A comprehensive model for Coulomb scattering in inversion layers

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(Received 28 June 1993; accepted for publication 8 October 1993)

A comprehensive model for Coulomb scattering in inversion layers is presented. This model simultaneously takes into account the effects of: (i) the screening of charged centers by mobile carriers, (ii) the distribution of charged centers inside the structure, (iii) the actual electron distribution in the inversion layer, (iv) the charged-center correlation, and (v) the effect of image charges. A Monte Carlo calculation to obtain the effective mobility of electrons in an $n$-Si(100) inversion layer by using the model proposed for Coulomb scattering has been developed. The importance of correctly taking into account the effects above to study Coulomb scattering in inversion layers is pointed out.

I. INTRODUCTION

It is well known that at least four types of electric charges exist at or near the interface of an insulator-semiconductor structure: the fixed insulator charge, the interface-state charge, the charge of the ionized impurities in the semiconductor bulk, and the mobile-carrier charge.$^{1,2}$ The first three types will be grouped hereafter under the name of external charges. The electric nature of the four types of charges causes a Coulombic interaction among them. This interaction is produced between the external charged centers themselves, between the mobile carriers themselves, and between the external charged centers and the mobile carriers. This last type of interaction is the topic dealt with in this article and so we group the scattering resulting from the interaction between external charged centers and mobile carriers under the general heading of Coulomb scattering. Nevertheless, we have also studied the influence of the charged-center correlation which can be considered to be a consequence of the interaction between the external charged centers themselves.

We have developed a general model for Coulomb scattering that can be directly applied to any heterointerface in which a quasi-two-dimensional electron gas is confined,$^3$ such as is formed in modulation-doped heterostructures, or in an inverted insulator-semiconductor heterointerface. Nevertheless, to demonstrate the usefulness of the method presented here, we have applied it to the study of an inverted insulator-semiconductor heterointerface. For this reason, we call one of the two sides of the interface insulator when, in a more general sense, it could also be a semiconductor layer.

The influence of the external charged centers in the electron transport in semiconductor inversion layers and in semiconductor heterostructures has been widely demonstrated in the past, mainly for low values of the electron concentration.$^4-10$ Coulomb scattering has thus received a great deal of attention by previous researchers and has been shown to be a matter of great complexity, so that most authors have centered their analysis on only partial aspects. The points that affect the mobility and that therefore we must consider are the following: (a) electron distribution in the inversion layer, (b) distribution of external charged centers, (c) screening of charged centers by mobile carriers, (d) charged-center correlation, and (e) image charges. It has been demonstrated that all these points influence the mobility, but none of them alone could account for the mobility values.$^7$ To reach good agreement between theoretical and experimental results, it is desirable to include all of these aspects simultaneously in a comprehensive model. Such a model is presented in this article.

The electron distribution in the inversion layer can be treated as a three-dimensional electron gas obeying classical laws$^5$ or as a quasi two-dimensional electron gas contained in electric subbands if quantum effects are taken into account.$^4,11$ This latter model seems more appropriate in most cases,$^12$ since the inversion layer is confined in a very narrow region, and has been adopted in this article. Some authors have considered that electrons are in a sheet of charge$^6$ and others include the spatial extension in the direction perpendicular to the interface with the envelope approximation, although sometimes only the ground subband has been considered$^4,11$ and the envelope function has been approximated by simple functions.$^5,13$ We have adopted a more accurate model$^{10}$ in which several subbands have been included and the envelope function has been obtained by self-consistently solving the Poisson and Schrödinger equations in the structure.

The screening of charged centers by mobile carriers was taken into account in early articles such as Ref. 4, where only the ground subband was considered to contain electrons. For low transverse fields, where Coulomb scattering dominates over other mechanisms, the electron gas is not as confined and the amount of electrons contained in excited subbands is significant.$^{14}$ The model of Ref. 4 was extended in Ref. 10, which is where we start from in this article, although we have incorporated significant improvements. The model considers the contribution of excited subbands to the mobility and allows the inclusion of the distribution of charged centers, but treats all of them as independent, thus overestimating the scattering. One of the improvements we have incorporated consists of including the effects of the correlation of charged centers. Correlation effects are important since the interaction among the charges causes the effect of one of them to partially overlap


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the effects of another and the potential fluctuations responsible for the electron scattering are weaker. This effect was considered in Ref. 6, but as a separate correction independent of the rest of the effects, and it has been included in this article in a comprehensive model. We have also formulated the model more generally, making it applicable with an arbitrary distribution of external charged centers placed anywhere in the structure.

Another improvement made here is the inclusion of image charges, both of the external charged centers, and of the charges responsible for the screening. Image charges are due to the differences in the permittivity of the two materials on either side of the interface,\textsuperscript{12} and their effect might be of little importance in compound-semiconductor interfaces where the permittivity is almost the same throughout the whole structure, but its influence is greater in inversion layers in other materials, such as in Si-SiO\textsubscript{2} interfaces.

In Sec. II, the Coulomb-scattering model is presented in detail. To illustrate its application, Sec. III contains the results of a one-electron Monte Carlo calculation\textsuperscript{16} in which Coulomb scattering has been included, adopting the model presented here, together with phonon and surface-roughness scattering. The model has been applied to a Si-SiO\textsubscript{2} structure, and the different aspects above have been discussed and compared with experimental results. Nevertheless, as presented here, the model can also be applied successfully to other materials and structures, such as heterointerfaces with compound semiconductors.

