Ni Schottky barrier on heavily doped phosphorous implanted 4H-SiC

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Abstract

The electrical behavior of Ni Schottky barrier formed onto heavily doped ($N_D > 10^{19} \text{ cm}^{-3}$) n-type phosphorous implanted silicon carbide (4H-SiC) was investigated, with a focus on the current transport mechanisms in both forward and reverse bias. The forward current–voltage characterization of Schottky diodes showed that the predominant current transport is a thermionic-field emission mechanism. On the other hand, the reverse bias characteristics could not be described by a unique mechanism. In fact, under moderate reverse bias, implantation-induced damage is responsible for the temperature increase in the leakage current, while a pure field emission mechanism is approached with bias increasing. The potential application of metal/4H-SiC contacts on heavily doped layers in real devices is discussed.

Keywords: 4H-SiC, electrical characterization, current transport, Schottky device

1. Introduction

In the last decades, wide-bandgap semiconductors have attracted great interest in the development of high-power electronic devices and systems [1, 2]. The interest towards these materials is based on their extraordinary physical and electronic properties, such as a wide bandgap, high breakdown electric field strength, high saturation electron velocity and high thermal conductivity [3]. In particular, the hexagonal polytype of silicon carbide (4H-SiC) plays a pivotal role thanks to the maturity reached in terms of material quality and technological implementation of the device fabrication steps [4]. In fact, 4H-SiC unipolar devices, such as Schottky barrier diodes (SBDs) and metal–oxide–semiconductor field effect transistors (MOSFETs), with high a performance (low on-state voltage drop, high breakdown voltage, high switching speed, possibility to operate at high temperature, etc), have become largely available on the market [4–6].

However, in order to fully exploit the potentialities of this material, significant efforts are currently being devoted to address some physical concerns, which still limits the performance of SiC devices [7]. For SiC devices, a full understanding of the Schottky barrier properties is particularly useful in several applications. For example, while in SBDs used as sensors and detectors a high Schottky barrier height is desired [8, 9], a reduction of the barrier is targeted in power electronics applications to minimize the device power consumption [10]. Typically, the Schottky barrier properties can be tailored by an optimized choice of metal (e.g. low work-function metals, tunable compositions, etc) [11–14], by suitable semiconductor surface treatments [15, 16] or by intentionally changing the electric field distribution below the interface by ion-irradiation [17]. In this context, many efforts have been dedicated to the basic understanding of the current transport in metal/semiconductor contacts on both lightly and heavily doped epitaxial 4H-SiC layers [18–20]. On the other hand, ion implantation is used to form heavily doped n-type and p-type regions in junction barrier Schottky (JBS) rectifiers and MOSFETs for the creation of ohmic contacts [21–23]. In such implanted...
layers, ohmic contacts can be formed by annealing at high temperature (>900 °C) of Nickel films, owing to the formation of nickel silicide (Ni$_2$Si) [23, 24]. Hence, the knowledge of the carrier transport mechanisms at metal/heavily doped SiC interfaces is a fundamental issue for the optimization of the contacts in these SiC devices. Recently, Hara et al [25] studied the forward carrier transport mechanism in Schottky diodes fabricated on 4H-SiC epitaxial layers with different donor concentrations (up to a doping concentration as high as 1.8 × 10^{19} cm$^{-3}$), observing a reduction of the barrier height with increasing the epilayer doping.

In this work, the electrical behavior of Ni Schottky contacts onto heavily doped (N$_D > 10^{19}$ cm$^{-3}$) n-type phosphorus-implanted 4H-SiC was investigated, in both the forward and reverse bias. Specifically, a reduced turn-on voltage was achieved under the forward bias, where the thermionic field emission (TFE) mechanism dominates the current transport through the interface. On the other hand, the behavior of the contact under reverse bias was explained considering a tunneling mechanism assisted by the presence of ion-implantation-induced defects for moderate reverse bias, while probably approaching a pure field emission regime with an increasing bias. Finally, numerical simulations of the potential distribution in a JBS diode structure demonstrate the feasibility of this approach in real devices.

2. Experimental details

The material used in our study was an n-type 4H-SiC epitaxial layer (with nitrogen doping of 1 × 10^{16} cm$^{-3}$) grown onto a heavily doped 4H-SiC (0001) substrate. First, the upper part of the epitaxial layer was implanted at 400 °C using phosphorus (P) ions at energies ranging from 30 to 200 keV and with ion doses between 7.5 × 10^{13} and 5 × 10^{14} cm$^{-2}$. In this way, an implantation profile extending over 200 nm and with a peak concentration of 1 × 10^{20} cm$^{-3}$ is obtained, as confirmed by secondary ion mass spectrometry reported in [26], which also showed a structural investigation by cross-section transmission electron microscopy analysis. Then, a post-implantation thermal annealing treatment was carried out at 1675 °C in Ar ambient, protecting the surface with a carbon capping layer [27], in order to achieve the electrical activation of the dopant.

