Characterization of 4H-SiC MOSFET Interface Trap Charge Density Using a First Principles Coulomb Scattering Mobility Model and Device Simulation

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Abstract: **We have developed a physics based device simulator for detailed numerical analysis of 4H-SiC MOSFETs. As part of the drift diffusion model implemented in the simulator, a first principles quasi-2D Coulomb scattering mobility model for SiC MOSFETs has been developed. This Coulomb scattering mobility model takes into account scattering by occupied interface traps, scattering by fixed oxide charges, distribution of mobile carriers inside the inversion layer, screening by mobile carriers and temperature. Using this mobility model it has been shown that Coulomb scattering plays a dominant role very close to the interface. The interface trap density of states profile has been extracted by comparing simulated I-V curves to experimental data for room temperature. Simulations show that interface trap density of states is low in the midgap region and very high near the conduction band edge in 4H SiC, and it severely limits device performance.**

Keywords: **4H-SiC MOSFETs, Coulomb scattering mobility model, interface traps**

I. INTRODUCTION

SiC is a material of great interest because it has a very large bandgap, and at the same time, has the ability to grow a natural oxide. This combination can facilitate the design and fabrication of SiC MOSFET devices for extremely high power and high temperature applications. In fact, it presents the opportunity of extending the micro-electronic revolution to very high power IC's. However, before high performance SiC MOSFETs are realized, their performance limitations due to low surface mobility must be understood and overcome. Currently, high interface trap densities pose the biggest challenge to SiC device operation. Developing a density profile for the interface traps and predicting their effect on device operation will help manufacturers to refine their process and produce better SiC devices. We have developed a physics based device simulator for detailed numerical analysis of 4H-SiC MOSFETs. A key unique aspect of the simulator is an advanced mobility model that accounts for the effects of surface phonon scattering, surface roughness scattering and Coulomb scattering of mobile carriers by occupied interface states and fixed oxide charges. We have developed a first principles quasi-2D Coulomb scattering mobility model for SiC MOSFETs that takes into account occupied interface traps, fixed oxide charges, distribution of mobile carriers inside the inversion layer, screening by mobile carriers and temperature dependence. Using this mobility model we have shown that Coulomb scattering plays a dominant role very close to the interface. A few nanometers away from the interface, Coulomb scattering is greatly reduced, and other scattering mechanisms control the total low field mobility. We have extracted values for the fixed oxide charge density and the interface trap charge density profile by comparing our simulated I-V curves to experimental data. Our simulations show that interface trap density values are low in the midgap region and very high near the conduction band edge in 4H SiC, and that they severely limit device operation.

II. INTERFACE TRAP DENSITY PROFILE

The model we use for the interface trap density for 4H SiC has a constant distribution in the midband region and an exponential increase near the band edge [1]. Our analysis indicates that the traps are acceptor type above midgap and donor type below it. For the acceptor type interface traps, the energy dependent density of states is represented as:

$$D_{it}(E) = D_{it_{mid}} + D_{it_{edge}} \exp\left(\frac{E - E_c}{\sigma_{it}}\right) \tag{1}$$

where, E_c is the energy at the conduction band edge, $D_{it_{mid}}$ and $D_{it_{edge}}$ represent the densities at the middle and the edge of the bandgap, and σ_{it} defines the curvature of the density of states curve. Values for $D_{it_{mid}}$, $D_{it_{edge}}$ and σ_{it} are obtained through comparisons of simulations and experiments. The density of states profile extracted by comparing simulations to experimental data is shown in Figure 1. The exponential rise in trap density near the band edges gives a large number of filled acceptor traps when the *n*-channel MOSFET is given a positive gate bias. These filled acceptor traps cause Coulomb scattering of mobile charges in the inversion layer and also cause a positive shift in the threshold voltage. With increase in temperature, the number of filled traps decreases. Hence the threshold voltage should decrease with increase in temperature. Also Coulomb scattering due to these traps would decrease with increase in temperature giving better mobility at higher temperatures. The occupied interface trap density is calculated by weighting the density of states with a probability density function which is dependent on the density of mobile charges near the interface. The larger is the density of free charges, the larger is the probability of filling up the traps. The density of occupied acceptor type interface traps is given by:

$$N_{it} = \int_{E_{neutral}}^{E_c} D_{it}(E) f_n(E)\, dE \tag{2}$$

where, $f_n(E)$ is the Fermi probability distribution function [1]:

$$f_n(E,x)=\frac{1}{1+\frac{1}{2}\frac{N_C}{n(x)}\exp\left(\frac{E-E_C}{k_BT}\right)} \quad (3)$$

