An Improved Model for Electron Mobility Degradation by Remote Coulomb Scattering in Ultra-Thin Oxide MOSFETs

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Abstract

This paper presents a new model for the electron mobility degradation in MOSFETs due to Remote Coulomb Scattering. We improved previous theoretical treatments by including screening in polysilicon and removing the approximation of quantum limit transport. Our results demonstrate that the ingredients included in our model are of remarkable quantitative importance.

1. Introduction

An impressive research effort has been recently devoted to the use of ultra-thin oxides in CMOS technologies in relation to either oxide leakage or reliability issues. However, so far only a few papers have discussed how extremely thin dielectrics and the proximity of the gate polysilicon can affect carrier transport in the MOSFET channel [1, 2, 3] despite some concerns were raised by the degradation of current drivability in decananometer MOSFETs with gate oxides thinner than 1.3nm [4].

This paper focuses on the modeling of the Remote Coulomb Scattering (RCS) in n-MOSFETs and on its possible impact on electron effective mobility ($\mu_{\text{eff}}$). Previous works on this topic [1, 2] rely on semi-analytical expressions for the Momentum Relaxation Time (MRT) due to RCS, as originally derived by Stern et al. [5] for coulomb centers in substrate silicon or in the oxide. Those derivations assume that only the lowest subband of the 2D inversion layer contributes to electron transport (Quantum Limit - QL) and, furthermore, neglect the screening effect due to free electrons in the polysilicon.

In this paper we use a fully-numerical procedure for the determination of mobility. Starting from the Schrödinger-Poisson solution of the 1D electrostatics, the first step is the calculation of the Coulomb Scattering (CS) perturbation potential induced by a point charge, obtained by solving the corresponding Poisson Equation [5] throughout the polysilicon/oxide/substrate stack. Once the screened CS potential is known, the matrix elements and MRTs for all subbands can be calculated using an improved version of the MRT approximation that accounts for both intra- and inter-subband electronic transitions.

Using our model, we found that to neglect screening in polysilicon and to treat transport in the QL lead to a severe underestimate of RCS limited mobility. By including also all other relevant scattering mechanisms, we discuss the dependence of the overall $\mu_{\text{eff}}$ on the oxide thickness ($T_{\text{ox}}$) and the polysilicon doping concentration ($N_{\text{poly}}$).

2. Calculation Procedure

The determination of the RCS limited mobility consists, in our model, of a two step procedure. First the CS perturbation potential and the scattering rates are computed. Then the MRTs and mobility are calculated.

2.1. RCS Scattering Rates

Our calculation of the screened CS potential is based on the perturbative approach introduced in [5]. If we let $\phi(q, z, z_0)$ be the 2D Fourier component of the CS potential of a point charge located at $z_0$, then the Poisson Equation can be written as [6]:

$$\phi(q, z, z_0) = \int_0^\infty dz_1 K(z, z_1)\phi(q, z_1) + \frac{2}{\epsilon_s q} \times$$

$$\times \exp(-q|z - z_0|) + A \exp(-qz) + B \exp(qz) \tag{1}$$

where $q$ is the space wave vector, $A$ and $B$ are constants to be determined as explained below, and:

$$K(z, z_1) = -\sum_i |\xi_i(z_1)|^2 S_i \times$$

$$\times \int_0^\infty dz_2 |\xi_i(z_2)|^2 (1/q) \exp(-q|z - z_2|) \tag{2}$$

is the kernel of the integral equation (1), $\xi_i$ is the i-th eigenfunction (in the polysilicon or in the substrate) and $S_i$ the screening constant given in [5, 6, 7]. In the oxide $K(z, z_1) \simeq 0$ and Eq.1 gives an explicit solution for $\phi$, whereas in the polysilicon and in the substrate the integral in Eq.1 accounts for the screening.

In the literature Eq.1 has been solved in the substrate only (i.e. neglecting the screening of free electrons in the polysilicon), and one can find either approximate solutions in the quantum limit [5] that have been recently used to study RCS [1, 2], or numerical solutions based on iterative schemes [6, 7]. However, using the definition of $K(z, z_1)$, Eq.1 can be recognized as a Fredholm Equation and solved using the Nyström method discussed in [8]. By solving Eq.1 in the poly/oxide/substrate stack we can account for impurities located in any of the regions, or at any...
interface. The unknown constants have been determined by imposing appropriate boundary conditions for \( \phi \) and its first derivative at each boundary and for \( z \rightarrow \pm \infty \).

Once the screened CS potential is known, the scattering matrix elements are calculated by summing the contributions of all possible scattering centers [6, 10] and the scattering rate is obtained using the Fermi Golden Rule.

