Numerical Analysis of the Schottky Contact Properties on the Forward Conduction of MPS/JBS SiC Diodes

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Abstract. In this paper, the impact of the anode contact in SBDs, PiN, JBS and MPS diodes is analyzed through TCAD simulations. The focus of the investigation is the correct simulation of the Schottky barrier height on the different areas of the device to correctly simulate a JBS or MPS structure. It is found that the splitting of the anode contact and an accurate selection of the Schottky barrier height on p-zone is necessary to allow the onset of the bipolar conduction in MPS devices. In this way, it is possible to correctly analyze the behavior of an MPS diode, including the snapback phenomenon.

Introduction

Diodes are the most mature components in Silicon Carbide, with the Schottky barrier diode (SBD) being the first to be commercially released [1]. SBDs are unipolar devices, so they exhibit a higher voltage drop at high current compared to PiN diodes. Lately, Silicon Carbide (SiC) diodes are usually designed with regularly spaced p+-wells in a n-type substrate. The resulting device is referred to as Junction Barrier Schottky (JBS) diode if the metal chosen for the anode contact inhibits the current conduction of the p+-zones, or merged-PiN-Schottky (MPS) diode if the metal on the p+-wells forms an Ohmic contact that allows their conduction. In Fig. 1, the idealized elementary cells of an SBD, PiN and MPS/JBS diodes are reported. The latter combines the advantages of SBDs and PiN diodes (Fig. 2), so the p-wells can reduce the leakage current by shifting the peak of electric field away from the metal-semiconductor interface and, possibly, assist the current conduction during surge events. It is worth clarifying that, although JBS and MPS diodes are different devices, they can be simulated with the same elementary cell, considering different types of contact on the p+-zone [2]. More in detail, to ensure that the p+ implantations can actually help the forward conduction by minority injection, the selection of the Schottky barrier height forming at the p+/metal interface is essential.

In this paper, the methodology to build an accurate TCAD model of a SiC MPS/JBS diode is reported, in order to correctly simulate the different Schottky barrier height on the different areas of the anode contact.



Fig. 1. 2-D TCAD models of the elementary cell of an (a) SBD (b) PiN diode (c) MPS or JBS diode.



Fig. 2. Comparison of PiN diode, SBD and MPS diode forward IV-characteristics.

Metal/semiconductor Junction

The study of the contact between metals and semiconductors has been widely undertaken in [3, 4] for narrow-bandgap material and in [5, 6] for SiC. When a metal and an n-type semiconductor are interfaced, a space charge region (SCR) expands from the junction into the semiconductor and an electric field develops within this region with the consequent formation of a potential barrier. This is illustrated in the idealized band diagram at thermodynamic equilibrium of Fig. 3a for a metal/n-type semiconductor junction with $\Phi_M > \Phi_S$, where Φ_M and Φ_S are the work-function in the metal and in the semiconductor, respectively.

The shape of the potential barrier depends on the charge distribution within the SCR. In a first order approximation, the thickness (W_D) of the potential barrier can be calculated according to Eq. 1, where ε_S is the permittivity of the semiconductor, ψ_{bi} is the built-in potential, q is the electron charge, K is the Boltzmann constant, T is the absolute temperature and N_D is the donor concentration.

$$W_D = \sqrt{\frac{2\varepsilon_s}{qN_D} \left(\psi_{bi} - \frac{kT}{q}\right)}.$$
(1)

Qualitatively, increasing N_D shrinks the potential barrier and, therefore, the electron tunneling probability through the latter increases. For very narrow values of W_D, the electrons are very likely to tunnel, and the contact becomes of near-Ohmic nature. Specular considerations hold for holes in the valence band when metal/ptype semiconductor junction is analyzed (Fig. 1b). In addition to the tunneling enhancement given by a narrowing of the barrier width, the Ohmic behavior of the junction can be also achieved by selecting a metal with a work function so that $\Phi_{\rm M} < \Phi_{\rm S}$ ($\Phi_{\rm M} > \Phi_{\rm S}$) for a metal/n-type semiconductor junction (metal/p-type semiconductor junction). More in detail, $\Phi_{\rm M}$ and $\Phi_{\rm S}$ determine the Schottky barrier