Here N_c is the effective conduction band density of states for 4H-SiC, n is the density of electrons which is calculated self-consistently, E_c is the conduction band minimum at the temperature T, and $E_{neutral}$ is the neutrality point.

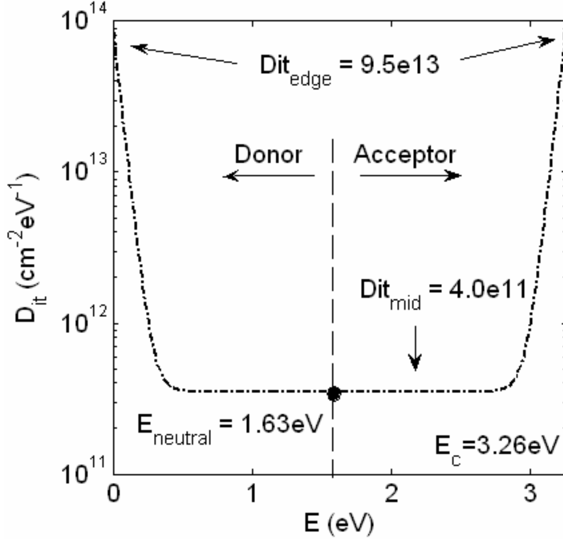

Figure 1. Extracted interface trap density of states profile for 4H-SiC, showing a constant distribution in the midband region, and an exponential rise near the band edges.

III. 4H SiC MOSFET MOBILITY MODEL

The extremely high density of occupied interface traps in 4H-SiC MOSFETs required the development of an advanced Coulomb scattering mobility model for the device simulator. As the effect of Coulomb scattering decreases with increasing distance from the interface, the Coulomb mobility was required to have a depth-dependence. As the traps are screened by the mobile electrons, it was necessary to put in a screening model for the Coulomb scattering. In addition to the Coulomb scattering mobility, the bulk mobility, surface phonon mobility and surface roughness mobility together give the total low field mobility. The saturation velocity and parallel component of the electric field give the high field mobility. The total mobility is a combination of the low field mobility and the high field mobility.

A) Quasi 2D Coulomb Scattering Mobility: To extract the quasi 2D Coulomb mobility, we start with a screened Coulomb potential:

$$V(\vec{r})=\frac{e^2}{4\pi\bar{\varepsilon}}\cdot\frac{1}{\vec{r}}\cdot e^{-q_{sc}r} \quad (4)$$

where, $\bar{\varepsilon}$ is the average permittivity of SiO_2 and 4H-SiC, and q_{sc} is the screening factor.

In order to get the 2D matrix element (H_{2D}) for applying the Fermi Golden Rule, we first take the 3D Fourier Transform of the Coulomb potential (5) and then take its 1D inverse transform (6).

$$H_{3D}=\left\langle e^{-i\vec{k}\cdot\vec{r}}\ |V(\vec{r})|\ e^{i\vec{k}'\cdot\vec{r}}\right\rangle=\frac{e^2}{\bar{\varepsilon}}\cdot\frac{1}{q_{3D}^2+q_{sc}^2} \quad (5)$$

$$H_{2D}=\frac{1}{2\pi}\int_{-\infty}^{\infty}H_{3D}\cdot e^{iq_z z}dq_z=\frac{e^2}{2\bar{\varepsilon}}\frac{e^{-\sqrt{q_{2D}^2+q_{sc}^2}\cdot z}}{\sqrt{q_{2D}^2+q_{sc}^2}\cdot z} \quad (6)$$

where, q_{3D} and q_{2D} are the 3D and 2D scattering wavevectors respectively.

