The influence of polarisation and image charges on Electron-Impurity Scattering in High Degeneracy, Nanometre Scale Silicon wrap-round gate MOSFETs

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Abstract. Atomistic impurities in the channel of a nano-wire silicon MOSFET with wrap-round gate and highly doped and degenerate source and drain are shown to be strongly screened by polarisation (image charge effects) arising from carriers that are confined to source and drain when the channel screening length exceeds the channel length. The image charge effects on a given atomistic ionized impurity depend significantly on its location in the channel. The model is based on an exact analysis of the Poisson equation using Fourier-Bessel analysis in cylindrical coordinates. Close to source or drain the analytically computed total and differential scattering rates correspond to a form of dipole scattering. The source and drain may separately or together contribute to the screening of the atomistic impurity depending on its location and the channel screening length. The net effect of the infinite sequence of fully developed screened image charges induced by the atomistic impurity is to substantially reduce impurity scattering by at least an order of magnitude and to enhance the back scattering. The theory is illustrated for a 5 nm channel device.

1. Introduction

Projected ultra-small silicon semiconductor devices such as double-gate MOSFETs [1] and wrap-round gate nanowire MOSFETs [2, 3] (Fig. 1, 2) will involve channel regions (4-10 nm length) of nominally undoped small volume surrounded by very highly doped \((\gg 10^{18}\ \text{cm}^{-3})\) or metallic regions corresponding to source, drain and gate. Unwanted impurities are expected to occur as highly deleterious scattering centres (Fig.1) within the channel although actual numbers will be very small. Atomistic impurities have been associated with strong variations in threshold voltage and channel conductance between technologically identical devices. At present the consequences of atomistic scattering on device variability are modelled using Monte Carlo simulation that employs simple isotropic screened Coulomb potentials. That procedure cannot be correct for realistic devices. In particular, when the channel is constricted, the effective idealised potential “seen” by carriers will contain an effective barrier of width equal to the channel length caused by the spatial variation of the conduction band edge due to confinement (Fig. 3). It follows that not all the carriers in source and drain are free to travel along the channel but instead they provide a pool of polarisable charge that can influence the screening of impurities in the channel through image charge effects. Similarly the confined charge on the gate acts a polarisable region that may give rise to image charge effects in the electrostatics of the device. Evidently if the screening length in the channel is greater than or
comparable to the channel length there is the enticing possibility that the atomistic impurity may be screened-out by the polarisation of charge source, drain and gate regions (Fig. 2, 4). In a recent study [4] we reported briefly on an approximate theory of the image charge effects due to source/channel or drain/channel interface that influence electron-impurity screening in relatively long channels. In the present paper this analysis has been extended to an exact analysis of the more complex case of a very short channel device where an impurity in the channel sets up polarisation in both source and drain and indeed, where source and drain charges interact. Remote plasmon scattering and Coulomb drag are already known but the remote image charge has not been previously studied.

2. Screening model

Using the model geometry of Figures 2 and 4, we determine the inhomogeneously screened position-dependent self-consistent scattering potential of an ionised impurity located at position \( \mathbf{r}_I \) relative to an origin located on the central symmetry \( z \)-axis of the channel (length \( L_c \)) at the source–channel boundary by a direct analytical solution of Poisson’s equation for a cylindrical geometry channel coupled to degenerately doped source and drain using 3D Fourier-Bessel analysis. In the source region \( (z<0) \) the electrostatic potential \( \phi=\phi_S \) is considered to satisfy Poisson’s equation in the linearised form:
\[ \nabla^2 \phi_s = -\rho_s / \kappa \varepsilon_0 \quad (1) \]

where \( \rho_s \) the free charge density in the source is assumed to be related to the inverse bulk screening length \( k_s = 1 / \lambda_s \) (Thomas-Fermi) in the source by:

\[ \rho_s = -\kappa \varepsilon_0 k_s^2 \phi_s \quad (2) \]