Fig. 3. Idealized band diagram at thermodynamic equilibrium for (a) a metal/n-type semiconductor junction with $\Phi_M > \Phi_S$ and (b) a metal/p-type semiconductor junction with $\Phi_M < \Phi_S$.

height viewed by electrons (Φ_{Bn}) and the Schottky barrier height viewed by holes (Φ_{Bp}). Since Φ_{Bn} and Φ_{Bp} are related by Eq. 2, increasing one of the two barriers results in a reduction of the other.

$$E_G = q\Phi_{Bn} + q\Phi_{Bp},\tag{2}$$

Consequently, defining a single anode contact that behaves as Schottky when interfaced with n-regions and as Ohmic when interfaced with p-wells might not be possible.

Simulations and Results

In this section the isolated behavior of an SBD and PiN diode are firstly investigated. Successively, their interaction obtained by merging the two structures into a MPS or JBS diode is analyzed. The considered structures are based on the devices described in [7]. All the simulations are performed on elementary cells and an appropriate area factor is set to consider a total area of all the devices of 1.56 mm^2 . The simulated devices are characterized by a 35 µm-thick drift region with a $4 \times 10^{15} \text{ cm}^{-3}$ constant doping concentration (N_{epi}) and a substrate with a thickness of 10 µm with constant doping concentrations are performed donor doping material is Nitrogen. The simulations are performed varying the contact type of the anode, while the cathode electrode is always implemented as ideal Ohmic. The used software is the TCAD simulator Sentaurus from Synopsys.

SBD Simulation. In this subsection, an SBD is analyzed. An elementary cell of an SBD was implemented in the TCAD simulator, where the anode electrode was modelled as a Schottky contact, and the simulations were performed varying the value of the Schottky barrier height viewed by the electrons(Φ_{Bn}). The idealized cell with some design parameter is reported in Fig. 4.

The simulations were performed with a Schottky barrier height of 0.87 eV, 1.1 eV and 1.6 eV, which correspond to the typical values of the barrier resulting from technological processes where the contact metallization is implemented by titanium (Ti), molybdenum (Mo) and nickel (Ni), respectively [7].

The obtained forward current-voltage (IV) characteristics are reported in Fig. 5, that shows that for a fixed current value, the voltage drop across the anode and cathode terminals increases as the Schottky barrier increases due to the higher built-in potential.



Fig. 4. 2-D TCAD model of the elementary cell of an SBD.

Fig. 5. Forward isothermal IV-characteristics at 25°C for an SBD for different barrier heights.

PiN Diode Simulation. The second diode design analyzed is the PiN diode, whose design parameters are reported in Fig. 6. The anode region was modeled according to the structures described in [7]. More in detail, it is composed by two different aluminum implantations: a shallow one, modeled by a Gaussian function with a peak concentration of 3×10^{19} cm⁻³ and a depth of 200 nm,

and a deep one, described by an error function with a maximum value of 2×10^{17} cm⁻³ that yields a junction depth of 700 nm. The resulting doping profile is reported in Fig. 7.

The operation of a PiN diode is characterized by bipolar conduction. To allow that, the anode contact should act as Ohmic. A contact between a metal and a semiconductor is defined as Ohmic if it has a negligible impedance compared to the series impedance of the bulk of the semiconductor. This implies that the free carrier density near the contact is much larger than that in the bulk of the semiconductor [8]. Moreover, an Ohmic contact represents the ideal case of neutral contact that leads to the flat-bands condition, i.e., no depletion or accumulation of free carriers will exist at the interface, and no band banding will be present. In simulation, a contact can be defined as ideal Ohmic, but can be more physically accurate to define it as Schottky to correctly represent the barrier formed by the metal-semiconductor junction. Specifically, for a metal that contacts a p-type semiconductor, to ensure a non-rectifying behavior, it is necessary to choose a metal of high work-function so that $\Phi_{\rm M} > \Phi_{\rm S}$.

