The influence of carbon in the back-barrier layers on the surface electric field peaks in GaN Schottky diodes

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***Abstract*—Technology Computer Aided Design simulations are used to assess the influence of carbon in the back-barrier layers of GaN-on-Si wafers on the voltage distribution in GaN Schottky diodes. It is shown that carbon cannot be present as an acceptor only – as it is commonly assumed. The carbon needs to be compensated by donors or partly electrically inactive in order to explain the observed high hard breakdown voltage in GaN-on-Si Schottky diodes. Furthermore, it is shown that the level of donor compensation of the carbon will have a significant influence on the two-dimensional voltage distribution in the devices, and, hence, on the surface electric field peaks. This conclusion is important to consider in the design of field plate extensions of the Schottky diode.**

Keywords— Technology Computer Aided Design (TCAD), GaN, Schottky diodes, Carbon defect

I. Introduction

GaN-on-Si power technology is considered to be the next paradigm shift for various power electronic applications [1]. The AlGaN/GaN material system has superior properties compared to conventional silicon such as high critical electric fields, high electron mobility and saturation velocity due to the wide band gaps and conduction at (undoped) heterointerfaces. Technology computer aided design (TCAD) has been a guide for device design and development in silicon technologies for several decades. This numerical tool allows one to gain insight in the physical operation of devices. Especially for Si power devices, TCAD has proven to be very useful since the space dimensions typically remain in the micrometer range and, thus, drift-diffusion based device simulations remain valid.

Since the advent of GaN as an alternative semiconductor, the TCAD tool that served well for Si is now being used for GaN power devices [2]. However, TCAD cannot yet be used as a predictive tool to a similar extent as in Si. One of the major reasons is the lack of detailed knowledge about the defects in GaN that determine important aspects of device operation. Not only is the simulation of the passivation interface related traps a challenging task [3], also the stress relief layers under the active GaN channel region need to be simulated as these layers play a vital role at high-voltage operation.

This work focuses on these deeper layers in the epitaxial stack, especially on the carbon doped back-barrier layers and the influence of the carbon related defects on the two-dimensional (2D) electrostatic potential distribution. As it will be shown, the level of donor compensation of the carbon deep acceptor trap will determine the height of the surface electric field peaks. This means that the design of the back-barrier layers has to go hand in hand with the design of the dielectric passivation layers and the field plate configuration. As we have shown in the past, this is important both for reducing the dynamic on-resistance dispersion [4] and for improving the reliability and time-dependent breakdown [5][6].

The TCAD simulation results are discussed in Section III and are illustrated on a high-voltage Schottky diode (described in Section II). The results can however easily be transferred to other high-voltage GaN-on-Si devices, such as the p-GaN high-electron-mobility transistor (HEMT).

II. Technology, GaN-on-Si Schottky Diode, and TCAD Simulation Set-Up

Imec's GaN-on-Si technology is used to process the Schottky diodes. The epitaxial stack is grown on a Si (111) substrate by means of metalorganic chemical vapor deposition (MOCVD). It consists of a 200 nm AlN nucleation layer, a 3.22 µm AlGaN stress relieve layer stack, a 1.0 µm GaN:C back-barrier, a 300 nm unintentionally doped (UID) GaN channel, a 0.5 nm AlN spacer, a 10 nm $Al_{0.25}Ga_{0.75}N$ barrier, and a 5 nm SiN cap. Further details on the processing and design of the gated edge termination (GET) Schottky diode can be found in [7]. The GET Schottky diode is the primary choice in imec's GaN-on-Si technology, and will be referred to simply as the Schottky diode. A scanning electron microscope (SEM) cross-section image of the Schottky diode with a certain field-plate configuration is shown in Fig. 1 (bottom).