From (1) and (2) we find for \( z < 0: \)

\[ \nabla^2 \phi_s - k_s^2 \phi_s = 0 \quad (3) \]

For the potential in channel (\( 0 < z < L_c \)), is similarly:

\[ \nabla^2 \phi_c - k_c^2 \phi_c = -(Q / \kappa \varepsilon_0) \delta(\mathbf{r} - \mathbf{r}_i) \quad (4) \]

and for the drain region (\( z > L_c \))

\[ \nabla^2 \phi_d - k_d^2 \phi_d = 0 \quad (5) \]

where \( k_c = 1 / \lambda_c \ll k_s, k_d \) is the inverse bulk screening length in the channel and the rhs of (4) describes an atomistic impurity of charge \( Q \) at \( \mathbf{r}_i \). Equations (3) - (5) may be solved exactly by Fourier-Bessel analysis (\( J_0 \) denotes Bessel function) using a cylindrical coordinate system and matching conditions at the interface derived from the continuity conditions on the fields \( \mathbf{E} \) and \( \mathbf{D} \).

3. Model potential: spatial dependence

The electrostatic potential in the source, channel and drain regions are found exactly as:

\[ \phi_s = \int_0^\infty dk \ J_0(k | \mathbf{R} - \mathbf{R}_i |) \exp[z | k^2 + k_s^2 |^{1/2}] a_s(k) \quad (6) \]

\[ \phi_c = \int_0^\infty dk \ J_0(k | \mathbf{R} - \mathbf{R}_i |) \{ \frac{Q}{4 \pi \kappa \varepsilon_0} \frac{k}{| k^2 + k_c^2 |^{1/2}} \exp[-(z - z_i) (k^2 + k_c^2)^{1/2}] 
   + a_c(k) \exp[-z | k^2 + k_c^2 |^{1/2}] + b_c(k) \exp[z | k^2 + k_c^2 |^{1/2}] \} \quad (7) \]

\[ \phi_d = \int_0^\infty dk \ J_0(k | \mathbf{R} - \mathbf{R}_i |) \exp[-z | k^2 + k_d^2 |^{1/2}] a_d(k) \quad (8) \]

\[ | \mathbf{R} - \mathbf{R}_i | = \sqrt{(x - x_i)^2 + (y - y_i)^2}^{1/2} \quad (9) \]

The coefficients \( a_s, a_c, b_c, a_d \) are determined from the boundary conditions using the matrix equation:

\[
\begin{bmatrix}
1 & -1 & -1 & 0 \\
0 & e^{-\sqrt{k^2 + k_s^2} L_c} & e^{-\sqrt{k^2 + k_c^2} L_c} & e^{-\sqrt{k^2 + k_d^2} L_c} \\
\sqrt{k^2 + k_s^2} & \sqrt{k^2 + k_c^2} & -\sqrt{k^2 + k_c^2} & \sqrt{k^2 + k_d^2} \\
0 & -\sqrt{k^2 + k_s^2} e^{-\sqrt{k^2 + k_c^2} L_c} & \sqrt{k^2 + k_c^2} e^{\sqrt{k^2 + k_c^2} L_c} & \sqrt{k^2 + k_d^2} e^{-\sqrt{k^2 + k_d^2} L_c}
\end{bmatrix}
\begin{bmatrix}
[a_s] \\
[a_c] \\
b_c \\
[a_d]
\end{bmatrix}
= 
\begin{bmatrix}
[\gamma_s] \\
[\gamma_c] \\
[\gamma_{CA}] \\
[\gamma_{CB}]
\end{bmatrix}
\]

\( (10) \)
\[ \alpha = \frac{Q}{4\pi \varepsilon_0}; \quad \gamma_s = -\frac{a_k}{\sqrt{k^2 + k_c^2}} e^{-\sqrt{k^2 + k_c^2} z_i}; \quad \gamma_c = -\frac{a_k}{\sqrt{k^2 + k_c^2}} e^{-\sqrt{k^2 + k_c^2} (L_c - z_i)}, \]
\[ \gamma_{CB} = c_k e^{-\sqrt{k^2 + k_c^2} z_i}; \quad \gamma_d = c_k e^{-\sqrt{k^2 + k_c^2} (L_c - z_i)} \] (11)

