Modeling of Metal-Semiconductor interface and anisotropic Drift-Diffusion model for simulating 4H-SiC Schottky diode and MESFET devices

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Abstract

Many computer-aided design (CAD) programs for simulating semiconductor devices structures are broadly available. However such tools developed prevalently for modeling Silicon devices, are used to study/model other semiconductors presenting anisotropic and/or wide bandgap properties. From the users point of view, CAD simulator is like a black box and what exactly it solves for or how it does is hidden. Concerning its usage, many physical parameter may be unknown and the used-simulator simply replace them with default values, bringing along errors. In this paper, we investigate the anisotropic features of Silicon Carbide (SiC) tackling its wide band gap features with its corresponding extremely low intrinsic concentration of free carriers. We have focused our interest on the 4H polytype, however similar conclusions may be satisfactory applied to the 6H-SiC as well. In the context of the work, boundaries conditions necessary for simulating the metal-semiconductor interface are exploited. A digression about the adopted physical model and the solution technique are given as well. Our model was also applied successfully for simulating devices of practical interest, i.e. 4H-SiC Schottky diode and MESFET. Results of the above-mentioned devices are presented.

1. Introduction

So far, silicon carbide (SiC) has been under extensively research due to its remarkable physical and electronic properties. Wide bandgap SiC devices hold superior electrical and thermal performance over silicon devices, of all the polytypes the 4H- and 6H-SiC crystals presents an anisotropic behavior of physical quantities in e.g. dielectric constant, electrons and holes mobility and the thermal conductivity. However our investigation was based prevalently on the former mentioned polytype. We have developed our own CAD namely ELTER-II [1] which was applied to investigate the anisotropic effect of a Schottky diode and a MESFET, in order to tackle robustly and efficiently the hexagonal SiC polytype. In the following coming sections a detailed description both for of our toll and results carried out are given.

2. Physical Model

The well defined Drift-Diffusion (DD) model has been adopted for our investigation. We have approached a tensor formalism to describe the anisotropic nature which influence the permittivity \( \tilde{\varepsilon} \), as well both the electrons and holes mobility \( \tilde{\mu}_{n,p} \), and the diffusion coefficients \( \tilde{D}_{n,p} \). The tilde over the previous signs denote their tensorial form. The DD model used in the context of modeling read as follow:

\[
\begin{align*}
F_n &= \nabla \cdot (\tilde{\varepsilon} \nabla \psi) + q (p - n + C) \\
F_p &= -\nabla \cdot J_n - q R_{\text{net}} \\
F_p &= \nabla \cdot J_p - q R_{\text{net}}
\end{align*}
\]

(1)

C is the net doping profile \( N_D - N_A \). \( J_n \) and \( J_p \) are the electron and hole current densities, \( n \) and \( p \) are the electron and hole concentrations, instead \( R_{\text{net}} \) is the net recombination rate and \( \mathbf{E} \) is the electric field, nonetheless expressed as \( \mathbf{E} = \nabla \psi \). The current equation for \( J_n \) and \( J_p \), read instead as:

\[
\begin{align*}
J_n &= q n \tilde{\mu}_n \mathbf{E} + q \tilde{D}_n \nabla n \\
J_p &= q p \tilde{\mu}_p \mathbf{E} - q \tilde{D}_p \nabla p
\end{align*}
\]

(2)

respectively. The permittivity tensor is expressed as:

\[
\tilde{\varepsilon} = \begin{pmatrix}
\varepsilon_\parallel & 0 & 0 \\
0 & \varepsilon_\parallel & 0 \\
0 & 0 & \varepsilon_\perp
\end{pmatrix}
\]

(3)
While the mobility tensors for electron and hole is expressed as:

$$\tilde{\mu}_n = \begin{pmatrix} \mu_{n,\perp c} & 0 & 0 \\ 0 & \mu_{p,\perp c} & 0 \\ 0 & 0 & \mu_{n,\perp c} \end{pmatrix}$$ (4)

and

$$\tilde{\mu}_p = \begin{pmatrix} \mu_{p,\perp c} & 0 & 0 \\ 0 & \mu_{p,\perp c} & 0 \\ 0 & 0 & \mu_{p,\perp c} \end{pmatrix}$$ (5)