SBDs were fabricated on this material. Prior to the front-side processing of the sample, a large-area back-side contact was fabricated by Ni-deposition followed by rapid thermal annealing at 950 °C in N$_2$-atmosphere [23]. Successively, a 100 nm thick Ni-layer was deposited on the P-implanted surface by direct current magnetron sputtering and defined in circular structures (radius of 250 µm) by optical lithography and lift-off process. These Ni-Schottky contacts were deliberately not subjected to annealing treatments to avoid interface reactions, which would induce a consumption of the SiC layer and/or a degradation of the barrier properties [28].

The Schottky contacts were characterized by means of current–voltage ($I$–$V$) measurements, under both forward and reverse bias, at various temperatures in the range 25 °C–115 °C (step of 15 °C). The measurements were performed on a Karl-Suss MicroTec probe station equipped with a parameter analyzer.

3. Results and discussion

First, figure 1 compares the forward room-temperature current density–voltage ($J$–$V_F$) characteristics of Ni Schottky contacts formed on an n-type 4H-SiC epilayer, with or without a heavily doped n-type implanted layer.

As one can see, the $J$–$V_F$ curve of the contact on the heavily doped n-type implanted 4H-SiC exhibits a lower turn-on voltage with respect to the reference contact formed on the 4H-SiC epilayer without implant.

Under the forward bias, the electrical behavior of 4H-SiC Schottky diodes is typically described by the thermionic emission (TE) model [29–31], with the current density–voltage ($J_{TE}$–$V_F$) relationship expressed by:

$$J_{TE} = A^* T^2 \times \exp \left( \frac{-q \Phi_{BTE}}{k_B T} \right) \times \exp \left( \frac{q V_F - J_{TE} R_{on}}{n k_B T} \right)$$

(1)

where $A^*$ is the effective Richardson’s constant of 4H-SiC (146 A cm$^{-2}$ K$^{-2}$) [32], $k_B = 1.38 \times 10^{-23}$ J K$^{-1}$ is the Boltzmann’s constant, q is the elementary charge, $V_F$ is the voltage applied across the metal/semiconductor interface and T is the absolute temperature. The relevant diode parameters in equation (1), i.e. ideality factor n, Schottky barrier height $\Phi_{BTE}$ and specific on-resistance $R_{on}$, were derived as best fit parameters. The experimental value of the barrier height measured in Ni-Schottky contacts on 4H-SiC epitaxial layer typically ranges between 1.3 and 1.6 eV [10, 33–35].

In our case, Ni Schottky contacts fabricated directly on the 4H-SiC epilayer (without implanted layer, black curve in
on the other hand, the TE model applied to the Ni Schottky contacts in the heavily doped n-type implanted layer gives a barrier height \( \Phi_{BTE} = 0.94 \) eV and an ideality factor \( n = 1.8 \). Such a strong discrepancy with respect to the ideal behavior (\( n = 1 \)) suggests that the current transport at the Ni/heavily doped 4H-SiC interface cannot be described by a pure TE regime. More reasonably, considering the high doping concentration of the implanted region, the presence of a tunneling contribution to the forward current transport must be taken into account. Thus, for analyzing the forward characteristics we considered a TFE model \([36, 37]\), that is a thermal-assisted tunneling. Figure 2 (open symbols) reports the semilog plot of the experimental forward \( J - V_F \) characteristic of a representative diode acquired at room temperature with the inset depicted a not-to-scale schematic energy band diagram of a thermal-assisted tunneling transport. In this scheme, \( n^+ \) and \( n^- \) represent the implanted and the epitaxial regions, respectively, while \( E_C \) and \( E_F \) are the bottom of the conduction band and the Fermi level in the semiconductor. The experimental forward characteristics were fitted by the TFE relationship (continuous line in figure 2), that is expressed by [37]:

\[
J_{TFE} = J_{0,TFE} (V_F) \times \exp \left( \frac{q (V_F - J_{TFE} R_{on})}{k_B T} \right)
\]  

(2)

where the saturation current \( J_{0,TFE} (V_F) \) is given by:

\[
J_{0,TFE} (V_F) = \frac{A^{*} T}{k_B \cosh \left( \frac{q E_0}{k_B T} \right)} \times \sqrt{\frac{2}{\pi}} \left( \Phi_{BTE} - \Delta E_F - (V_F - J_{TFE} R_{on}) \right) \times \exp \left( \frac{q \Delta E_F}{k_B T} - \Phi_{BTE} - \Delta E_F \right)
\]  