The full exact expressions for the coefficients \( a_s, a_c, b_c, a_d \) are lengthy and are not reproduced here. Instead we examine various limiting forms. It should be noted that \( a_c \) controls the screened fields produced by image charges in the source regime, whereas \( b_c \) controls screened fields from image charges in the drain. Figure 5 plots the (a) the bulk screened Coulomb potential, (b) the modified potential due to interaction with an image charge in the source region only, (c) the exact channel potential of an atomistic impurity interacting with polarisation in source and drain for a channel of length \( L_c = 5 \) nm and for successive impurity locations \( z_i = 0.1 \) nm, 2.5 nm, 4.9 nm.

### 3.1 Long channel limit

The long channel limit is defined as \( L_c \gg \lambda_c = 1/k_c \). In this case the atomistic impurity will induce a single image charge in: (a) the source when \( z_i \leq N\lambda_c \) where \( N \sim 3 \); (b) the drain when \( L_c - z_i \leq N\lambda_c \). The self-consistent atomistic impurity for case (a) is

\[ \phi_s(R,z) = \frac{Q}{4\pi \varepsilon_0} \frac{2\exp[z^2 + k^2] \exp[-z_i \sqrt{k^2 + k_c^2}]}{\sqrt{k^2 + k_s^2 + \sqrt{k^2 + k_c^2}}} (1 - \theta(z)) \] (12)

\[ \phi_c(R,z) = \frac{Q}{4\pi \varepsilon_0} \frac{\exp[-z + z_i \sqrt{k^2 + k_c^2}]}{\sqrt{k^2 + k_c^2}} \theta(z) \]

\[ - \frac{Q}{4\pi \varepsilon_0} \frac{\exp[-z_i \sqrt{k^2 + k_c^2} + k_s^2]}{\sqrt{k^2 + k_c^2}} \left( \frac{\sqrt{k^2 + k_s^2} - \sqrt{k^2 + k_c^2}}{\sqrt{k^2 + k_c^2}} \right) \theta(z) \] (13)

It is noted that when \( k_s = k_c \) we recover the usual simple screened Coulomb potential as expected.

In the limit of strong screening in source and drain: \( k_s \approx k_d \gg k_c \); \( n_s \sim n_d \gg n_c \) the potential is reduced to zero (screened out) in the source whereas the channel potential from (13) reduces to:

\[ \phi_c(r) = \theta(z) \frac{Q}{4\pi \varepsilon_0} \frac{\exp[-|r - r_i| k_c]}{|r - r_i|} \frac{\exp[-|r - r^*| k_c]}{|r - r^*|} \] (14)

\[ r_i^* = [x_i, y_i, -z_i] \]

where the second term in (13) is the field of the image charge to the impurity at \( r_i \) located at \( r^* \).

This limit corresponds to Fig. 5(b). A similar form exists for the case when the impurity is close to the drain interface.

### 3.2 Short channel limit

The short channel limit is defined as \( L_c \ll \lambda_c \). In this case the atomistic impurity will induce a single image charge: (a) in the source when \( z_i \leq N\lambda_c \) where \( N \sim 3 \); (b) in the drain when \( L_c - z_i \leq N\lambda_c \). In...
the strong screening limit, \(k_s \sim k_D >> k_C\); \((n_S \sim n_D >> n_C)\), the field of the atomistic impurity is screened out inside the source and drain regions but in the channel it comprise the screened Coulomb potential plus the screened Coulomb potentials of an infinite sequence of image charges \(Q_j\), induced in source and drain at locations \(\mathbf{r}_j\) (this situation corresponds to Fig 5(c)): 

\[
\phi_c = \frac{1}{4\pi\varepsilon} \left\{ \frac{Q}{|\mathbf{r} - \mathbf{r}_j|} + \sum_{j=1}^{\infty} \frac{Q_j}{|\mathbf{r} - \mathbf{r}_j'|} \right\}
\]

(15)

The different approximate models are summarised in Figure 5.