Strictly speaking, analytical solution is not feasible. Numerical approach must be followed instead. Such system of equations must be solved self-consistently, in order to follow this strategy the scaled/normalized set were used instead, principally because the high order of magnitude of some parameters leads to buffer overflow which appears trying to solve such system. We have chosen the quasi-Fermi electron and hole formulation in order to solve system (1). The whole set for which the system is solved read as \{ψ, φ, ψ\}, where ψ is the electrostatic potential, while φn and φp are the electron and hole quasi-Fermi levels, respectively. In principle the choice of which set of variable to solve for is arbitrary. For instance another possible set is \{ψ, n, p\}. We have adopted the former mentioned formulation since such set has the same unit and moreover the same order of magnitude. The Poisson equation and both the electron and hole continuity equations were rewritten in residual form, and the discretized form were solved with appropriate boundary conditions. Concerning the boundaries, what pose the main difficulty on modeling the Schottky and the MESFET devices is their own metal-semiconductor interface. Such boundaries must be implemented differently in order to gain the correct I-V characteristics. Contextually the solution flow, the final solution was achieved by iterations using a Gummel scheme [2]. Each iteration is substantially performed by the Newton method which imply the evaluation of the Jacobians for (1). We have considered feasible to use sparse matrix system in order to tackle the fine meshes needed to model accurately the MESFET in particular. In our model were also introduced the SRH and Auger recombination rates [3].

3. Boundary conditions for contacts

Boundaries for the \{ψ, φ, ψ\} set have to be properly defined. In the next section are presented ohmic, artificial and the metal-semiconductor boundaries conditions.

3.1 Ohmic contacts

The boundary conditions for the potentials, (ohmic boundary conditions) are expressed as:

$$\psi = V_{\text{Applied}} + \psi_b$$ (6)

where ψb for an n-type and p-type regions are given as:

$$\psi_b = V_i \ln \left( \left( C^2 + 4n_i^2 \right)^{0.5} + C \right) \frac{1}{2n_i}$$ (7)

and

$$\psi_b = -V_i \ln \left( \left( C^2 + 4n_i^2 \right)^{0.5} - C \right) \frac{1}{2n_i}$$ (8)

respectively. $V_i$ is the thermal voltage formally as $k_B T / q$, where $k_B$ is the Boltzmann constant, $T$ the device temperature set to 300K for our investigation and q the elementary charge. The intrinsic carrier concentration $n_i$ and the relative density of states in the conduction band $N_C$ and in the valence band $N_V$ are modelled as in [1].

The quasi-Fermi potentials instead are set as:

$$\phi_n = V_{\text{Applied}}$$
$$\phi_p = V_{\text{Applied}}$$ (9)

The artificial boundaries, which are intended to isolate the device are well approximated with a zero Neumann boundary, given as

$$\frac{\partial \psi}{\partial n} = \frac{\partial \phi_n}{\partial n} = \frac{\partial \phi_p}{\partial n} = 0$$ .

3.2 Schottky contacts

The Ohmic and Neumann boundaries conditions present less difficulty than the metal-semiconductor interface. This complexity arise since several mechanisms contribute to the current transport across the metal-semiconductor interface, such as the 1) thermionic emission over the potential barrier, 2) quantum-mechanical tunneling of carrier through the potential barrier, 3) carrier recombination in the depletion region and 4) carrier recombination in the neutral region of the semiconductor. Of the four mechanisms, in our model is implemented only the first one. In our model we have neglected the interface state, that is, image force lowering [3] was not included since the overall metal-semiconductor model faced our attention. For the electrostatic potential we set:

$$\psi = V_{\text{Applied}} - \phi_b + \frac{E_F}{2q} - \frac{k_B T}{2q} \ln \left( \frac{N_C}{N_V} \right)$$ (10)
In (10) the barrier height $\phi = \phi_{metal} - \chi$, where $\phi_{metal}$ is the metal work function and $\chi$ is the electron affinity of the semiconductor, while $E_g$ is the bandgap of the simulated semiconductor. The boundaries conditions for the current densities are relatively complicated. Since we are dealing with the quasi-Fermi levels they are:

$$\frac{\partial n}{\partial n} = -\frac{v_{mn}}{\mu_{n0,LC}} \left[ 1 - \frac{n_{0n}^B}{n} \exp \left( -\frac{\psi - \phi_n}{k_BT/q} \right) \right]$$

and

$$\frac{\partial p}{\partial n} = -\frac{v_{mp}}{\mu_{p0,LC}} \left[ 1 - \frac{p_{0p}^B}{p} \exp \left( -\frac{\phi_p - \psi}{k_BT/q} \right) \right]$$