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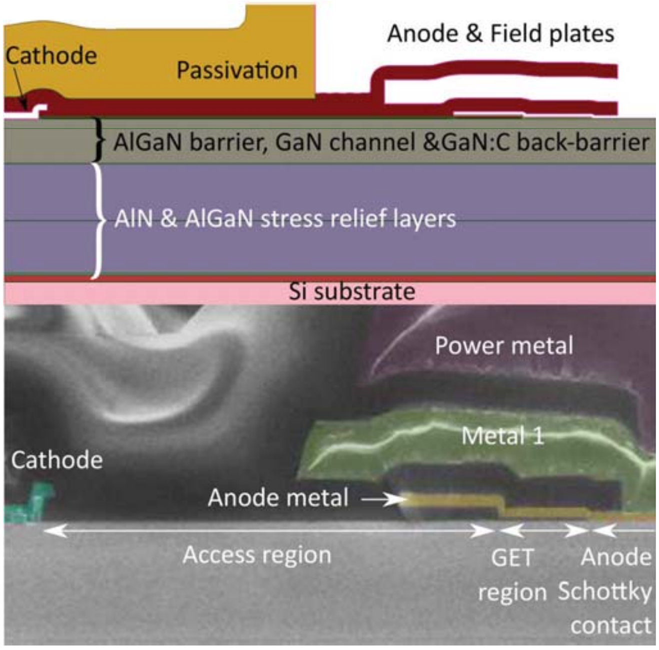

Fig. 1. 2D TCAD simulated cross-section (top) and SEM image (bottom) of the Schottky GET diode, indicating the field plate configuration and multiple dielectric layers. Note that the pictures do not have the same scale and have a slightly different field plate configuration.

The two-dimensional (2D) simulated cross-section of the Schottky diode is shown in Fig. 1 (top). These structures were generated using Synopsys' Sentaurus Process Simulation [8]. The gated edge terminated and recessed anode with various field plates are vital parts of the Schottky diode, and, need to be included into the simulated structure as precisely as possible based on the actual process flow and e.g. SEM pictures such as the one shown in Fig. 1 in order to be able to simulate the electric field peaks at the surface as precisely as possible.

The most important quantity determining the ON-state is the density of the two-dimensional electron gas (2DEG). This 2DEG density is governed on the one hand by the polarization charges – for which the strain model including the spontaneous and piezoelectric polarization is used; and on the other hand by the top and bottom boundary conditions: the Fermi level pinning at the surface passivation and in the GaN:C back-barrier. The 2DEG density is calibrated in the access regions based on Hall measurements and sheet resistance R_{sh} measurements on Transmission Line Method (TLM) structures. The calibration method is described in [2]: a thin (2.5 to 5.0 nm) 'border trap region' together with interface states is used to pin the Fermi level at the surface. The 2DEG density is also partly determined by the boundary condition at the bottom of the GaN channel. However, since the GaN channel itself is relatively thick (300 nm), the Fermi level pinning at the GaN/GaN:C interface does not have a large influence on the 2DEG density. Yet, the back-barrier boundary condition is also important for the 2D voltage distribution in the OFF-state as discussed in the next section.

Fig. 2 shows a typical measured OFF-state characteristic, where the substrate and anode are grounded and the cathode is

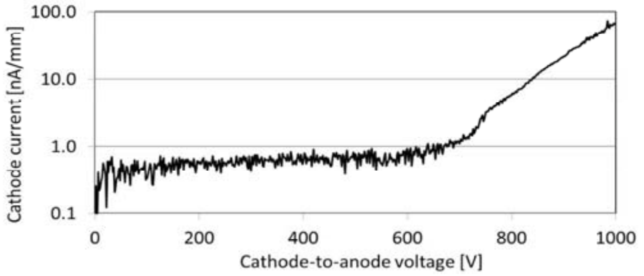

Fig. 2. Typical measured OFF-state I-V curve of a Schottky diode. Hard breakdown occurs well beyond 600 V.

positively biased (cathode-to-anode voltage V_{ca} high). The hard breakdown is typically above 1 kV for these devices, and the increase in leakage current above the $V_{ca} > \sim 700$ V is dominated by buffer leakage (i.e. cathode to substrate leakage). The leakage current I-V characteristics do not vary to a large extent between different field plate configurations and the measured curve (Fig. 2) corresponds to a Schottky diode with a field plate configuration as shown in Fig. 1 (top). Note, however, that the reliability and time-dependent breakdown can significantly vary between different field plate configurations, which is attributed to the difference in the electric field peak distribution at the surface – as described in [5] and [6]. Therefore, a better understanding of the role of the back-barrier on this surface electric field peak distribution is needed.

