Influence of the Oxide-Charge Distribution Profile on Electron Mobility in MOSFET's

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Abstract—To characterize the effect of oxide-charge distribution on electron mobility in a MOSFET channel, a more precise method for obtaining the oxide-charge profile than C-V measurements is needed. We have shown by Monte Carlo simulation that the effective interface-charge concentration obtained from threshold voltage measurements does not reproduce the actual effect that the oxide charge has on electron mobility. It is therefore absolutely necessary to know the real profile of the charge distribution. An analytical expression to obtain the interface-charge concentration which correctly models the effect of the actual oxide-charge distribution is calculated from Monte Carlo results.

I. INTRODUCTION

IT is well known that oxide charge and interface traps can adversely affect MOS-device performance due to the strong influence that the concentration and position of these electrically active centers have on device characteristics [1]–[4]. Both the density and position of charged centers can change during MOSFET operation, thus involving modification of the device's electric properties [1], and causing parametric failure of the device. This fact poses a serious stability and reliability problem that it is imperative to control. To do so, a thorough understanding of the roles all these charges play in carrier-transport properties is required.

Together with the threshold voltage, the mobility of the electrons in the channel is one of the fundamental parameters in MOS devices. The electron mobility directly establishes, for example, the current level in the device, and thus the transconductance. It is therefore indispensable to develop a characterization of electron mobility that includes the effects of the charge distributed in the oxide.

It has been accepted for years that the generation of interface states is the only mobility-degradation mechanism [5]–[7]. However, recent works have reported on the nonnegligible contribution of the oxide-trapped charge to mobility degradation in MOS devices in ionizing-radiation environments [4], [8]–[11]. Mobility degradation due to interface traps and oxide charges trapped right at the interface has been previously modeled [12]–[15]. However, since radiation-induced oxide charges may be located in the oxide bulk, they will degrade carrier mobility differently as compared to surface charges. (For example, in MOS devices irradiated at cryogenic temperatures, the charge is frozen in the oxide, rather than transported and subsequently trapped at the interface). A model for mobility degradation due to scattering from bulk oxide charges has recently been proposed [11]. Although the authors found that the experimental results are in good agreement with their model predictions, they used the relaxation time approximation and a very simple screening approximation to calculate electron mobility due to oxide-charge. In addition, they used Matthiessen's rule to obtain the total mobility.

On the other hand, although Zupac et al. [4], [8]–[9] demonstrated experimentally the significant contribution of the oxide-trapped charge to mobility degradation, they used charge densities derived from voltage shifts [16], which are not always adequate from the mobility viewpoint [2]. As we will show, different oxide-charge distributions can produce the same threshold-voltage shift but very different electron mobility.

In this work we have studied the influence of the oxide charges on the electron mobility, solving the Boltzmann transport equation by Monte Carlo simulation [17], and considering the actual profile of the oxide-charge distribution. The calculation has been applied to the case of a silicon-inversion layer in a MOS structure with a (100) p-type substrate. Different oxide-charge distributions have been considered in order to determine the actual effect that charges trapped in the oxide bulk have. The validity of our Monte Carlo simulator has already been proved by reproducing experimental results [14]–[15], [18]. It is worth noting that a Monte Carlo study is specially suitable in this case since it not only allows the parameters of the device to be precisely controlled, but also provides information of great importance for device production and modeling that is unavailable experimentally.

II. MONTE CARLO SIMULATION

The effective mobility has been obtained by the one-electron Monte Carlo procedure described below [14]: Electrons in the MOSFET channel have been treated as a quasi-two-dimensional electron gas contained in energy subbands. The position of the subband minima and the electron concentration in each of them were obtained by the self-consistent solution of the Poisson and Schroedinger equations for each value of the effective transverse electric field [19], [20]. The simulation begins with an electron in a given subband and a wave vector \( k_z \). The longitudinal electric field modifies the electron wave vector according to the semiclassical model. The history of
the electron is divided into different subhistories, and each subhistory is continued until the effective scattering events exceed 25,000 to obtain good convergence for the electron-drift velocity. The number of subhistories considered is that necessary for the standard deviation of the velocity data to fall below 5% of the final mean value. The average drift velocity is calculated in this way for several values of the longitudinal electric field, and the low-field effective mobility is obtained by extrapolating to zero electric field. The upper limit of the longitudinal field is chosen sufficiently high to allow calculations without excessive numbers of subhistories, but low enough to avoid electron heating.