(11) and (12)

Such complexity is externalized somehow from the normal electron and hole current density components, respectively. However in the proposed way is visible the role played by the anisotropic electron and hole mobilities. The higher mobility forces the current to increase very slowly, that is, the anisotropic mobility will not change drastically the IV curves. In (11) and (12) $v_{nm}$ and $v_{np}$ are the surface recombinations velocities for electrons and holes, respectively. While $n_{0n}^B$ and $p_{0p}^B$ are the equilibrium electron and hole densities. They may be set equal to the $N_D$ and $N_A$, respectively. The above metal-semiconductor model has been applied for simulating the Schottky diode, however it may not be used straightforward for simulating MESFET. Mainly this is owed to the fact, that its numerical formulation enable current flowing across the gate contact. To avoid this complication the normal component of the current density at the metal-semiconductor interface is set to be zero, this is equivalent to set the right hand side of (11) and (12) to nil, that is, having the artificial boundary set. This conditions is needed in order to guarantee the correct operation.

4. Numerical investigation

Our DD model was tested first investigating the 4H-SiC Schottky diodes. The device had 20 µm drift layer with a doping concentration of $10^{16}$ cm$^{-3}$ and the n$^+$ substrate of $8\times10^{18}$ cm$^{-3}$. The length and the height were 90 µm and 30 µm. The contact metal used in our simulation was Nickel for both Schottky and MESFET. This choice is simply due in order to verify the overall metal-semiconductor model for both devices. In Fig.1 and Fig.3 are depicted the schematic cross-sections for both devices, the inset exemplify the crystallographic orientation. In Fig.1 it is shown also how the boundaries were set.

Fig.1. Schematic cross-section of a Schottky diode.

The current characteristics plotted in Fig.2 seem to be slightly affected by the anisotropic mobility. This result was expected and clear verified by (11) and (12). The simulations were performed switching the anisotropic coefficients once parallel to the x- and y-axes. The slightly higher current is gained when the c-axes is set to be parallel to the y-axes. Equivalently, the higher current is led by the highest mobility value present in the specified direction. The lower current instead correspond the case where the c-axes is perpendicular to the y-axes, in this situation is the lowest mobility set along the main axes which leads to the lowest current.

Fig.2. I-V characteristics for the 4H-SiC Schottky diode.

Along our investigation, the second structure we modeled with our DD simulator was a simple MESFET. However the second investigation was carried out considering the Neumann boundary condition for the gate contact. In Fig.3 it is drawn the schematic cross-section. The anisotropic feature are handled as well. The gate length is 3 µm, while the source and drain length are 1µm, the drift layer was set 0.25 µm with doping level of $5\times10^{16}$ cm$^{-3}$, the n$^+$ regions have a doping level of $1\times10^{18}$ cm$^{-3}$ and thickness of 0.1 µm. As previously mentioned the metal type in this second investigation is again Nickel.
In Fig.4 are plotted the I-V characteristics carried out with our simulator. Differently from the Schottky diode, the IV characteristics are broadly influenced by the anisotropic mobilities more specifically by the crystallographic direction. Here again the simulations were performed switching the anisotropic coefficients once parallel to the x- and y-axes. The higher current is visible gained when the higher mobility values is oriented parallel to the x-axes, that is when c-axes is parallel to the x-axes. The inset in Fig.3 schematically shows the case when the main crystal axes is parallel to y, however this situation leads to the lower current, as plotted in Fig.4.

**Fig.3. Schematic cross-section of a MESFET.**

**Fig.4. I-V characteristics of the 4H-SiC MESFET**

### 5. Conclusions

A semi-classical approach was used to investigate the metal-semiconductor interface characteristics for 4H-SiC Schottky and MESFET devices. The DD model was exploited, tensorial features for the macroscopic physical quantities was considered as well. Numerical results have shown that the anisotropy is enhanced particularly for the MESFET, despite the fact both structure present similar metal-semiconductor interface. These major differences arise from the boundary condition used for the Schottky diode and for the MESFET. The formally equal metal-semiconductor boundaries must be treated differently in order to carry out the correct IV characteristic.

**Bibliography**


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