The scattering rate is obtained by applying the Fermi Golden Rule:

$$\Gamma_{\vec{k}\to\vec{k}'}=\frac{2\pi}{\hbar}\left(\frac{e^2}{2\bar{\varepsilon}}\frac{e^{-\sqrt{q_{2D}^2+q_{sc}^2}\cdot z}}{\sqrt{q_{2D}^2+q_{sc}^2}\cdot z}\right)^2\delta\left(E_{\vec{k}}-E_{\vec{k}'}\right) \quad (7)$$

The scattering charges are of two types. The occupied interface traps which are located at the interface and the fixed oxide charges that are distributed inside the oxide close to the interface. In order to incorporate this distribution of fixed oxide charges, we calculate the scattering rate as a function of both, the distance of the mobile charge from the interface (z) and the distance of the fixed charges from the interface (z_i). At a distance z_i inside the oxide, the total density of charges is given as:

$$N_{2D}(z_i)=\begin{cases}N_{it}+N_f(0) & \text{for } z_i=0\\ N_f(z_i) & \text{for } z_i<0\end{cases} \quad (8)$$

where N_{it} is the occupied interface trap density, and N_f is the fixed oxide charge density.

The total quasi 2D scattering rate for a $N_{2D}(z_i)$ density of scattering charges can be written from the Fermi Golden Rule as:

$$\frac{1}{\tau(z,z_i)}=\frac{N_{2D}(z_i)}{4\pi^2}\int k'dk'\int\Gamma_{k\to k'}(1-\cos\theta)d\theta \quad (9)$$

The screened Coulomb scattering mobility as a function of depth is obtained from this scattering rate as:

$$\frac{1}{\mu_C(z,z_i,T_e)}=\frac{m^*e^3N_{2D}(z_i)}{16\pi\bar{\varepsilon}^2\hbar k_BT_e}\cdot F(z,z_i,T_e) \quad (10)$$

It has an inherent exponential dependence on the distance between the mobile charge and the scattering charge center given by the form factor:

$$F(z,z_i,T_e)=\int_{\alpha=0}^{\pi/2}\left(1-\frac{q_{sc}^2}{\frac{8m^*k_BT_e}{\hbar^2}\sin^2\alpha+q_{sc}^2}\right)\exp\left[-2\sqrt{\frac{8m^*k_BT_e}{\hbar^2}\sin^2\alpha+q_{sc}^2}\,(z-z_i)\right]d\alpha \quad (11)$$

The screening factor in the Coulomb potential depends on the amount of inversion charge present and also on an average depth of the inversion layer and is given as the inverse of the Debye length for semiconductors:

$$q_{sc} = \sqrt{\frac{e^2 N_{inv}}{\varepsilon_{SiC} Z_{av} k_B T_e}} \quad (12)$$

Due to screening, Coulomb scattering reduces drastically over a short distance when a large number of mobile carriers are present. Our method of treating Coulomb scattering gives us a Coulomb mobility for a mobile charge at any location inside the semiconductor. This can be directly incorporated in the device simulator. Similar results were obtained by previous investigators using analytical approximations and did not provide a form suitable for device simulation [2][3].

The Coulomb scattering mobility model shows that the scattering rate is directly proportional to the density of occupied interface traps and the fixed charge density at the interface. Hence reducing the interface trap density will reduce Coulomb scattering and improve surface mobility. Occupied interface state density decreases with increase in temperature thereby increasing the surface mobility and causing a negative shift in threshold voltage.

B) Total Mobility: In addition to the Coulomb scattering mechanism described above, the scattering mechanisms included in calculating the total low field mobility are the surface phonon scattering and surface roughness scattering. The low field mobility is combined with saturation velocity dependent high field mobility by Matheissen's rule, to get the total mobility [1].

IV. SIMULATION RESULTS

We can extract values for fixed oxide charge density and the interface trap density of states (D_{it} – E) profile by comparing simulated I_D-V_{GS} curves to experimental data. A fixed oxide charge density of 1.8×10^{12} cm^{-2} and the D_{it} – E profile shown in Figure 1 has been obtained. The energy dependent interface trap density of states profile agrees with experimentally measured values reported in literature [4][5][6].