II. THEORY

The transport properties of the electrons in a semiconductor inversion layer are modified by the presence of charged centers near the interface.\textsuperscript{7,9} Let \( \rho_{\text{ext}} \) be the external charge density responsible for the Coulomb scattering. As a consequence of this charge density, the electrostatic potential is modified and its perturbation, \( \Phi' \), obeys Poisson’s law:\textsuperscript{4}

\[
\nabla [\varepsilon(z) \nabla V(r,z)] = 2\varepsilon_\infty \sum_i S g_i(z) \int V(r,z_2) g_i(z_2) dz_2 - \rho_{\text{ext}}(r,z),
\]

where \( r \) is a vector parallel to the interface and \( z \) is the coordinate perpendicular to it (the insulator-semiconductor interface is assumed to lie in the \( z=0 \) plane), \( \varepsilon(z) \) is the position-dependent permittivity overall, and \( \varepsilon_\infty \) is the permittivity of the semiconductor. The first term of the right-hand member of Eq. (1) is the induced charge, which is the local modification of the electron charge density and is responsible for the screening. \( g_i(z) \) is the square of the electron envelope-function in the \( i \)th subband, and \( S_i \) is the screening constant given by\textsuperscript{4,10}

\[
S_i = \frac{\varepsilon^2}{2} \frac{N_i}{E_d},
\]

where \( \varepsilon \) is the modulus of the electron charge, \( N_i \) is the number of electrons contained in the electric subband whose minimum energy is \( E_i \):

\[
N_i = \frac{K_B T}{\pi \hbar^2} n_d m_{di} \ln [1 + e^{(E_F - E_i)/K_B T}],
\]

and

\[
E_{d,i} = K_B T [1 + e^{(E_i - E_F)/K_B T}] \ln [1 + e^{(E_F - E_i)/K_B T}],
\]

where \( E_F \) is the Fermi level, \( n_d \) the degeneracy of the considered electric subband, \( m_{di} \) the density-of-states mass, \( K_B \) the Boltzmann constant, and \( T \) the temperature.

Equation (1) had been solved for a pointed charge, \( Z \varepsilon \), located in the insulator, in the semiconductor, or at the interface between them when only the ground subband is occupied and assuming an approximate distribution function for the inversion-layer charge.\textsuperscript{4} Yokoyama and Hess\textsuperscript{10} solved Eq. (1) for a point charge located at \( r=(0,z_0) \), using self-consistently calculated envelope wave functions.\textsuperscript{11} In this article, the latter formulation is used to solve Eq. (1) for an arbitrary distribution of charge although significant improvements have been incorporated. Details of the calculation are given below.

Multiplying expression (1) by \( e^{-Q \cdot r} \) and integrating over \( r \), one obtains the following integro-differential equation for the Fourier transform of electrostatic potential perturbations:

\[
\left( \frac{\partial}{\partial z_1} \varepsilon(z_1) \frac{\partial}{\partial z_1} - e(z_1) Q^2 \right) V(Q,z_1) - 2\varepsilon_\infty \sum_i S g_i(z_1)
\times \int dz_2 V(Q,z_2) g_i(z_2) = -\rho_{\text{ext}}(Q,z_1).
\]

Multiplying Eq. (5) by \( (1/Q) e^{-Q |z-z_1|} \) with \( z>0 \) and integrating for \( z_1>0 \) [assuming that \( V(Q,z) \) and its derivative must be zero when they are far from the interface], the Fourier transform of the electrostatic potential perturbations for \( z>0 \) is then written as

\[
V(Q,z) = \frac{1}{Q} \int_{0}^{L_2} dz_1 e^{-Q |z-z_1|} \sum_i S g_i(z_1)
\times \int_{-L_1}^{L_1} dz_2 V(Q,z_2) g_i(z_2)
+ \frac{1}{2\varepsilon_\infty Q} \int_{0}^{L_2} dz_1 \rho_{\text{sc}}(Q,z_1) e^{-Q |z-z_1|}
+ \frac{e^{-Qz}}{2} \left( V(Q,0) - \frac{1}{Q} \frac{dV}{dz} \bigg|_{z=0^+} \right).
\]

\[ L_2 \text{ and } L_1 \text{ are the semiconductor and the insulator width, respectively, and } \rho_{\text{sc}}(Q,z) \text{ is the Fourier transform of the semiconductor charge density responsible for Coulomb scattering. Similarly, the Fourier transform of the potential perturbations for } z<0 \text{ can also be obtained.} \]
\[ V(Q, z) = -\frac{\epsilon_{sc}}{\epsilon_{ins} Q} \int_{-L_1}^{L_2} dz_1 e^{-Q|z-z_1|} \sum_i S_i \rho_{g_i}(z_1) \]

\[ \times \int_{-L_1}^{L_1} dz_2 V(Q, z_2) \rho_{g_i}(z_2) \]

\[ + \frac{1}{2\epsilon_{ins} Q} \int_{-L_1}^{0} dz_1 \rho_{ins}(Q, z_1) e^{-Q|z-z_1|} \]

\[ + \frac{\rho_{Q2}}{2} \left( V(Q, 0) + \frac{dV}{dz} \bigg|_{z=0} \right) \quad (6b) \]

with \( \rho_{ins}(Q, z) \) being the Fourier transform of the insulator charge density responsible for Coulomb scattering.