### 2.2. Momentum Relaxation Times

Besides ionized impurity scattering, our model also includes phonon and surface-roughness scattering. As for phonons, we accounted for both intra- and inter-valley transitions, using appropriate selection rules for \( f \) and \( g \)-type processes [9]. Both optical and acoustic phonons were considered to be isotropic since we used the energy equipartition approximation of the acoustic phonon number [9, 10]. Surface roughness is treated according to Ando’s approach [11] using a gaussian spectrum and accounting for the screening through the 2D dielectric function \( \epsilon \) [10, 12].

If we let \( f_0(E) \) be the equilibrium Fermi-Dirac occupation function and \( S_{i,j}(q) \) the scattering rate between the \( i \)-th and \( j \)-th subbands then the MRT for isotropic scattering, accounting for carrier degeneracy, is given by [13]:

\[
\tau^{-1}_{i}(E) = \sum_{j,k'} S_{i,j}(q)(1 - f_0(E'))/(1 - f_0(E))
\]  

(3)

whereas for elastic, anisotropic scatterings the MRTs of the different subbands are coupled by the relation [10]:

\[
\tau^{-1}_{i}(E) = \sum_{j,k'} S_{i,j}(q)[1 - (k'\tau_{j}(E)/k\tau_{i}(E))\cos \theta]
\]  

(4)

where \( \theta \) is the angle between \( k' \) and \( k \). Inter-subband transitions for coulomb and surface scatterings were restricted to the same valley, since the much larger \( q \) involved in inter-valley transitions results in negligible values of the corresponding scattering matrix elements [6, 7]. In Eq.4 the relaxation times are considered to be dependent on energy only, because we assumed parabolic, isotropic bands throughout the work. When the summation in Eq.4 is converted to an integral, a system of non-linear, algebraic equations for each energy is found, which finally allows us to calculate the MRT of each subband accounting for both intra- and inter-subband transitions.

When different scattering mechanisms are considered, the inverse of the MRTs are summed according to the Mathissen’s rule, and the average value of the total relaxation time within each subband is used to calculate the corresponding mobility. Total mobility is the average mobility weighted on subband occupancy [10].

### 3. RCS Limited Mobility

The simulated structure consists of an \( n^+ \) polysilicon and a \( p \)-type silicon throughout the work. The first point worth discussing about RCS limited mobility \( (\mu_{RCS}) \) is the role of screening in polysilicon, in our opinion previously overlooked. Fig.1 shows the CS potential of a point charge located inside polysilicon at 0.5\( nm \) from the oxide interface together with polysilicon and substrate electron concentrations. Electron quantization was accounted for both in the polysilicon and in the substrate. As can be seen, the free charge density in the polysilicon is much larger than in the substrate at this modest inversion density \( (N_{inv} \approx 10^{12} cm^{-2}) \), so that its screening effect should not be neglected.

In fact, the CS potential obtained neglecting poly screening (open squares) is much larger than its counterpart obtained using the polysilicon QM electronic structure (filled circles). Furthermore a closer analysis reveals that, due the QM boundary conditions at the poly/oxide interface, a \( QM \) depletion region is developed in polysilicon resulting in an electron concentration much smaller than the doping density \( (N_{poly}) \) and also smaller than its classical counterpart [14]. At this regard, Fig.1 also illustrates the CS potential obtained using a classical screening length in the polysilicon (open triangles) calculated from a constant electron concentration equal to \( N_{poly} \). It is evident that neglecting the QM depletion region has a strong...
impact on the CS potential and this fact claims for the fully QM treatment of the screening employed in this work.

Fig. 2 shows RCS limited mobility versus $N_{\text{inv}}$. Consistently with the results of Fig. 1 $\mu_{\text{RCS}}$ is severely reduced when poly screening is neglected and the difference is the largest at small $N_{\text{inv}}$ because in this condition the relative importance of the poly screening is maximum. In fact, at large $N_{\text{inv}}$ the screening effect of the channel inversion layer increases while, on the contrary, the screening in polysilicon becomes less effective due to the widening of the QM depletion region. When $N_{\text{inv}}$ increases the two counteracting effects of a stronger screening in the channel but weaker in polysilicon are also responsible for the relatively weak and possibly non-monotonical dependence of $\mu_{\text{RCS}}$ on $N_{\text{inv}}$. A classical screening in polysilicon with $n \approx N_{\text{poly}}$ results in much larger $\mu_{\text{RCS}}$ than what obtained with the fully QM treatment.

The second topic addressed in this section is the error related to the QL approximation. Fig. 3 shows the same CS potential as in Fig. 1 together with the squared eigenfunctions of the first unprimed (quantization mass of $0.916m_0$) and of the first primed subbands (quantization mass of $0.19m_0$).