III. Simulation Results & Discussion

The first back-barrier layer is a carbon doped GaN layer and the Fermi level is pinned at the C_N level (0.9 V above the valence band [9][10]). This deep acceptor can be partly compensated by donors (the C_{Ga} defect as main donor contributor), an effect that is used by Uren et al. [11] to calibrate the hole density in a carbon doped GaN layer and by Rackauskas et al. [12] to suppress a 2D hole gas (2DHG) at a GaN/AlGaN heterointerface. We will use the same defect levels to study the influence of the donor compensation on the 2D potential distribution and on the surface electric field peaks.

A. 2D potential distribution and surface electric field peaks

Fig. 3 shows the 2D potential distribution in the Schottky diode at reverse bias ($V_{ca} = 600$ V, substrate grounded) for four different ratios of donor compensation $R = C_{Ga}/C_N$ in the GaN:C layer (where C_{Ga} and C_N are the *concentration* of the carbon on a gallium site C_{Ga} and on a nitrogen site C_N, respectively). It can be seen that without donor compensation ($R = 0$), the electrostatic potential drops mainly at the cathode side. This is due to the large concentration of carbon ($\approx 4 \times 10^{19}$ cm^{-3}, based on SIMS measurements) which is defined as a deep acceptor trap and is able to hold an equal amount of space charge. This space charge effectively blocks the extension of the depletion layer into the deeper layers (similar to a conventional heavily doped p^+ region). With increasing donor compensation, not only does the absolute value of the deep acceptor trap density decrease (as the donor compensation is assumed to be C_{Ga} and the total amount of carbon remains constant); but, more importantly, the net negative space charge is reduced. Indeed, since $C_{Ga} < C_N$, the Fermi level is always

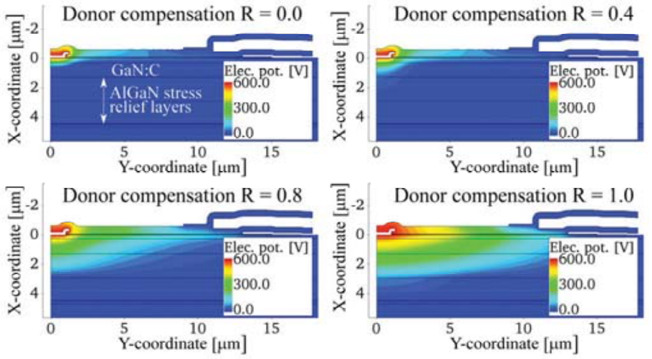

Fig. 3. The electrostatic potential distribution (Elec. pot.) at 600 V for four different ratios of donor compensation in the GaN:C layer. The upper passivation layer (see Fig. 1) has been omitted in these plots (but was simulated). Without donor compensation (top left) the electrostatic potential drops close to the cathode contact – yielding high electric field peaks around the cathode. With donor compensation, the electrostatic potential distribution is able to spread more.

pinned near the C_N level and all C_{Ga} are ionized – i.e., these defects hold positive charge as it is a donor. As a result, the potential drop can spread deeper (analog to a wider depletion region in a more moderately doped p-type region). This has an impact on the 2D potential distribution, also at the surface of the device, which is the most obvious in the full donor compensation case (*R = 1*), where all deep acceptors are compensated by donors and there is no net negative charge possible in the GaN:C. Hence, the potential drop occurs deeper in the epitaxial stack. It is worth noting that the donor compensation also results in a suppression of the 2DHG at the GaN:C/AlGaN interface for donor compensation levels of *R > 0.2*. Since the carbon was not included in the deeper layers, the 2DHGs are still present at the deeper interfaces. This effect is further discussed in the following subsection.

The compensation of the deep acceptor C_N and the suppression of the first 2DHG have a large impact on the potential distribution and the electric field peaks at the surface. Fig. 4 shows the electric field peaks along a cut-line taken in the AlGaN barrier at 600 V reverse bias for the four levels of donor compensation of Fig. 3. The lower compensation levels (*R < 0.4*) yield electric field peaks at the cathode side which are larger than the critical electric field (≈ 4 MV/cm; these simulations were done without avalanche generation). This indicates that with low donor compensation ratios the simulated breakdown voltage should be below 600V, in contrast with the measurements where a hard breakdown well beyond 600 V is observed (Fig. 2).