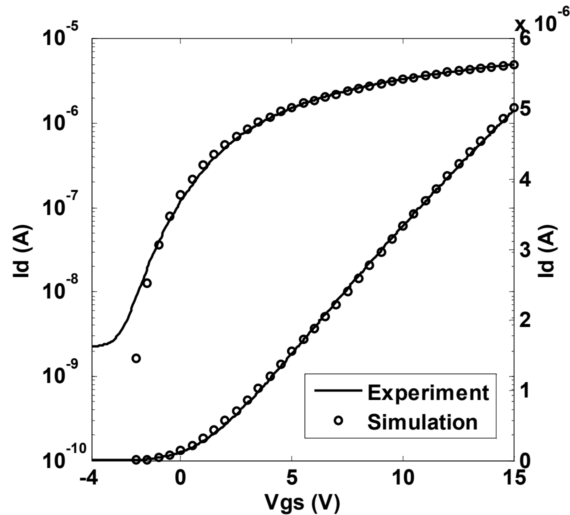

Figure 2. Agreement between simulated and experimentally measured Id-Vg characteristics for a 4H-SiC MOSFET at room temperature is shown.

Room temperature I_D-V_{GS} agreement with experiment is shown in Figure 2. The linear and log-scale plots show that the simulated curves match the experimentally measured I-V characteristics in the subthreshold and linear regions of MOSFET operation.

Even though our 2D model shows maximum electron concentration at the interface, because of the large amount of Coulomb scattering, surface mobility is very low and most of the current flows some distance away from the interface. Surface mobility is around 20 cm^2/Vs at the interface, but it increases rapidly with depth. We get a mobility of around 100 cm^2/Vs at the depth where we observe the peak of the current density curve. We found that the peak of the current density is 2 - 3 nm away from the interface. With increase in gate voltage, electrons are pulled closer to the interface; hence we can see the peak of the current density curve shift towards the interface with increase in gate voltage. (We note that this is a classical result, the Schrödinger Wave Equation was not solved here.)

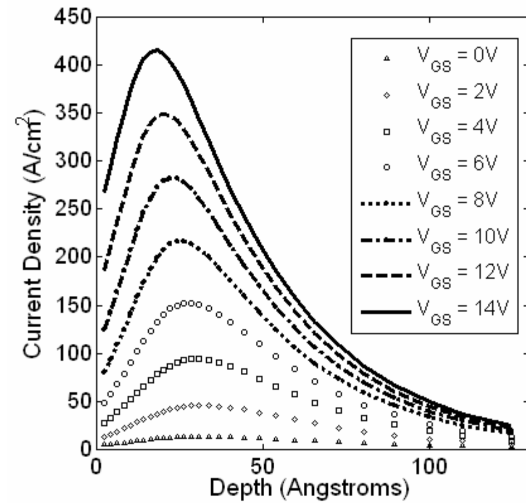

Figure 3. Current density variation with depth for a 4H-SiC MOSFET at room temperature.

Figures 4 and 5 show comparisons between Coulomb scattering mobility and surface roughness mobility varying with depth, at two different gate voltages. At low gate voltages, Coulomb scattering is the dominant mobility limiting mechanism and the total mobility curve (μ_{Total}) follows the Coulomb mobility (μ_C) curve. But at higher gate voltages, owing to increased screening of scattering charges by inversion layer electrons, Coulomb scattering decreases and surface roughness becomes the dominant scattering mechanism. The total mobility curve now follows the surface roughness mobility (μ_{SR}) curve for most of the depth. The current density curves varying with depth are also plotted.

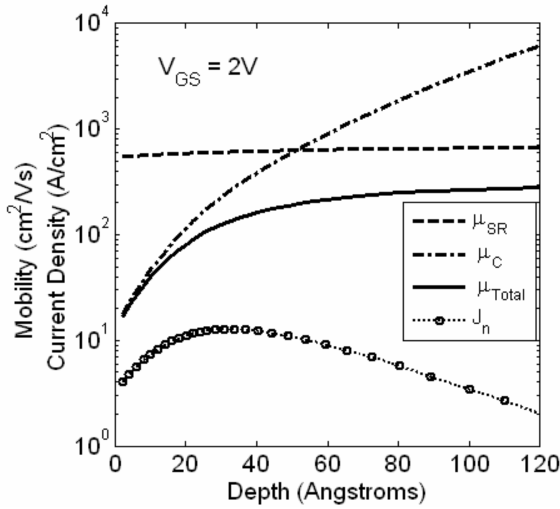

Figure 4. Comparison between various mobilities at high gate voltage and at room temperature showing that Coulomb scattering is the dominant mobility limiting mechanism at low gate voltages.