Several simulations were performed, first defining the anode contact as ideal Ohmic, then modelling such contact as Schottky with a barrier height of 2.75 eV, 2.80 eV, 2.85 eV, 3.05 eV. The latter value corresponds to the value of the Schottky barrier height (Φ_{Bn}) to obtain a nearly flat-band condition, as shown in Fig. 8. In Fig. 9, the resulting simulated IV-characteristics are reported. The simulations show that the device conducts a non-negligible current only for a Schottky barrier height grater than 2.75 eV, with the current increasing as the barrier height increases. As shown in Fig. 3 and according to Eq. 2, the increase of Φ_{Bn} causes the decrease of the barrier Φ_{Bp} viewed by the holes in the metal, that leads to an increase of the current. Notice that simulating barrier height values greater than the bandgap of the semiconductor could lead to non-physical results [9].

Furthermore, simulations show that if the Schottky barrier height is far from the flat-band condition, for high applied voltage the current saturates. Specifically, the structure can be schematized as two diodes back-to-back, representing the metal/p-type semiconductor junction and the p/n junction, and a resistance, representing the bulk. When the device is forward biased, the metal/p-type semiconductor junction is reverse biased, so if the applied voltage is low it operates in the linear region and acts as a resistance. When the voltage increases, the current through the whole device saturates to the value of the leakage current of the metal/ p-type semiconductor junction. Moreover, the characteristics saturate at different current value because the leakage current of the diode increases as the Schottky barrier height increases.





Fig. 6. 2-D TCAD model of the elementary cell of a Fig. 7. Profile of the net doping concentration in the PiN diode.

anode region of the simulated PiN diode.



Fig. 8. Band diagram near the metal/semiconductor junction at thermodynamic equilibrium (overlapping constant quasi-Fermi levels) of the simulated PiN diode for different values of Φ_{Bn} . Inset: band diagram through the whole device.



Fig. 9. Forward isothermal I/V characteristics at 25°C for a PiN diode with different types of anode contact.

Simulation of MPS Diode with Single Anode Contact. After comparing the behaviors of the SBD and the PiN diode, they were merged to create JBS and MPS diodes. Although the cross section of an elementary cell of a JBS diode is identical to the one of a MPS diode, the capability of the p+-zone to conduct denotes if the diode is MPS or JBS and it is determined by the Schottky barrier

of the metal/semiconductor interface. The n-zone and the p-zone must be simulated in the same structure due to the interaction between the two regions. According to this, usually a single contact is used for the anode electrode, therefore the same Schottky barrier height (either Φ_{Bn} or Φ_{Bp}) is imposed on the two zones, as shown in Fig. 10a.

In this subsection, the simulations of an MPS elementary cell with a single anode contact are reported. The structure is based on the design 4 reported in [7], where the p-zone and n-zone are 2 μ m and 3 μ m-wide, respectively, while the other geometrical and doping specifications are the same of the structures described in the previous subsections. In Fig. 11, the IV-characteristics for a Schottky barrier height of 1.7 eV and 3.05 eV are shown. While



Fig. 10. 2-D TCAD models of an MPS with (a) a single Schottky contact and (b) two different Schottky contacts with different barrier heights.

 $\Phi_{Bn} = 1.7 \text{ eV}$ inhibits the conduction of the p-zone leading to a JBS behavior, $\Phi_{Bn} = 3.05 \text{ eV}$ forms an Ohmic contact for holes and allows the injection of minority carriers into the epi-layer, thus resulting in an IV-characteristic like that of a PiN diode. This is also clarified by the current density distributions for a current of 100 A shown in Fig. 12. This analysis asserts that using a single anode contact is too simplifying to simulate an MPS diode, but it is suitable to simulate a JBS diode.





Fig. 11. Forward IV-characteristic resulting from the isothermal simulation at 25°C of an MPS diode with a single anode contact for different values of the Schottky barrier height.

Fig. 12. Maps of the total current density distribution for a barrier height of (a) 1.7 eV and (b) 3.05 eV.