![Figure 5: Contour plots of atomistic potential for impurity at various locations in channel and for different approximations](image)

**Figure 5:** Contour plots of atomistic potential for impurity at various locations in channel and for different approximations channel length \(L_c=5\) nm; screening length \(\lambda_c=20\) nm.

### 4. The model potential: Fourier transform

In order to compute the scattering rate between \(k\)-states we require the Fourier transforms of expressions (6) - (8) which may be obtained in closed analytical form. Scattering between size quantized states is similarly straightforward to compute. In the long channel, strong screening limit \(k_s,k_D >> k_C\)

\[
\phi[\mathbf{q}_\perp,q_z] = \phi_c[\mathbf{q}_\perp,q_z] = \frac{Q}{4\pi\varepsilon_0\kappa} 2\pi \exp[-iq_\perp \cdot \mathbf{R}_j] \left\{ \exp[-iq_z z_j] - \exp[-z_j \sqrt{q_z^2 + k_C^2}] \right\} \frac{q_z}{q^2 + k_C^2}
\]

(16)

Eqn (16) describes case of impurity close to the source. It also describes impurity close to drain if we replace \(z_j \rightarrow L_c - z_j\). In the limit \(z_j > N\lambda_c\) eqn. (16) gives the Fourier transform of the usual bulk-screened Coulomb potential. For the opposite limit: \(z_j \sim 0\), eqn. (16) reduces to essentially an averaged screened dipole form (compare [5]):

\[
\phi[\mathbf{q}_\perp,q_z] = \frac{Q}{4\pi\varepsilon_0\kappa} 2\pi \frac{z_j}{\sqrt{q_z^2 + k_C^2}}
\]

(17)
5. Scattering rates

The Golden rule scattering rate may be computed from the Fourier transformed potentials. In the long channel limit, strong source screening limit, with \( z_i << L_c \), and using (16) we obtain

\[
R[q \cdot q_z] = \frac{1}{4} R_{\text{Coulomb}}[q \cdot q_z] (1 + \exp[-2z_f \sqrt{q_z^2 + k^2 c^2}] - 2 \exp[-z_f \sqrt{q_z^2 + k^2 c^2} \cos(q_z z_i)])
\]

where \( R_{\text{Coulomb}}[q = k - k'] \) is the scattering rate for scattering between states \( k \) and \( k' \) for the bulk screened Coulomb potential.

![Figure 6: Ratio \( R[q \cdot q_z]/R_{\text{Coulomb}}[q \cdot q_z] \)](image_url)

A similar set of results holds for the impurity close to the drain interface.

6. Discussion and Conclusions

From Figure 5(c) it is clear that the single image charge model (corresponding to the closest interface) is a good approximation valid except at the shortest channel lengths. The single image charge model results shown in section 5 indicate two main effects: (a) the overall scattering rate is strongly reduced (by a factor of 6 in Figure 7) compared with the bulk screened model when the impurity is close to the source or drain; (b) from Figs. 6-7 it is clear that the back-scattering is enhanced compared with the screened Coulomb result. The single image charge picture resembles a half-dipole produced by the impurity potential and the virtual image charge. In the limit that the impurity is very close to source or drain interface, the corresponding scattering rates may be shown to be \( \frac{1}{4} \) of the rates computed for the Stratton degenerate randomized dipole model. In the extreme case of a very short channel the atomistic potential is strongly screened out by the image charges although it is possible that the same effect may partially screen the gate potential. Total scattering rates suitable for incorporation into Monte Carlo modelling are easily obtained from the theory outlined here and will be discussed elsewhere. Finally, we predict that the strong screening of atomistic impurities due to image charge effects in very short channel nanowire MOSFETs effectively suppresses the deleterious effects of atomistic impurities such as threshold voltage and channel conductance variability.

7. References

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