Using Eqs. (6a), (6b), and the boundary condition

\[ \epsilon_{sc} \frac{dV}{dz} \bigg|_{z=0^+} - \epsilon_{ins} \frac{dV}{dz} \bigg|_{z=0^-} = -\sigma_{st}(Q), \quad (7) \]

where \( \sigma_{st}(Q) \) is the Fourier transform of the interface charge density responsible for Coulomb scattering, the Fourier transform of the potential perturbations in the semiconductor \((z > 0)\) is written as

\[ V(Q, z) = -\frac{1}{Q} \int_{-L_1}^{L_1} dz_1 \left( e^{-Q|z-z_1|} + \frac{\epsilon_{sc} - \epsilon_{ins}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right) \sum_i S_i \rho_{g_i}(z_1) \int_{-L_1}^{L_2} dz_2 V(Q, z_2) \rho_{g_i}(z_2) \]

\[ + \int_{-L_1}^{L_1} dz_1 \left[ \frac{\rho_{sc}(Q, z_1) + \rho_{ins}(Q, z_1)}{2\epsilon_{sc} Q} \left( e^{-Q|z-z_1|} + \frac{\epsilon_{ins} - \epsilon_{sc}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right) \right], \quad z > 0, \quad (8) \]

where

\[ \bar{\epsilon} = \frac{\epsilon_{sc} + \epsilon_{ins}}{2}. \]

If we define a three-dimensional function for \( \sigma_{st}(Q) \),

\[ \rho_{st}(Q, z) = \sigma_{st}(Q) \delta(z), \quad (9) \]

Eq. (8) could finally be written as

\[ V(Q, z) = -\frac{1}{Q} \int_{-L_1}^{L_1} dz_1 \left( e^{-Q|z-z_1|} + \frac{\epsilon_{sc} - \epsilon_{ins}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right) \sum_i S_i \rho_{g_i}(z_1) \int_{-L_1}^{L_2} dz_2 V(Q, z_2) \rho_{g_i}(z_2) \]

\[ + \int_{-L_1}^{L_1} dz_1 \frac{\rho_{st}(Q, z_1) + \rho_{ins}(Q, z_1)}{2\epsilon_{sc} Q} \left( e^{-Q|z-z_1|} + \frac{\epsilon_{ins} - \epsilon_{sc}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right), \quad z > 0, \quad (10a) \]

where

\[ \rho_{ext}(Q, z) = \rho_{sc}(Q, z) + \rho_{ins}(Q, z) + \rho_{st}(Q, z). \]

Similarly, the Fourier transform of the potential perturbations in the insulator \((z < 0)\) is written as

\[ V(Q, z) = -\frac{\epsilon_{sc}}{\epsilon_{ins} Q} \int_{-L_1}^{L_2} dz_1 \left( e^{-Q|z-z_1|} + \frac{\epsilon_{ins} - \epsilon_{sc}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right) \sum_i S_i \rho_{g_i}(z_1) \]

\[ \times \int_{-L_1}^{L_2} dz_2 V(Q, z_2) \rho_{g_i}(z_2) + \int_{-L_1}^{L_2} dz_1 \frac{\rho_{ext}(Q, z_1)}{2\epsilon_{ins} Q} \left( e^{-Q|z-z_1|} + \frac{\epsilon_{ins} - \epsilon_{sc}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right), \quad z < 0. \quad (10b) \]

In Eq. (10) two terms proportional to the difference between the two dielectric constants can be noted. These terms account for the image charges, one of them for the induced-charge image and the other for the external-charge image. Expressions (10a) and (10b) can be expressed more succinctly by using Green's function,\(^{18}\) defined here as

\[ G_{Q}(z_1, z_1) = \frac{1}{2\epsilon_{sc} Q} \left( e^{-Q|z-z_1|} + \frac{\epsilon_{ins} - \epsilon_{sc}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right), \quad z > 0, \]

\[ (11a) \]

\[ G_{Q}(z_1, z_1) = \frac{1}{2\epsilon_{sc} Q} \left( e^{-Q|z-z_1|} + \frac{\epsilon_{ins} - \epsilon_{sc}}{\epsilon_{sc} + \epsilon_{ins}} e^{-Q(z_1+|z_1|)} \right), \quad z < 0. \]

\[ (11b) \]
Hence, the integro-differential equation for the two-dimensional Fourier components of the potential fluctuations is reduced to

\[ V(Q,z) = -2\epsilon_s \sum_i S_i \int_{-L_1}^{L_2} dz_1 G_Q(z_1)g_i(z_1) \]

\[ \times \int_{-L_1}^{L_2} V(Q,z_2)g_i(z_2) \]

\[ + \int_{-L_1}^{L_2} dz_1 \rho_{eext}(Q,z_1)G_Q(z_1). \]  \hfill (12)

Equation (12) has been formulated in terms of an arbitrary external-charge density. To solve this equation we make the ansatz equal to

\[ V(Q,z) = \int_{-L_1}^{L_2} dz' \frac{\rho_{eext}(Q,z')}{e} \phi(Q,z,z'). \]  \hfill (13)