(3)

and \( E_0 = E_{00} \times \cos \left( \frac{\Phi_{BTE}}{k_B T} \right) \), with \( q \) is the elementary charge, \( k_B \) is the Boltzmann’s constant and \( T \) is the absolute temperature. The parameter \( E_{00} \) is dependent on the doping concentration \( N_D \), according to \( E_{00} = \frac{h^2}{2\pi} \sqrt{\frac{N_D}{m^* \epsilon_S C}} \), with \( m^* = 0.38 m_0 \) the effective mass (\( m_0 \) is the electron mass) and \( \epsilon_S C = 9.66 \epsilon_0 \) the dielectric constant of the semiconductor (\( \epsilon_0 \) is the vacuum permittivity) \([37-40]\), while \( \Delta E_F \) is the difference between the bottom of the conduction band and the semiconductor Fermi level.

The barrier \( \Phi_{BTFE} \) and the doping concentration \( N_D \) were determined as parameters of the TFE fit to the experimental \( J - V_F \) curve, obtaining \( \Phi_{BTFE} = 1.77 \) eV and \( N_D = 1.97 \times 10^{19} \) cm\(^{-3}\). The ratio \( k_B T/q E_{00} \) gives an indication of the relevance of the TE process with respect to the tunneling one and allows us tofor the evaluation of which current transport mechanism is predominant for a given doping concentration \([38]\). Using \( N_D = 1.97 \times 10^{19} \) cm\(^{-3}\), the ratio \( k_B T/q E_{00} = 0.61 \), which confirms the appropriateness of the TFE model to describe our data.

Furthermore, considering the doping concentration \( N_D = 1.97 \times 10^{19} \) cm\(^{-3}\) derived by the TFE fit, a depletion width \( W_D = 10 \) nm at the Ni/4H-SiC interface can be estimated at zero bias \([41]\). Such a donor concentration is in agreement with the value measured by scanning capacitance microscopy of the active dopant profile on a 4H-SiC sample implanted and annealed under the same conditions \([24]\).

The temperature-dependence of the forward and reverse characteristics of the diode were then studied to gain additional insights into the dominant current transport mechanisms.

First, the temperature-dependence of the forward \( J - V_F \) characteristics was monitored between 25 °C and 115 °C (figure 3), showing an increase in the current with the temperature. Specifically, by fitting the experimental curves to TFE model for each temperature, we observed a decrease in the barrier \( \Phi_{BTFE} \) (from 1.77 to 1.66 eV) with increasing temperature. On the other hand, an almost constant value of doping \( N_D \) (1.96 ± 0.02) \( \times 10^{19} \) cm\(^{-3}\) was found as the temperature increases, in agreement with our previous Hall measurements carried out on similar samples \([24]\). The temperature-dependence of the barrier height \( \Phi_{BTFE} \) and the doping concentration \( N_D \) is reported as insets in figure 3.

Moreover, as reported in figure 4, the effective Richardson’s constant determined from the plot \( \ln (I/JT^2) \) vs 1/(k_B T)
Figure 3. Experimental $J−V_F$ curves for Ni/4H-SiC Schottky diode under forward bias at different measurement temperatures in the range 25 $^\circ$C–115 $^\circ$C. The insets show the temperature-dependences of the barrier height and doping concentration values, derived by the TFE fits of the forward $J−V_F$ curves at the different measurement temperatures.

Figure 4. Richardson’s plot $\ln \left( \frac{I_S}{T^2} \right) vs \frac{kT}{q}$ for Ni Schottky diode on n-type implanted 4H-SiC. From the linear fit of the effective barrier height and Richardson’s constant could be determined.

Figure 5. $nkT$ vs $kT$ plot for the ideal case $n = 1$ (red solid line), for an inhomogeneous barrier described by the ‘$T_0$ anomaly’ (dashed lines) and for our experimental data (black open circles). The $nkT$ vs $kT$ curves calculated with the TFE for three different doping concentration values are also reported.

Figure 6. (a) reports the reverse current density–voltage characteristic ($J−V_R$) of the Ni/4H-SiC Schottky diode acquired at various temperatures. As can be seen, the reverse current density increases from tenths of nA cm$^{-2}$ up to a few units of A cm$^{-2}$ with increasing reverse bias. Noticeably, while the reverse current exhibits a clear dependence on the measurement temperature for lower voltages, it becomes almost independent of the temperature at higher bias values.

The field emission (FE) regime through a metal/semiconductor interface predicts only a weak temperature dependence of the reverse current, with the reverse current density expressed as [37]

\[
I_S = A^* T^2 \times \exp \left( -\frac{q\Phi_B}{kT} \right)
\]

where $I_S = AA^* T^2 \times \exp \left( -\frac{q\Phi_B}{kT} \right)$ is the saturation current of equation (1), was $4.7 \times 10^{-4}$ A cm$^{-2}$ K$^{-2}$. This experimental value is lower than the expected one of 146 A cm$^{-2}$ K$^{-2}$ for 4H-SiC [42]. This discrepancy has often been attributed to deviations from the TE model and/or to lateral inhomogeneity of the barrier [42, 43].