B. The role of the 2DHGs at the deeper interfaces

2DHGs must exist at the interface between GaN/AlGaN and $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ ($x < y$) layers for Ga face defect-free material due to negative polarization charges at these interfaces and based on the charge neutrality. As the MOCVD grown GaN-on-Si is Ga face with a decreasing Al mole fraction for the stress relief layers from the bottom AlN nucleation layer to the GaN channel, 2DHGs should be present at each interface in the stress relief layer stack (except for AlN/Si, where an electron inversion layer in the Si is formed). However, these 2DHGs can be suppressed if defects are present that trap

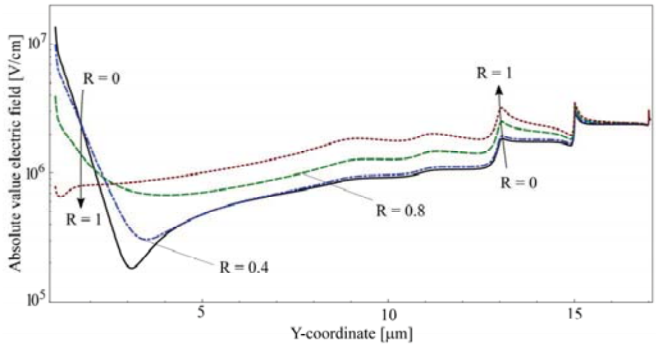

Fig. 4. Absolute value of the electric field along a (surface) cut-line taken in the AlGaN barrier at 600 V reverse bias. The electric field peaks depend on the level of donor compensation.

positive charge. The trap density must be high so as to be able to screen the high polarization charge densities [12][13].

Fig. 5 shows the band diagrams at equilibrium without (*R = 0*) and with full donor compensation (*R = 1*) in the GaN:C layer. These two values illustrate how the Fermi level gets de-pinned from the valence band in case there is donor compensation. Since a large concentration of electrically active carbon is assumed (4 x 10^{19} cm^{-3}), the suppression of the 2DHG happens for values of R > 0.2 (analog to [12], yet here the total carbon density is twice as large). Since no carbon was added in the deeper layers, the Fermi level is still pinned at the valence band for the deeper interfaces, yielding 2DHGs. These 2DHGs also play a role when reverse biasing the device. This can be seen in Fig. 3: the spreading of the potential lines stops at the first interface within the AlGaN stress relief layer stack with a 2DHG (~3 μm deep). The 2DHGs thus act as shields for the extension of the depletion region. This is further illustrated in Fig. 6 where the hole density at 600 V is plotted (same conditions as in Fig. 3). Without donor compensation (*R = 0*) all 2DHGs are still present within the structure at 600 V as the potential drop is provided solely by the deep acceptor C_N in the GaN:C layer. The higher the donor compensation in the GaN:C layer, the more the first 2DHG gets screened, and for full donor compensation (*R = 1*), the deeper 2DHGs (~3 and ~4.5 μm deep) get depleted at 600 V under the cathode side.

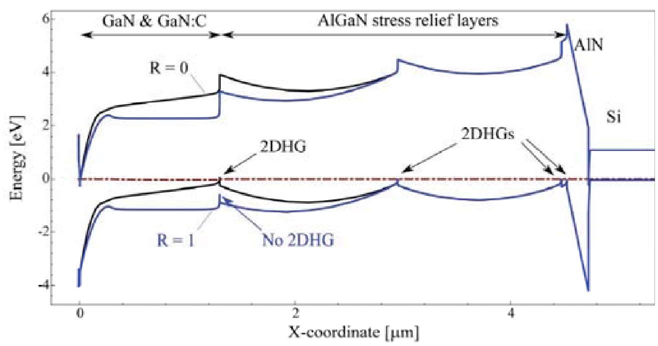

Fig. 5. Band diagrams at equilibrium in the access region (see Fig. 1) for a structure with full donor compensation (*R = 1*) and without donor compensation (*R = 0*) in the GaN:C layer. The 2DHG vanishes at the GaN:C/AlGaN stress relief layer interface for *R = 1*.