Simulations of MPS Diode with Two Anode Contacts. To simulate an MPS diode, the PN junction should conduct a current during surge events. To ensure that the p+-implantations can contribute to the forward conduction by minority injection, it is essential to accurately select the Schottky barrier height forming at the p+/metal interface, so that the contact could behave as Ohmic (Fig. 3b). At the same time, the n-zone should preserve its rectifying behavior. To achieve this in simulation, it is possible to split the anode contact into two parts, one placed on the n-zone and the other on the p-well, in order to differentiate the contact type on the two zones, as shown in Fig. 10b. The former should exhibit a Schottky barrier for electrons, while the latter should act as Ohmic for holes. However, it is not recommended to define the contact on the p-zone as ideal Ohmic because it can lead to incorrect simulation results around PN junctions [10]. A general approach consists in defining both contacts as

Schottky with different values for the barrier height, also in order to more accurately model the actual metals used to build the device. Fig. 13 shows the holes current density map at I = 100 A in the MPS structure with two different anode contacts, with a Schottky barrier height of 1.7 eV on the n-zone, and of 3.05 eV on the p-zone, that leads to the nearly flat-band condition. The holes current distribution shows that the p-zone injects holes into the epi-layer contributing to the current conduction of the device, unlinke the structure with a single anode contact. It follows that considering two different anode contacts allows the bipolar operation of the device. Fig. 14 reports the IV-characteristics of an MPS diode with two different Schottky contacts for the p-zone and the n-zone obtained by varying the Schottky barrier height on p-zone. The Schottky barrier height on the n-zone is fixed at 1.7 eV, whereas the barrier height values considered on the p-zone were 2.75 eV, 2.80 eV, 2.85 eV and 3.05 eV. The current conducted by the device is equal to that through the device with a single anode contact with the same Schottky barrier height on the n-zone (1.7 eV) up to 10 V. Above 10 V, if the barrier height of the contact on the p-region is greater than



Fig. 13. Map of the holes current density at I=100 A in the MPS structure with a two different anode contacts.

2.75 eV, the p-well starts injecting holes into the epi-layer, the resistivity of which is then reduced by the conductivity modulation phenomenon. As this mechanism occurs, an overall reduction of the voltage drop across the device takes place, causing a negative differential resistance (NDR) [11]. This

phenomenon is known as snapback, that is a serious issue for the operation of diodes in parallel [12]. Therefore, taking into account the possible rising of the snapback is fundamental to correctly design reliable MPS diodes and this can be done only by splitting the anode electrode into two contacts.

It is worth noticing that for values of the Schottky barrier heights far from the flat-band condition, at a certain value of the current, the resistance of the epi-layer becomes constant due to the saturation of the conductivity modulation, caused by the saturation of the current conducted by the metal/p-semiconductor junction, as described in the previous pharagraphs.

Moreover, the variation of the epi-layer doping changes the slope of the IV-characteristic, hence the current from which the NDR region strarts, as shown in Fig. 15. More in detail, increasing N_{epi} determines an increase of the concentration of minority carriers needed to trigger the conductivity modulation of the epi-layer.



Fig. 14. Forward IV-characteristics resulting from the isothermal simulation at 25°C of an MPS diode with the double Anode contact.



Fig. 15. Forward IV-characteristics resulting from the isothermal simulation at 25° C of an MPS diode with two anode contacts for different values of N_{epi}.

Conclusion

From the analysis conducted in this paper, it has been shown that the selection of the metal to ensure a Schottky barrier height that allows the conduction of the p-wells in MPS diodes is a design parameter of primary importance. According to this, to have a methodology to correctly simulate the behavior of an MPS diode is fundamental. In particular, it has been shown that with a single anode contact, it is not possible to correctly simulate the bipolar behavior of an MPS diode during surge events. On the other hand, splitting the anode contact into two has been found to better model the conduction of the p-zones, also by enabling the occurrence of possibly detrimental phenomena, such as the snapback.

Summary

In this paper, a TCAD analysis of the impact of the type of anode contact on JBS and MPS SiC diodes has been presented. Firstly, the analysis has been conducted on the constituent cells of those devices, i.e., Schottky and PiN elementary cells. Afterwards, their interaction in JBS and MPS diodes has been analyzed and several case-studies has been investiged.

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