In our Monte Carlo procedure we have allowed the electron to travel in six subbands and to move between them [14]. In addition, we have considered phonon [17], [21] and surface-roughness [22], [23] scattering. Phonon scattering mainly causes one of two types of electron transitions: a) intravalley acoustic transitions and b) intervalley transitions, both of which have been adapted from their treatment in silicon bulk for use in Si(100) inversion layers. The phonon scattering rates have been deduced by using Price’s formulation [24]. The intervalley transitions are described according to Jacoboni’s bulk phonon model [17]. Expressions for the phonon scattering rates can be obtained from [25]. In accordance with [21], we have not taken into account the effect that screening may have on phonon scattering, since unscreened models give reasonably good results. Surface-roughness scattering has been considered in Ando’s approach with a Gaussian model dependent on the spectral distribution of roughness at the interface. The Gaussian model has been widely used in the literature [22], although it has been proved [26] that other models, which may have more physical basis, such as the exponential one, provide the same results as the Gaussian model. An improvement of our surface-roughness-scattering model could perhaps be achieved by introducing screening. Nevertheless, this would not modify the conclusions of this paper at all, because roughness scattering affects mobility at high transverse electric fields where the Coulomb scattering is very weak as a consequence of screening.

III. COULOMB-SCATTERING MODEL

Coulomb scattering is essential in this study on the influence of oxide-charge distribution on electron mobility. We have therefore developed a comprehensive Coulomb-scattering model in semiconductor inversion layers (to be found in [14] and [15]) that allows the actual profile of the oxide-charge distribution to be taken into account. A brief description of this model is given below.

The transport properties of an electron in a semiconductor inversion-layer are modified by the presence of charged centers (both silicon bulk-impurities and oxide charges) near the Si-SiO₂ interface [1], [13], [27], since they induce local fluctuations of the electric potential, thus modifying the position and occupation of the electric subbands. These local fluctuations of the electric potential are responsible for the scattering of the electrons in the inversion layer.

To calculate them, we solved the Poisson equation due to the spatial variations of external point-charge distributions (both silicon bulk-impurities and oxide interface charge), taking into account screening due to mobile carriers. Once the potential local fluctuations were evaluated, the scattering rate was calculated by the Golden rule. Such a Coulomb-scattering model, simultaneously takes into consideration the effects of i) screening by mobile carriers, ii) space correlation of the external charged centers (which may be important at high concentrations), iii) distribution of the charged centers in the oxide and semiconductor bulk, iv) distributions of the electrons in the inversion layer, and v) image effects caused by the difference in the dielectric constants of Si and SiO₂. For simplicity, we assumed that the external-charge distributions responsible for Coulomb scattering were conceptually divided into two-dimensional sublayers parallel to the insulator-semiconductor interface [14]. Thus the actual profile of the oxide-charge distribution could easily be taken into account. The complete development of this Coulomb scattering model can be seen in [14] and [15].

IV. POSITION OF THE CHARGE INSIDE THE OXIDE BULK

It is obvious that a charge remote from the interface will scatter carriers less effectively than one close to it [14]. Nevertheless, we have quantitatively studied this behavior using Monte Carlo simulation in order to see the actual effect of the oxide charges on electron mobility when they are kept away from the interface. Fig. 1 shows the effective mobility of electrons in a silicon inversion layer versus the transverse effective field for a charged layer parallel to the interface, located inside the oxide bulk at different distances from the Si-SiO₂ interface. In this figure we can observe that all the curves coincide in the high-field region, even when oxide charges are so far from the interface that they do not contribute to electron scattering (curve 6). This fact suggests that in this region, effective mobility is dominated by surface-roughness and phonon scattering. The differences in the curves are observed at low electric fields, which means that Coulomb scattering (which is different in all the curves due to different charge positions) dominates in that field region. An initial growth and a later decrease of the mobility curves can be observed as the effective field increases. This behavior
of the mobility curves, also experimentally observed, has been attributed to experimental uncertainties. Since this study relies on simulation, however, this phenomenon cannot be attributed to any such experimental uncertainties. The shape of the mobility curves can be nevertheless justified by the superposition of two tendencies: i) the tendency of the phonon and surface-roughness scattering to increase with an increasing electric field, and ii) the tendency of Coulomb scattering to decrease as the effective electric field rises because the higher the electric field, the higher the electron concentration in the inversion layer and the higher the screening of the oxide charge. This last tendency is dominant at low electric fields where Coulomb scattering is dominant, as we have just seen above.