The $J−V_F$ measurements, reported in figure 3, revealed a temperature dependence of the ideality factor, which in turn confirms a deviation from the ideal TE and suggests the formation of an inhomogeneous Schottky barrier. A way to visualize the deviation from the TE behavior is to report a plot of $nkT$ as a function of $kT$, as shown in figure 5. In particular, besides our experimental data (black open circles), this graph also reports the ideal TE case with $n = 1$ and the case of an inhomogeneous Schottky barrier described by the so-called ‘$T_0$ anomaly’, with $T_0$ values typically observed in Schottky contact to 4H-SiC, i.e. varying in a range between 20 and 40 K [44–46]. Moreover, the $nkT$ vs $kT$ curves, calculated with the TFE model for three different doping concentration values, are also reported. As can be seen, an excellent agreement between our experimental data and the calculated TFE curve is obtained for a concentration of $1.96 \times 10^{19}$ cm$^{-3}$.

(continues)
with the meaning of symbols as mentioned above.

At room temperature (inset of figure 6(a)), the FE model can fit the experimental data with a barrier height $\Phi_B = 1.77$ eV and a doping concentration $N_D = 1.0 \times 10^{19}$ cm$^{-3}$. In this case, the effect of the series resistance at high current level (high reverse voltage) cannot be ruled out. Moreover, the FE model cannot well describe the experimental curves at all measurement temperatures. Hence, it is possible to argue that an additional mechanism must be taken into account to explain the more pronounced temperature behavior of the reverse current at low voltage.

Figure 6(b) reports an Arrhenius’ plot of the current density for three representative reverse biases (at 1 V, 3 V and 8 V). From these plots, it was possible to determine the activation energy $E_A$ that varies from 0.387 eV at 1 V down to 0.205 eV at 3 V. Interestingly, the Arrhenius’ plot gives a much lower activation energy of 0.052 eV at 8 V, where the current is almost independent of temperature. This latter is consistent with the prevalence of a tunneling mechanism coexisting with the series resistance contribution of the epilayer. In fact, since the FE is almost independent of temperature, the activation energy determined from the Arrhenius’ plot of the leakage current significantly decreases with increasing the reverse bias, i.e. where FE becomes dominant.

As observed in the literature [36, 42, 47–51], a large variety of defects can be induced in 4H-SiC by ion-implantation and post thermal treatments, introducing energy levels within the band gap of the material, which can have an impact on the leakage current of Schottky diodes. Plausibly, the defects in our high dose P-ion implanted sample induce energy levels that can assist the current transport in the moderately reverse bias range, explaining the temperature-dependence of the reverse characteristics (inset figure 6(b)). At higher voltages, the direct tunneling FE becomes progressively dominant, due to the barrier thickness reduction.

A possible application of these results in a real device is considered by performing a numerical simulation of the potential distribution in a JBS diode structure. The JBS consists in embedding p$^+$-type regions (usually achieved by ion implantation) within an n-type Schottky area. In this layout, the leakage current of the Schottky contact in an n$^+$-doped surface region can be mitigated by the lateral depletion of the p$^+$-n junctions. The numerical simulation, carried out using a drift diffusion solver implemented in the open source FEniCS platform [52] and employing a heavily doped n$^+$-type region below the Schottky metal, is shown in figure 7 for a reverse bias of −10 V. FEniCS allows accurate and robust implementation of user defined coupled partial differential models, as the drift-diffusion one, whilst an efficient implementation of user defined coupled partial differential models, as the drift-diffusion one, whilst an efficient computer aided design of the structure and the meshing algorithm is obtained coupling the FEniCS python modules with the Gmsh package (again, in an open source licensing format) [53]. The JBS structure (inset of figure 7) assumes ideally 0.6 $\mu$m thick rectangular p$^+$-regions ($N_A = 2 \times 10^{19}$ cm$^{-3}$) placed around a 1.4 $\mu$m wide Schottky contact formed on a
diode demonstrated the possibility of applying this process to improve the performance of real 4H-SiC Schottky

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Figure 7. (a) Numerical study of the potential distribution for a JBS structure (schematically depicted in the inset) employing a heavily doped n+ -type region below the Schottky metal, for a reverse bias of −10 V. The potential reference in the bulk n-epi region is aligned to its quasi-Fermi energy. (b) Cut line of the potential distribution 50 nm above the p+ -regions, showing the pinch-off effect.