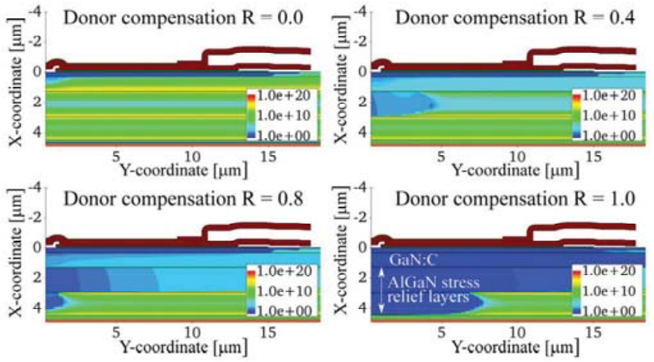

Fig. 6. The hole density (legend is in cm^{-3}) at 600 V for four different ratios of donor compensation in the GaN:C layer. The upper passivation layer (see Fig. 1) has been omitted in these plots (but was simulated). Without donor compensation (top left) the 2DHGs are not yet depleted. With higher donor compensation, the 2DHGs get more and more depleted.

Fig. 7 plots the surface electric field in the AlGaN barrier for a high donor compensation ratio $R = 0.8$ where the carbon was included in the entire stack with concentrations based on SIMS measurements (and compared to the situation of Fig. 4 with donor compensation in the GaN:C layer only). It shows that the incorporation of carbon in the deeper layers still has an influence on the surface electric field peaks. Although the influence on the surface electric field peaks seems small, it was the simulation with the lowest value of donor compensation that did not yield critical electrical fields above 4 MV/cm in the vicinity of the cathode contact for a simulation up to 1 kV – as expected from the measured OFF-state I-V curves (Fig. 2).

C. High donor compensation or electrically inactive carbon

From the above observations we infer that the carbon cannot be incorporated as a deep acceptor trap only and needs to be compensated to a larger amount than assumed until now [11][12], or is less electrically active than expected. The latter would mean that the carbon is not incorporated as C_N or C_{Ga} – e.g. the carbon could be decorating dislocation lines, or the carbon forms complexes with other defects. The formation of large amounts of complexes is unlikely based on density functional theory (DFT) calculations [10] and since no other defect has concentration levels comparable to the one of carbon (with the important exception of the dislocation lines). The exact level of donor compensation (or electrically inactive carbon decorating dislocation lines) is hard to determine and will be the topic of future investigations where e.g. back-gating I-V curves will be calibrated based on these new findings.

IV. Conclusion

In this work we have illustrated, by means of TCAD simulations on Schottky diodes, the impact of the donor compensation of the deep acceptor level C_N and of the 2DHG suppression at the deeper interfaces on the 2D voltage distribution in the device and subsequently on the surface electric field peaks. We conclude that a large amount of the carbon either must be compensated by donors or must be electrically inactive. These observations are important to consider when designing high-voltage GaN-on-Si devices.

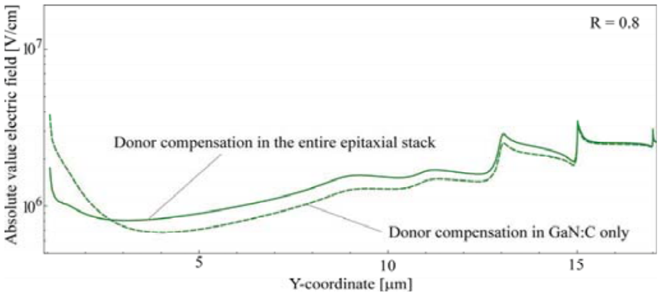

Fig. 7. Absolute value of the electric field along a cut-line taken in the AlGaN barrier at 600 V reverse bias for the case of a donor compansation ratio $R = 0.8$. The electric field peak distribution changes as the carbon is included in the deeper layers or not.

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