In addition, note that the scattering of electrons by charged centers quickly decreases when the charge is kept away from the interface. It is also evident that for charges placed at 100 Å or more from the interface, Coulomb scattering is negligible: Fig. 2 shows mobility curves for different concentrations of a charged layer located right at the interface or at 100 Å from it. When the charged layer is located right at the interface, the electron mobility is strongly affected by the charge concentration. In contrast, when the charged layer is located at 100 Å from the interface, the oxide charge hardly modifies the electron mobility.

At cryogenic temperatures, the influence on the effective mobility of the charges located far from the interface is still lower.

V. OXIDE-CHARGE DISTRIBUTION PROFILE

Both mobility and threshold voltage are influenced by oxide-trapped charge and interface-trapped charge [1], [4]. The effect that the oxide-charge distribution has on the threshold-voltage or flatband-voltage is modeled by defining an effective oxide charge placed at the Si-SiO₂ interface which is actually the first moment of the oxide-charge distribution [11]:

\[
qN_{ox}TH = \frac{1}{d_{ox}} \int_0^{d_{ox}} x \rho_{ox}(x) dx
\]  (1)

\( x \) being the distance to the gate, and \( d_{ox} \) the oxide thickness. This effective oxide charge is the magnitude measured when analyzing flatband voltage shifts with capacitive techniques.

However, oxide-charge distributions corresponding to the same effective oxide charge (providing therefore the same threshold voltage shift), can actually lead to very different mobility curves. This means that, from the mobility viewpoint, a simple C-V measurement is not enough to model the influence of the oxide charge on device behavior and therefore a better characterization is needed.

It follows that a detailed knowledge of the oxide-charge profile is strongly required. Nevertheless, the experimental determination of the charge density as a function of distance in the oxide is not an easy task since it requires complex experimental methods (Etch-off, and photo I-V) [1], [29]. This means that an experimental study on the influence of the oxide-charge distribution profile on electron mobility is quite difficult, complicated, and very expensive. All these difficulties can be successfully bypassed, however, by doing a mobility study by Monte Carlo simulation.

To do so, we assumed an NMOS-Si(100) structure with an oxide-layer thickness of 200 Å, and considered different oxide-charge distributions, all corresponding to the same effective oxide-charge at the interface (1). Therefore, the threshold voltage has the same value in all cases. Doping concentration was assumed to be \( N_A = 9 \times 10^{14} \) cm\(^{-3}\), low enough that the bulk-impurity charge does not modify electron mobility. In the simulation we also considered no charge trapped in the interface, thus avoiding any influence of this charge on electron mobility, which could conceivably mask the effects of the oxide-charge profile. In fact, however, the interface-trap charge is expected to smooth the effects of the oxide charge.

The following oxide-charge distributions were taken into account:

1) A uniform distribution throughout the oxide, with a concentration per unit volume of \( N_{ox} = 5 \times 10^{17} \) cm\(^{-3}\).
2) A charged layer located inside the oxide at 100 Å from the interface, with a concentration of \( 1 \times 10^{12} \) cm\(^{-2}\) per unit area.
3) Two charged layers located inside the oxide in the following two situations:

   a) (c-1) One layer located at 50 Å from the interface with a concentration per unit area of \( 5 \times 10^{11} \) cm\(^{-2}\), and a second one at 150 Å with a concentration of \( 5 \times 10^{11} \) cm\(^{-2}\).
   b) (c-2) One layer at 10 Å from the interface with a concentration of \( 1 \times 10^{11} \) cm\(^{-2}\), and a second one at 110 Å with a concentration of \( 9 \times 10^{11} \) cm\(^{-2}\).

