepancy could well be explained by a combination or combinations of the effects studied in this paper. For example, let us consider the mobility at $T = 77\,^\circ\mathrm{K}$. If we assume a classical electron distribution proportional to $e^{(-eE_S z/k_B T)}$, as in case (ii) of Fig. 6, where E_S is the surface electric field and $eE_S z$ is the electron potential energy, then for the experimental conditions, where $E_S \simeq 2.5\times 10^4$ V/cm,[5] most of the electrons are localized within a distance of $\alpha = k_B T/eE_S = 26$ Å from the interface. That is, the finite distribution of the electrons in the surface channel could account for a factor of about 4 (see Fig. 6). If we further assume an exponential distribution of the surface-oxide charges, as in case (ii) of Fig. 5, with a reasonable mean distance of 25 Å, then we could account for another factor of about 3 (see Fig. 5). The remaining discrepancy by a factor of 1.7 could very well be accounted for by the screening effect (see Fig. 2) and the effect of position correlation of the surface-oxide charges (see Fig. 3).

It is interesting to note that none of the effects studied here could alone account for the discrepancy between experiment and the theoretical value of μ_0. This would indicate that a combination of these effects should be taken into consideration simultaneously in a more refined theory of electron transport in semiconductor surface channels.

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Spatial Dispersion Effects in Resonant Polariton Scattering. I. Additional Boundary Conditions for Polarization Fields*

Roland Zeyher,[†‡] Joseph L. Birman,[‡] and Wilhelm Brenig[§]
Department of Physics, New York University, New York, New York 10003

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The normal-incidence propagation of transverse modes in a medium with spatial dispersion is analyzed. A careful examination of discrepancies existing in the literature concerning the boundary conditions shows that they are due to the use of different susceptibilities. Thus they originate from a discrepancy in the solution of Schrödinger's equation and not of Maxwell's equations.

I. INTRODUCTION

In the present paper we shall propose a resolution of a long-standing controversy concerning the additional boundary conditions (ABC) appropriate for the description of the electrodynamics of a bounded spatially dispersive medium.[1–7] From the analysis we give here it is apparent that the different ABC's are intimately related to different assumptions made concerning the proper nonlocal susceptibility $\chi(\vec{r}, \vec{r}\,')$ governing the spatially dispersive medium. In turn, the susceptibility directly reflects assumptions made concerning the boundary conditions for excitons (the most relevant elementary excitation here) in the bounded medium. Hence, different boundary conditions for the Schrödinger equation produce different ABC's.

To illustrate the essential point, we may focus on the case of spatial dispersion resulting from the coupling of bare photons with wave vector $k_0 = \omega/c$ to a dispersive discrete bare exciton (with center-of-mass motion). In the absence of coupling, the Fourier-transformed susceptibility $\chi(\vec{k}, \omega)$ due to this single-exciton level has a simple pole [see (3.7)] at the wave number $k_e(\omega)$, for each frequency ω. Owing to the coupling, polariton modes are formed which in an infinite medium satisfy the well-known dispersion equation

$$(k_i/k_0)^2 = 1 + 4\pi\chi(k_i, k_0) . \tag{1.1}$$

In this case two linearly independent degenerate polaritons can propagate with wave vectors $k_1(\omega)$