Expression (12) then reads as

\[ \int_{-L_1}^{L_2} \frac{\rho_{eext}(Q,z')}{e} \phi(Q,z,z') \]

\[ = \int_{-L_1}^{L_2} dz' \frac{\rho_{eext}(Q,z')}{e} \]

\[ \times \left( -2\epsilon_s \sum_i S_i \int_{-L_1}^{L_2} dz_1 G_Q(z_1)g_i(z_1) \right) \]

\[ \times \int_{-L_1}^{L_2} dz \phi(Q,z_2,z')g_i(z_2) + eG_Q(z,z'). \]  \hfill (14)

And \( V(Q,z) \), given in expression (13), is the solution of Eq. (12) if \( \phi(Q,z,z') \) is the solution to the following equation:

\[ \phi(Q,z,z') = -2\epsilon_s \sum_i S_i \int_{-L_1}^{L_2} dz_1 G_Q(z_1)g_i(z_1) \]

\[ \times \int_{-L_1}^{L_2} dz \phi(Q,z_2,z')g_i(z_2) \]

\[ + eG_Q(z,z'). \]  \hfill (15)

Expression (15) is the application of expression (12) to the case of a pointed charge located at \((0,z')\). [It would have been obtained directly from Eq. (12) if \(\rho_{eext}(Q,z_1) = e\delta(z_1-z')\).] We have thus managed to convert a problem involving many charges, even several kinds of charges distributed anywhere, to easier problems involving only one charge in each of them. In order to solve Eq. (15) a self-consistent method has been used. We have developed an improved procedure which offers good initial results for the entire range of \(Q\) values. To estimate the initial value (for the numerical iterative procedure) of \(\phi(Q,z,z')\), \(g_i(z_2)\) is approximated by a sum of weighted delta functions located at the \(g_i(z_2)\) maxima,

\[ g_i(z_2) \approx \sum_{\mu=1}^{\infty} a_{\mu,\delta}(z_2-z_{\mu}), \]  \hfill (16)

where \(z_{\mu}\) are the relative maxima of \(g_i(z_2)\), and \(a_{\mu}\) the corresponding weights proportional to the maximum amplitudes, obtained by imposing normalization to unity. By assuming that all the maxima of \(g_i(z_2)\) fall in the semiconductor \((z>0)\), Eq. (15) is then written as

\[ \phi(Q,z,z') = eG_Q(z,z'), \quad z<0. \]  \hfill (17a)

With this approximation, it is only necessary to obtain \(\phi(Q,z_\mu,z')\) for all the subbands considered to calculate the first estimation of \(\phi(Q,z,z')\). By applying expression (17) to each of the maxima of \(g_k(z)\) \(z=z_{kv}\) is the position of the \(v\)th maximum of \(g_k(z)\), we obtained

\[ \sum_i A_{j_{kv}} \phi(Q,z_{kv},z') = eG_Q(z_{kv},z'), \]  \hfill (18)

where

\[ A_{j_{kv}} = \delta_{ij} + 2\epsilon_{sc} \delta_{j_{kv}} S_{i_0} \int dz_1 g_i(z_1)G_Q(z_{kv},z_1). \]  \hfill (19)

and \(\delta_{ij}=1\) for \(i=j\) and 0 otherwise.

Expression (18) is a linear equation system where the unknowns are \(\phi(Q,z_{kv},z')\). Once system (18) has been solved, the initial estimation of \(\phi'(Q,z,z')\) can be obtained from expression (17). Based on these initial values, Eq. (15) is solved iteratively.

Once the Fourier transform of the potential perturbations due to a pointed charge located at \((0,z')\) has been evaluated by this procedure for every \(z'\), we can obtain the Fourier transform of the potential perturbations due to the external-charge density responsible for Coulomb scattering by evaluating expression (13).

The Coulomb scattering rate for an electron of wave vector \(k\) in the \(i\)th subband, when the final state is in the \(j\)th subband, can now be calculated by the Golden rule:

\[ \mu_{ij}(k) = \frac{S}{2\pi \hbar} \int \left| \int dz \xi_i(z)H'(Q,z)\xi_j(z) \right|^2 \times \delta(E-E') dk', \]  \hfill (20)

where \(\xi_i(z)\) is the envelope function in the \(i\)th subband and \(H'(Q,z) = -eV(Q,z)\) is the perturbation Hamiltonian given by

The scattering rate between subbands $i$ and $j$ is then given by

$$
\frac{\varrho_{ij}(k)}{2\pi\hbar} = \sum_{t} \left[ |M_{ij}(Q,z_{t})|^2 \right] \delta(E-E') dk' 
+ \sum_{t=t+u} \left[ |M_{tu}(Q,z_{t},z_{u})|^2 \right] \delta(E-E') dk' ,
$$

(23)

where

$$
|M_{ij}(Q,z_{t})|^2 = \tilde{\phi}_{ij}^{(ij)}(Q,z_{t}) \tilde{\phi}_{ij}^{*(ij)}(Q,z_{t}),
$$

(24)

and

$$
|M_{tu}(Q,z_{t},z_{u})|^2 = \tilde{\phi}_{tu}^{(ij)}(Q,z_{t}) \tilde{\phi}_{tu}^{*(ij)}(Q,z_{t}),
$$

(25)

where

$$
\tilde{\phi}_{ij}^{(ij)}(Q,z_{t}) = \int_{-L_{1}}^{L_{2}} dz' \tilde{\phi}_{ij}(z') \phi(Q,z_{t},z_{t}').
$$

(26)

In order to evaluate expression (23) and thus obtain the scattering rate, we need to know $\sigma_{t}(r,z_{t})$, that is to say, the external charge density which is responsible for Coulomb scattering. In a simplified model of an insulator-semiconductor interface, charged centers are considered to be uniform charge sheets. In this idealized model, the electrons in an $n$-type inversion layer would not be scattered by charged centers, but only the average values of charges and their mean positions (by combining several techniques), and on the other hand it is a useless exercise, since the results obtained by these means will only be valid for this particular distribution. We therefore need an averaged Coulomb scattering rate related to the averaged macroscopic properties of the device.