The distributions considered here are not likely to occur in practical devices having thermal oxide as the gate insulator (e.g., two charge layers at different distances from the interface). However, since it is very difficult to know the exact distribution of the oxide charge introduced due to radiation, we decided to use these simple distributions. In addition, and in spite of their lack of practical application, these distributions are even more appropriate than the actual charge distribution for clearly showing the effect of the distribution profile on
the mobility. In any case, we should note that this Coulomb scattering model allows the actual oxide-charge distributions to be considered, if they are known.

In all the above cases, the total amount of charge trapped in the oxide is \( Q_0 = e \times A \times (1 \times 10^{12} \text{ cm}^{-2}) \), where \( e \) is the electron charge and \( A \) is the transverse area of the structure. The mean position of the distribution is located inside the oxide, at \( z_0 = 100 \text{ Å} \) from the interface. The threshold voltage shift produced by all these charge distributions is equal to \(-0.464 \text{ V}\), and is the same in all cases. All these distributions would therefore appear to be the same when measured by C-V method, thus making it impossible to distinguish among them by this method. However, from a mobility viewpoint, they show very different behavior. To appreciate this, we calculated mobility curves both at room and low temperatures for each oxide-charge distribution.

In order to apply the Coulomb-scattering model to distribution (a), the oxide must be divided into sublayers. This is because the Coulomb-scattering model described in [14] was developed for oxide-charge distributions in the form of charge sheets, although there is no limitation to the number of sheets we can consider. This was done so that the actual profile of the charged-center distributions could easily be taken into account. In any case, the greater the number of sublayers, the better the approximation of the oxide-charge distribution to the actual profile. We have considered different partitions of the oxide in order to determine the optimum number of slices necessary to reproduce the effects of the oxide-charge distribution. To take into account distribution (a), the following three situations were considered:

1) The oxide is assumed to consist of only one slice. This slice is modeled by a charged layer located in the middle of the oxide, \( z = 100 \text{ Å} \), with a concentration of \( N_{ox} = 1 \times 10^{12} \text{ cm}^{-2} \).

2) The oxide is divided into ten slices 20 Å thick. Each slice is now modeled by a charged layer with a concentration of \( 1 \times 10^{11} \text{ cm}^{-2} \) in the middle of the slice.

3) The oxide is divided into twenty slices 10 Å thick. Each slice is modeled by a charged layer located in the middle of the slice, and with a concentration per unit area of \( 0.5 \times 10^{11} \text{ cm}^{-2} \).

Mobility curves in situations 1–3 have been obtained at different temperatures using the Monte Carlo procedure. The results can be observed in Fig. 3. As shown, mobility curves coincide when ten or more slices are taken into account, but are very distinct when only one slice is considered. This means that dividing the oxide into ten slices provides a good approximation of oxide-charge concentration. If the distribution was nonuniform, we would have to evaluate the concentration of each sublayer according to the actual profile of the distribution.

Fig. 4 shows mobility curves versus the transverse electric field calculated by Monte Carlo simulation for each of the oxide-charge distributions (a) to (c) detailed above at room temperature. Important differences between the mobility curves can be seen in extreme cases (a) and (b), a change of about 30% in mobility maximum occurs, and the effect is greater at low temperatures.

This result proves that the actual profile of the distribution can strongly modify electron mobility, even when the total amount of charge and the mean position of the distribution is kept fixed. In consequence, it is necessary to consider the oxide-charge distribution profile and not only the first moment of the distribution, nor even the total charge and its mean position.
TABLE I