Since $\phi(q, z, z_0)$ exponentially decreases as a function of $z$ from the polysilicon towards the substrate, scattering matrix elements are the largest for the lowest subbands which are the most confined ones toward the oxide interface, as can be recognized in Fig. 3. Fig. 4 reports $\mu_{\text{RCS}}$ for the first unprimed, the first primed subband and also the total $\mu_{\text{RCS}}$ versus the inversion density. Despite the larger conduction mass, the first primed subband exhibits a remarkably larger $\mu_{\text{RCS}}$ than the first unprimed because of a significant suppression in the RCS rate. The larger $\mu_{\text{RCS}}$ of higher subbands is due to the remoteness of the ionized centers and does not apply to the mobility limited by local coulomb centers in the channel of the transistor. This feature of the $\mu_{\text{RCS}}$ demands for simulations accounting for many subbands and leads to a significant underestimate of mobility if calculations are performed in the QL approximation.

4. Total Effective Mobility

Before we illustrate the predictions of our model in terms of $\mu_{\text{eff}}$ degradation in ultra-thin oxides, we report in Fig. 5 the comparison between electron $\mu_{\text{eff}}$ measurements [15] and the corresponding simulations obtained with our model.

Figure 3. Same CS potential as in Fig. 1 (QM Poly screening) and the squared eigenfunctions of the first unprimed and of the first primed subbands. The lowest subbands are the most confined ones toward the oxide interface.

Figure 4. RCS limited mobility versus the inversion density for the two lowest subbands and for the total, average mobility. Higher subbands have significantly larger $\mu_{\text{RCS}}$.

Figure 5. Measured electron mobility (symbols, [15]) and simulations with the model of this work (solid lines).

Figure 6. Effective mobility versus inversion density calculated with our model for different $T_{\text{ox}}$ (open symbols). Results with simplified assumptions are also shown (filled symbols). $N_{\text{sub}} = 2 \cdot 10^{16} \text{cm}^{-3}$. 
In order to reproduce the data for a substrate doping of $2 \times 10^{16} \text{cm}^{-3}$ we chose a deformation potential for acoustic phonons of 14.6 eV (in close agreement with [12]) while the RMS mean value and correlation length for the surface roughness spectrum were chosen to be 0.51 nm and 1.0 nm, respectively. The good agreement (within 10%) with the experiments for larger substrate dopings was obtained with no further parameter adjustments and this supports a reasonable confidence in our model for ionized impurity scattering.

Fig. 7 shows the simulation of total, effective mobility for a device with $N_{\text{sub}} = 2 \times 10^{16} \text{cm}^{-3}$ for different thin oxides ranging from 3.0 nm down to 1.2 nm. For the thinnest oxide our model predicts a $\mu_{\text{eff}}$ degradation induced by RCS of approximately 30% for $N_{\text{inv}} \approx 10^{12} \text{cm}^{-2}$ whereas at large $N_{\text{inv}}$ the effect of RCS is effectively suppressed by the screening of the inversion layer. It is also worth noticing in Fig.6 how simplified models for RCS predict a much stronger $\mu_{\text{eff}}$ degradation. The largest difference is due to the neglect of polysilicon screening (filled squares) but the QL approximation results in a further, significant $\mu_{\text{eff}}$ reduction (filled triangles). Fig.7 reports $\mu_{\text{eff}}$ versus the oxide thickness behavior for two different inversion densities, and the corresponding values obtained with no RCS (dashed lines).

At large $N_{\text{inv}}$ mobility is almost independent of $T_{\text{ox}}$ because it is mainly limited by surface roughness. For $N_{\text{inv}} \approx 8 \times 10^{11} \text{cm}^{-2}$, instead, our model predicts that mobility should be essentially unaffected by RCS for $T_{\text{ox}} > 5 \text{nm}$ and decreased by only a 7% for $T_{\text{ox}} = 3.0 \text{nm}$. If polysilicon screening is neglected, instead, a large $\mu_{\text{eff}}$ degradation is observed already for $T_{\text{ox}} = 5 \text{nm}$ or even thicker oxides. Finally, Fig.8 illustrates how effective mobility depends on the polysilicon electrically active doping, when a thin oxide and a modest inversion density are set. As can be seen, apart from the absolute values of $\mu_{\text{eff}}$, the inclusion of screening inside polysilicon results in a weaker dependence on $N_{\text{poly}}$ (compared to the simplified model) because the increase of the density of ionized scattering centers is partly compensated by a more effective screening.

5. Conclusions

In this paper we have presented an improved model for RCS in thin oxide n-MOSFETs. Compared to previous simplified approaches our results stress the importance of the polysilicon screening and of a multi-subband transport. Neglecting these ingredients results in a significant underestimate of RCS limited mobility.

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