Let $N$ be the total number of charged centers in the structure, and $P(r_{1},r_{2},...,r_{N})dr_{1}dr_{2}...dr_{N}$ the probability that charged-center 1 is located in $dr_{1}$, charged-center 2 is located in $dr_{2}$, and so on. The normalization condition is

$$
\int P(r_{1},r_{2},r_{3},...,r_{N})dr_{1}dr_{2}dr_{3}...dr_{N} = 1.
$$

(30)

The averaged Coulomb scattering rate in the $i$th subband is then

$$
\Gamma_{ij}(k) = \langle \varrho_{ij}(k) \rangle_{av},
$$

(31)

where by definition

$$
H'(Q,z) = -eV(Q,dz') \rho_{ext}(Q,dz') \phi(Q,z),
$$

(21)

where $Q = k - k'$, $E$ and $E'$ are the initial and final energies of the scattered electron and $S$ is the interface area.

For simplicity, we have assumed that the external charge distributions responsible for Coulomb scattering are conceptually divided into two-dimensional sublayers parallel to the insulator-semiconductor interface. Let $A_{zt}$ be the thickness of the $t$th sublayer, $z_{t}$ the center of the sublayer, and $\sigma_{t}(r,z_{t})$ the charge density per unit area in the $t$th sublayer, and $\sigma_{t}^{*}(Q,z_{t})$ its Fourier transform. Instead of (13) we now have

$$
V(Q,z) = \sum_{t} \frac{\sigma_{t}(Q,z_{t})}{e} \phi(Q,z,z_{t}i).
$$

(22)

The scattering rate between subbands $i$ and $j$ is then given by

$$
\varrho_{ij}(k) = \sum_{t} \left[ \frac{S}{2\pi\hbar} \int_{k'} |M_{ij}(Q,z_{t})|^2 \delta(E-E') dk' \right] 
+ \sum_{t=t+u} \left[ \frac{S}{2\pi\hbar} \int_{k'} |M_{tu}(Q,z_{t},z_{u})|^2 \delta(E-E') dk' \right],
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|M_{ij}(Q,z_{t})|^2 = \tilde{\phi}_{ij}^{(ij)}(Q,z_{t}) \tilde{\phi}_{ij}^{*(ij)}(Q,z_{t}),
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The scattering rate between subbands $i$ and $j$ is then given by

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\varrho_{ij}(k) = \sum_{t} \left[ \frac{S}{2\pi\hbar} \int_{k'} |M_{ij}(Q,z_{t})|^2 \delta(E-E') dk' \right] 
+ \sum_{t=t+u} \left[ \frac{S}{2\pi\hbar} \int_{k'} |M_{tu}(Q,z_{t},z_{u})|^2 \delta(E-E') dk' \right],
$$

(23)

where

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|M_{ij}(Q,z_{t})|^2 = \tilde{\phi}_{ij}^{(ij)}(Q,z_{t}) \tilde{\phi}_{ij}^{*(ij)}(Q,z_{t}),
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$$

(25)

where

$$
\tilde{\phi}_{ij}^{(ij)}(Q,z_{t}) = \int_{-L_{1}}^{L_{2}} dz' \tilde{\phi}_{ij}(z') \phi(Q,z_{t},z_{t}').
$$

(26)
\[ \langle f \rangle_{\text{avg}} = \int \text{d}r_1 \text{d}r_2 \cdots \text{d}r_N P(r_1, r_2, \ldots, r_N) f(r_1, r_2, \ldots, r_N). \]  

(32)

As \( |M_{tu}^{(ij)}(Q, z_t, z_u)|^2 \) and \( |M_{tu}^{(ij)}(Q, z_u)|^2 \) only depend on the distance of the sublayers to the interface but not on the position of the charged centers in the plane parallel to it, we obtain, using expressions (29) and (31),

\[
\Gamma_{ij}(k) = \sum_i \left( \frac{S}{2\pi \hbar} \int_{k'} \left[ q^2 \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_t) \rangle_{\text{avg}} \times |M_{tu}^{(ij)}(Q, z_t)|^2 \right] \delta(E - E') \text{d}k' \right) \\
+ \sum_{i \neq u} \left( \frac{S}{2\pi \hbar} \int_{k'} \left[ q^2 \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_u) \rangle_{\text{avg}} \times |M_{tu}^{(ij)}(Q, z_t, z_u)|^2 \right] \delta(E - E') \text{d}k' \right). 
\]