<table>
<thead>
<tr>
<th>Distribution</th>
<th>( \mu_{\text{max}} ) (cm²/Vs)</th>
<th>( N_{\text{th}} ) (cm⁻³)</th>
<th>( \mu_{\text{max}} ) (cm²/Vs)</th>
<th>( N_{\text{th}} ) (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>2950</td>
<td>1.54x10¹⁰</td>
<td>449</td>
<td>1.57x10¹¹</td>
</tr>
<tr>
<td>b</td>
<td>7266</td>
<td>1.1x10⁹</td>
<td>640</td>
<td>1.55x10⁹</td>
</tr>
<tr>
<td>c-1</td>
<td>3811</td>
<td>7.3x10⁸</td>
<td>484</td>
<td>9.7x10⁹</td>
</tr>
<tr>
<td>c-2</td>
<td>3525</td>
<td>9.0x10⁹</td>
<td>489</td>
<td>9.0x10⁹</td>
</tr>
</tbody>
</table>

Fig. 5. Electron mobility in a MOSFET for a uniform charge distribution inside the oxide (\( N_{ox} = 5 \times 10^{17} \) cm⁻³, \( d_{ox} = 200 \) Å): (*) Considering the actual distribution profile. (1): Modeling the actual distribution with a two-dimensional charge distribution located right at the interface and with a concentration of \( N_{th} = 1.7 \times 10^{11} \) cm⁻³.

Nevertheless, for device modeling and simulation purposes, it is still interesting to take into account the effects that oxide charges have on the electric parameters of MOSFET’s, by considering an effective-charge distribution located right at the interface [16]. For modeling the threshold voltage shift produced by oxide charge, an interface charge of \( N_{TH} = 5 \times 10^{11} \) cm⁻² must be set in all cases (a to c). However, we have found that the effective-charge concentration necessary to reproduce mobility behavior (\( N_{th} \)) strongly depends on the profile of the oxide-charge and is quite different from \( N_{TH} \).

To calculate \( N_{th} \), we simulated mobility curves and modified the amount of charge trapped right at the interface, comparing the results to the actual mobility curve. Table I shows the \( N_{th} \) values for the different oxide-charge distributions considered in this work. Fig. 5 also shows the comparison between mobility curves obtained assuming distribution (a) and taking into account the respective \( N_{th} \). Very good agreement can be observed both at room and low temperatures.

It is worth noting that the effective interface-charge concentrations needed to reproduce mobility results (\( N_{th} \)) strongly depend on the oxide-charge profile, and are much smaller than the effective interface-charge concentration needed to reproduce the threshold voltage (\( N_{TH} \)). In any case, \( N_{th} \) scarcely depends on temperature, as seen in Table I.

These simulation results can be used to model the effect that the profile of the oxide-charge distribution has on mobility by calculating an analytical expression for \( N_{th} \) versus the mobility-maximum value. To do so, we considered ten different oxide-charge profiles, and calculated the mobility maximum and \( N_{th} \) values that give each mobility curve. Applying a least-squares fitting to the resulting data, the following expressions were obtained:

\[
N_{th} = 2.823 \times 10^{18} (\mu_{\text{max}})^{-2.94}, \quad T = 77 \text{ K}
\]

\[
N_{th} = 3.411 \times 10^{28} (\mu_{\text{max}})^{-6.536}, \quad T = 300 \text{ K}
\]

with \( \mu_{\text{max}} \) expressed in cm²/Vs and \( N_{th} \) in cm⁻².

Knowing the mobility maximum, Expressions 2 and 3 provide the effective interface-charge concentration which, when located right at the interface correctly models the effect of the oxide-charge distribution.

VI. CONCLUSIONS

We have studied the influence of the position of the oxide-charge on the electron mobility in MOSFET’s by Monte Carlo simulation. We have proved that the charges located at 100 Å or more hardly modify electron mobility.

We have also shown that oxide-charge distributions providing the same threshold voltage shift can actually lead to very different mobility curves. Therefore, in order to characterize the effect of oxide charge on electron mobility in a MOSFET channel, it is highly desirable to know the actual profile of the charge distribution.
It has been seen that an effective interface-charge concentration obtained from threshold voltage measurements does not reproduce the effect that the oxide charge has on electron mobility. Nevertheless, for device modeling and simulation purposes, it is interesting to consider the effects of oxide charges on electron mobility by taking into account an effective-charge distribution located right at the interface.

We have calculated an analytical expression to obtain such an interface concentration from Monte Carlo results.

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