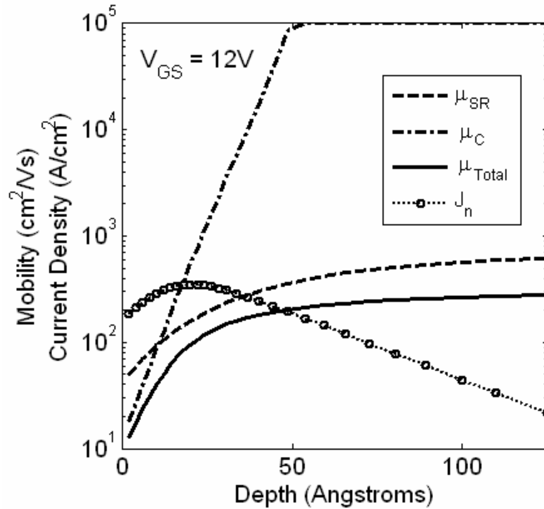

Figure 5. Comparison between various mobilities at high gate voltage and at room temperature. Coulomb scattering is the dominant scattering mechanism at this voltage only very close to the interface.

Figure 6 shows the improvement that is obtained in the Id-V_{GS} characteristics when the interface trap density of states near the band edge is reduced by factors of 10 and 100. It can be clearly seen that there is a significant improvement in the current at low gate voltages. At higher gate voltages, owing the increased effect of screening, Coulomb scattering is not very high, and so a reduction of interface traps does not have as significant an impact in current improvement.

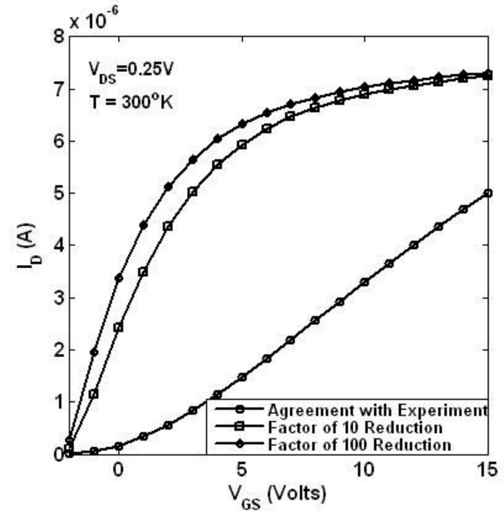

Figure 6. Improvement in 4H-SiC MOSFET performance by reduction in the interface traps at the band edges.

V. CONCLUSION

A first principles Coulomb scattering mobility model for SiC MOSFETs has been developed and implemented. The mobility model incorporates the effect of scattering of inversion layer mobile charges by occupied interface traps and fixed oxide charges at the semiconductor-oxide interface. It also accounts for distribution of mobile carriers inside the inversion layer at different depths, and the effect of screening. This model in conjunction with various other mobility models has given us a detailed picture of the physics of the inversion layer in SiC MOSFETs. The extracted energy dependent interface trap density of states profile for 4H-SiC MOSFET devices shows extremely large number of trap states near the band edges of 4H-SiC. This agrees very well with various experimental measurements. These large number of interface states give rise to excessive Coulombic scattering near the interface, which brings down the surface mobilities to around 20 cm^2/Vs in 4H-SiC MOSFETs. For low gate voltages, Coulomb scattering mobility controls the total low field mobility. But at higher gate voltages, because of increased screening due to high inversion layer charge density, its effect is limited to within only a few nanometers near the interface. A large improvement in device characteristics can be obtained by reducing the interface states near the band edges in SiC.

VI. REFERENCES

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