(33)

\[ \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_t) \rangle_{\text{avg}} \] is the density correlation function of charged centers in the same sublayer, and \( \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_u) \rangle_{\text{avg}} \) is the density correlation function of charged centers in different sublayers, defined according to expression (32). If we assume that there is no correlation among charged centers of different sublayers, then \( \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_u) \rangle_{\text{avg}} = 0 \) \( \neq u \) and the averaged Coulomb scattering rate is finally written as

\[
\Gamma_{ij}(k) = \sum_i \left( \frac{S}{2\pi \hbar} \int_{k'} \left[ q^2 \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_t) \rangle_{\text{avg}} \times |M_{tu}^{(ij)}(Q, z_t)|^2 \right] \delta(E - E') \text{d}k' \right). 
\]

(34)

Expression (34) is the Coulomb-scattering rate for a transition from subband \( i \) to subband \( j \). Transitions involving different valleys can be considered by taking into account the valley separation in the \( k \) space and accounting for the degeneracy of the final valleys. In general, the matrix element for the larger wave vectors involved in these intervalley transitions, \( |M_{tu}^{(ij)}(Q, z_t)|^2 \), is quite small,\(^{20}\) and the intervalley rate due to Coulomb scattering will then also be much smaller than that of the intravalley. Besides, the scattering rate for intersubband transitions in the same valley is much smaller than the intrasubband scattering rate due to the reduced overlap factor in the transition matrix element.\(^{10}\) Therefore, we have included below only intrasubband transitions:

\[
\Gamma_i(k) = \sum_i \left( \frac{S}{2\pi \hbar} \int_{k'} \left[ q^2 \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_t) \rangle_{\text{avg}} \times |M_{tu}^{(ij)}(Q, z_t)|^2 \right] \delta(E - E') \text{d}k' \right). 
\]

(35)

Equation (35) explicitly includes the charged-center distribution and correlation, while the effects of electron distribution, image charges, and screening are contained in the matrix element \( |M_{tu}^{(ij)}(Q, z_t)|^2 \). The screening constant \( S_i \) used in this work has been taken into account in the long wavelength limit. A more complete treatment would include a dependence in the \( Q \) vector.\(^{21}\) Stern\(^{22}\) has shown that at low temperatures this expression yields results significantly different from the expression employed in our article. However, we have also obtained the two-dimensional Fourier component of the potential fluctuations due to external charged centers taking into account the dependence of \( S_i \) on \( Q \) for the temperature range considered in our study. We have found that only for strong inverted layers at the lowest temperatures may our approximation be insufficient and the most complete expression need to be considered. In any case, the inclusion of one or the other expression is straightforward in the formulation.

To include the charged center correlation we have derived an expression for \( \langle \tilde{n}_i(Q, z_t) \tilde{n}_j^*(Q, z_t) \rangle_{\text{avg}} \) in terms of two-dimensional distribution functions considering the simple hard-sphere model, according to which the distribution of charged centers is assumed to be random to the extent that no two centers can be found within a radius of \( R_i \) from each other. In this case one obtains\(^{7}\)

\[ \langle \tilde{n}_i(Q) \tilde{n}_j^*(Q) \rangle_{\text{avg}} = \frac{N_i}{S} \left( 1 - \frac{2C \Gamma_i(QR_i)}{Q R_i} \right), \]

(36)

where \( \Gamma_i(x) \) is the first order Bessel function, \( C_i = \pi R_i^2 N_i \) is a parameter which is a measure of the degree of correlation \( (C_i=0 \text{ corresponds to a completely random distribution; } C_i=1 \text{ corresponds to uniform distribution of point charges}). \)

As it is assumed that Coulomb scattering assists intravalley transitions, the difference between the wave vector before and after the scattering is small and we can approximate \( Q \approx 2k \sin \theta/2 \), where \( \theta \) is the angle between initial and final wave vectors. Expression (35) is finally given as

\[
\Gamma_i(k) = \sum \frac{N_i m^*_i}{\pi \hbar^*} \int_0^\pi \left[ q^2 \left( 1 - \frac{2C \Gamma_i(QR_i)}{Q R_i} \right) \right] \times |M_{tu}^{(ij)}(Q, z_t)|^2 \text{d}\theta, 
\]

(37)

where \( m^*_i \) is the parallel mass of the electron in the \( i \)th subband.

Expression (37) can be used for calculating the Coulomb-scattering rate in simulation procedures; we have included it in a Monte Carlo calculation of the electron transport properties. Details of this calculation are given in the next section.

III. SIMULATION RESULTS AND DISCUSSION

We have employed this theory to study the effect that Coulomb scattering has on the mobility of electrons in an \( n\)-Si(100) inversion layer, for which a one-electron Monte Carlo method has been developed. Although our study of Coulomb scattering has been applied to the metal-Si-SiO\(_2\) structure, the proposed model in Sec. II is completely general and could be applied to any semiconductor inversion layer and any heterointerface. Most of the results and discussion presented here should therefore also apply to electronic transport in other structures.
We have considered the Si/SiO₂ interface to be parallel to a [100] plane and the ⟨011⟩ direction of the n-inversion layer to be the direction of the driving field. In these conditions, if an electric field is applied perpendicularly to the interface, the energy bands are bent down and a potential well is defined. The degeneracy of the six equivalent minima of the silicon conduction band breaks and the electrons are distributed in two sets of subbands. One set arises from the two equivalent valleys showing the longitudinal mass in the direction perpendicular to the interface \((E_0,E_1,...)\) and the other one from the four equivalent valleys showing the transverse mass in the same direction \((E'_0,E'_1,...)\). To obtain the effective transverse-electric field, the energy of the subbands, and the envelope function normal to the interface, we have self-consistently solved the Schrödinger and Poisson equations\(^{11}\) for each value of the surface potential. Although some authors have considered that it is an acceptable approximation to suppose that most of the electrons are in the lowest three subbands,\(^{23,24}\) we have observed appreciable differences when considering a greater number of subbands.\(^{25}\) We therefore decided to allow the electron to move in six subbands in our Monte Carlo calculation even though we considered twenty subbands for the solution of the Poisson and Schrödinger equations. The occupation of higher subbands forces us to include the contribution of several subbands in the transport and to allow transitions among them.\(^{26}\) In these conditions, phonon scattering mainly causes one of two types of electron transitions: \(^3\) (a) intervalley acoustic transitions and (b) intervalley optical transitions, both of which have been adapted from their treatment in silicon bulk\(^ {27}\) to use them in Si(100) inversion layers. The scattering probabilities of these mechanisms have been deduced from the matrix elements for the scattering of electrons by bulk phonons, and using Price's formulation.\(^ {28}\) The coupling constants, deformation potential, and phonon temperatures have been adjusted so that the phonon-limited mobility of the electrons in the silicon inversion layer approaches the bulk value as the transverse electric field approaches zero.\(^ {29}\)

We have considered interactions both in zero and first-coupling order. The low-energy intervalley phonons considered in the model are forbidden in zero order,\(^ {30}\) so they have been treated via first-order interaction.\(^ {31}\) The first-order intervalley scattering has been shown to play an important role in hot-electron transport in silicon-inversion layers;\(^ {32}\) our results show that this mechanism is also important in ohmic transport.\(^ {24}\) A detailed study of the electron-phonon interaction has been published recently.\(^ {33}\)

In addition to Coulomb and phonon scattering we have considered surface-roughness scattering in the Ando's approach with a Gaussian model which depends on the spectral distribution of the roughness at the interface.\(^ {3}\) Other models\(^ {34}\) have been proposed in the literature to take into account the effect of the separation of the interface from an ideal plane. Some models have included screening of this scattering.\(^ {25}\) We have centered this article on Coulomb scattering but have added surface-roughness scattering in order to reproduce the mobility behavior for high transverse-electric fields. We have chosen the values of the surface roughness parameters to achieve a good adjustment. Therefore, we will no longer include any further discussion on surface roughness in this article.

Taking into account all the above scattering mechanisms, (phonon, surface roughness, and Coulomb scattering) the mobility of the electrons in the inversion layer has been obtained by calculating the mean velocity along the inversion layer for several values of the longitudinal electric field and extrapolating to zero. We have chosen the lowest range of the longitudinal field that allows the calculation without excessive noise.

In order to study the effect that Coulomb scattering has on electron transport properties, we first determined in which conditions of temperature and transverse effective field (as defined in Ref. 36), Coulomb scattering is important. Figures 1 and 2 show the dependence of the total scattering rate, and of the rate for each scattering mechanism on the electron kinetic energy. Plotted data in each figure correspond to the ground subband for a low and a high transverse electric field, respectively. In Fig. 1 the temperature is \(T=300\) K while in Fig. 2 it is \(T=77\) K. The mean electron kinetic energy is marked in each figure with a vertical line. The total scattering rate is shown by a solid line. It is evident from these two figures (dashed-line) that Coulomb scattering is the main scattering mechanism.
at low electric fields regardless of temperature. However, the situation is completely different when the effective transverse field is higher. In this case, the induced charge density is much larger and thus the screening of charged centers by mobile carriers is much more effective, thereby decreasing the Coulomb-scattering rate. Both figures also indicate that phonon scattering acquires importance as the temperature increases. With regard to surface-roughness scattering, it is shown to increase as the effective electric field increases, being the main scattering mechanism for high electric fields.

Once we determined in what conditions Coulomb scattering is important, we studied its effects on the transport properties of electrons in silicon inversion layers. To do so, effective mobility curves versus the effective transverse electric field have been obtained in different conditions of temperature, charged-center density, correlation, and position of charged-center distributions. These aspects are studied below.

A. Effect of temperature

The influence of temperature on Coulomb scattering has already been seen in Figs. 1 and 2. It is apparent in these figures that the lower the temperature the more important the effect of Coulomb scattering versus the rest of the scattering mechanisms. In order to see the temperature effect, more clearly we obtained different effective mobility curves versus the effective transverse electric field for several temperatures. Figure 3 shows mobility values for a charged center density of \( N_q=4\times10^{16} \text{ cm}^{-2} \) and for a substrate doping of \( N_A=10^{16} \text{ cm}^{-3} \). We have assumed a single layer of charged centers located right at the interface (\( z_0=0 \)).

B. Effect of charged-center concentration

To demonstrate the effect of charged-center concentration on the transport properties we obtained mobility curves for different values of charged-center densities (Fig. 4). Here we have also assumed that all the charged centers are located in a layer parallel to the interface at the plane \( z=z_0 \). We have imposed \( C=1 \) (charge-center correlation) and a substrate doping of \( N_A=10^{10} \text{ cm}^{-3} \). As expected, the
higher the concentration, the lower the mobility. It is also apparent that all the curves are almost superposed at high electric fields, which indicates that Coulomb scattering loses its importance with respect to the other mechanisms, mainly surface-roughness scattering, as the electric fields grows, which is in agreement with the conclusions from Figs. 1 and 2.

C. Effect of the position of charged centers

Figure 5 shows the effective mobility of electrons in a silicon inversion layer versus the transverse effective electric field for different charge layers, parallel to the interface, located at \( z = z_0 \). It can be observed that the scattering of electrons by charged centers quickly decreases when the charge is kept away from the interface. For charges placed at 100 Å or more from the interface, Coulomb scattering is negligible.

The model we have developed and presented in this article has allowed us to study the influence of simultaneous charged-center layers. We have obtained the effective mobility by assuming that charged centers are distributed in two layers parallel to the interface: one is located within the oxide at the plane \( z = z_0 \), while the other is assumed to lie right at the interface. Curves shown in Fig. 6 were obtained at a temperature of \( T = 300 \) K and a substrate-doping concentration of \( N_A = 9 \times 10^{14} \) cm\(^{-3} \).

D. Effect of image charges

We have also applied the formulation developed in Sec. II to study the effect on the mobility of the difference in the permittivity of the two materials on either side of the interface. We have assumed that all the charged centers are located in a layer parallel to the interface at plane \( z = z_0 \), and that the temperature is \( T = 300 \) K. We have imposed the following values: \( C_1 = 1 \) (charge-center correlation), an oxide-charge density of \( N_{ox} = 0.8 \times 10^{11} \) cm\(^{-2} \), and a substrate doping of \( N_A = 10^{16} \) cm\(^{-3} \). Results are shown in Fig. 7 for three different cases: curve (1) was obtained by neglecting image charges (i.e., by assuming that the permittivity of the SiO\(_2\) coincides with that of silicon); curve (2) was obtained by considering only the image of the oxide charge; and the curve (3) all the image-charge effects have been taken into account. The data in Fig. 7(a) are for an external charge placed right at the interface, and Fig. 7(b) corresponds to a sheet of charge placed within the oxide, at 20 Å from the Si-SiO\(_2\) interface. These curves show the appreciable influence of image charges: if their effects are completely ignored, Coulomb scattering is underestimated, but if only the image of the external charge is considered, neglecting that of the induced charge, Coulomb scattering is overestimated due to an underestimation of the screening.

E. Effect of charged-center correlation

Figure 8 shows curves of effective mobility versus the effective field obtained for \( T = 300 \) K and \( N_{ox} = 0.8 \times 10^{11} \) cm\(^{-2} \) for different positions of the charge distributions. Dotted line curves correspond to a two-dimensional charge distribution in a plane parallel to the interface at 50 Å from it, and solid-line curves are for a distribution right at the interface. In both cases, correlation of the charged centers has the effect of reducing scattering, and hence increasing the mobility since if charges are randomly distributed the perturbation is locally greater than for uniform distribution. It is also apparent that the lower the transverse electric field the greater the correlation influence. This was expected, since at low fields the interaction with charged centers is stronger due to lower screening.

F. Comparison with experimental results

The Monte Carlo simulation, with our Coulomb-scattering model, has been observed to reproduce the experimental results quite well. We have used, for compari-
Electro mobility vs the effective transverse electric field in a silicon inversion layer, at $T=300$ K, for two different positions of the charge in the oxide: right at the Si-SiO$_2$ interface (a), and at 20 Å from the Si-SiO$_2$ interface (b). In both parts of the figure three curves are shown: curve (1) has been obtained by neglecting image charges; curve (2) has been obtained by considering only the image of the oxide charge; and curve (3) corresponds to the approach of this letter, in which all the image-charge effects have been taken into account.

In Fig. 9, experimental mobility curves (solid line) taken in our laboratory are compared to computed data (symbols) at three different temperatures. Both the magnitude and the bell-shaped behavior are well reproduced with our model.

**IV. CONCLUSIONS**

We have refined an existing theory to study the transport properties of electrons in semiconductor inversion layers, useful in both semiconductor inversion layers and in other heterostructures. We have proposed a comprehensive model for Coulomb scattering that simultaneously takes into account the effects of screening of charged centers by mobile carriers, the distribution of charged centers into the insulator, the actual electron distribution in the inversion layer, the charged-center correlation, the effect of image charges, and the influence of the rest of the scattering mechanism.

In order to study Coulomb scattering of electrons in semiconductor inversion layers we have developed a one-electron Monte Carlo procedure, and applied it to an $n$-Si(100) inversion layer.

The importance of Coulomb scattering versus the other mechanisms has been shown, mainly at low transverse-electric fields. We have also pointed out the importance of correctly taking into account the effect of image charges, both external and induced. The correlation of charged centers has been shown to play an important role, and considerably modifies the effective mobility. Finally, it has been shown that the higher the charged-center concent...
tration, the greater the scattering and the lower the electron mobility, and the farther from the interface the charged centers are, the smaller the influence they have on the electron mobility.

ACKNOWLEDGMENTS

We thank Professor J. Banqueri for providing experimental results, and the CICYT and the Junta de Andalucía for financial support for our research group.

20. The Fourier transform of the potential perturbation rapidly decreases with the increase of the Q value as can be observed in Green’s function expression [Eq. (11)].
33. A detailed study of the scattering mechanisms for electrons in silicon inversion layers, which was published during the revision process of this article, can be found in M. V. Fischetti and S. E. Laux, Phys. Rev. B 48, 2244 (1993).