Bias-dependence of surface charge at low temperature in GaN Self-Switching Diodes

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***Abstract*—In this work, with the help of a semi-classical two-dimensional Monte Carlo (MC) simulator, we study the DC current-voltage curves of Self-Switching Diodes (SSDs) fabricated on an AlGaN/GaN heterostructure from 100 K up to room temperature. Due to the very narrow channel of the SSDs, the presence of surface effects plays a key role not only on their DC behavior but also on their RF detection performance. The evolution with temperature of the negative surface charge density σ at the etched sidewalls of the SSD is the key quantity to explain the measurements. At 300 K, MC simulations with a constant value of σ are able to replicate very satisfactorily the experiments. However, to reproduce the shape of the *I-V* curve at low temperatures, a more realistic approach, where σ depends not only on *T*, but also on the applied bias *V*, is necessary.**

Keywords—Monte Carlo simulation; Self-Switching Diode; Gallium Nitride; surface effects.

I. INTRODUCTION

In recent decades, numerous efforts have been invested to develop compact semiconductor devices operating at room temperature in the terahertz range, due to their relevance in security, medicine, biology, and science applications [1]. One of the most widely used approaches to reach THz frequencies consists in reducing the size of devices to the nano-scale [2-3]. However, downscaling leads to a high surface-to-volume ratio of devices, their performance being significantly affected by the physical properties of the surfaces. Sidewall surface charge contributes to deplete the conductive channel as a consequence of Coulombian repulsion, resulting in a decrease of the electron density and changes in electron transport [3-5].

Among the electronic detectors able to operate at THz frequencies, Self-Switching Diodes (SSDs) are quite attractive thanks to their planar geometry and design flexibility. SSDs, originally proposed by A. M. Song *et al.* [4], are planar nanodiodes fabricated with a single lithography step, the etching of two L-shaped trenches defining an asymmetric channel, which in turn produces a rectifying behavior. It is worth noting that these devices are extremely affected by surface states, since the etching process originates numerous intermediate surface states at the semiconductor-air interfaces. Despite the above-mentioned problem, the good THz detection capability of SSDs based on several materials, like InAs, InGaAs and GaAs, has been reported [6-8]. Another semiconductor widely used more recently to fabricate microwave detector devices thanks to its good electrical and thermal properties is GaN. Devices fabricated with this semiconductor have exhibited a high responsivity at moderately high frequencies. Not only SSDs [9], but also other similar structures such as gated-SSDs (G-SSDs) [10], gated nanowires field-effect rectifiers (NW-FERs) [11], as well as high-electron mobility transistors (HEMTs) [12].

In this work, we deal with SSDs fabricated in AlGaN/GaN, where the presence of traps has been reported to play an important role, since an appreciable decrease of the current at low temperature is revealed. The characteristic times and energies of such surface states have been determined through impedance measurements [13-14]. The aim of this work is to extend the use of the Monte Carlo (MC) tool to analyze the evolution with temperature of the SSD *I-V* curves from 100 K to room temperature, paying special attention to the modelling of the surface states. Previous works of our group have demonstrated the great usefulness of the MC simulations in explaining the static, dynamic and noise performance of the SSDs [3,15-16].

The outline of this paper is as follows. In section II, the geometry of devices under test and the details about the surface charge models are described. In section III, by comparing at each temperature the experimental *I-V* curves and the MC simulations, we fit the value of σ for each applied bias. In section IV, the main conclusions are drawn.

II. DEVICES AND SURFACE CHARGE MODELS

A. Devices under analysis

The characterized SSDs were fabricated on an $Al_{30}Ga_{70}N$/GaN heterostructure grown on a Si substrate. The epitaxial stack consists of a 25 nm AlGaN barrier on a 1.5 µm GaN buffer. The asymmetric shape of the channel was defined by dry etching. More details about the technological process for the fabrication can be found in [17]. The results shown in this work correspond to an SSD consisting of a single channel, 1 µm long and 80 nm wide (see inset of Fig 1). On-wafer measurements over a temperature range from 100 K to room temperature were carried out using a cryogenic probe station (LakeShore CRX-VF) connected to a Keysight B2900A Source Measurement Unit (SMU), which was controlled via an in-house made LabVIEW code.

B. *Monte Carlo Model*

An in-house-made MC simulator coupled with a two-dimensional (2D) Poisson solver will be employed for the calculations, which has proved to be a powerful tool for simulating a wide range of devices [18-20]. The model considers electron heating, degeneracy and contact injection with appropriate statistics. To account for surface charges, we have used the model known as Constant Charge Model (CCM), which assigns a negative surface charge density σ independent of the position at the etched interfaces. Initially, a bias independent σ is considered. In a second step, the value of σ for each bias (V) and temperature (T) is determined from the fitting of the measured *I-V* curves. Note that the lateral depletion at each side of the channel can be calculated as $W_d=\sigma/N_{Db}$, being N_{Db} (10^{17} cm $^{-3}$) the net background doping assigned to the GaN channel to solve Poisson's equation (while impurity scattering is switched off, see [3] for details). The electron dynamics in the SSD is simulated during a time series of 100.000 steps of 1 fs for each bias point. Simulations have been performed in the same T range as experimental results.

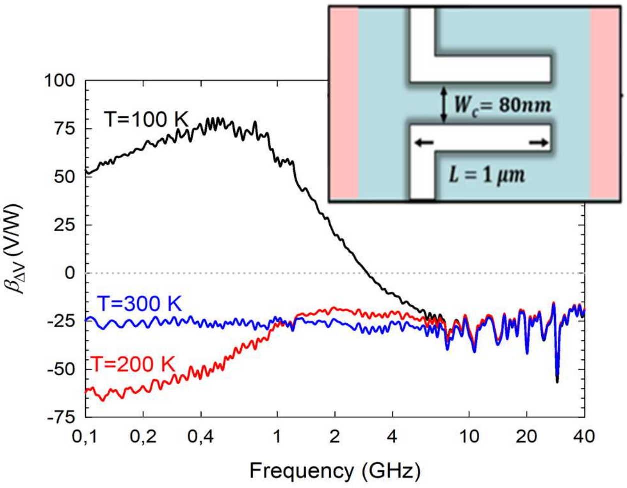

Fig. 1. Zero-bias responsivity, $\beta_{\Delta V}$, as a function of frequency between 100 MHz and 40 GHz for 100 K, 200 K and 300 K. The inset shows the geometry of the SSD under study.

III. RESULTS

The existence of surface states in the device under study is unambiguously evidenced by the presence of undesirable effects on its detection capability. The behavior of the zero-bias responsivity (shown in Fig. 1) with temperature clearly shows the signature of the traps, which originate a change in the sign of the voltage response at the lower measured frequencies when the temperature decreases [13-14].

Since the square law detection of small signals is related to the features of the *I-V* curve, the previous findings suggest the need of a deep analysis of the impact of temperature on the *I-V* characteristic, as shown in Fig. 2. The inspection of the experimental *I-V* curves reveals a surprising decrease of the current (and the consequent increase of the resistance, see the inset) at low T, most likely related to a significant increase of the surface charge at the sidewalls of the trenches. Electrons from the two-dimensional electron gas (2DEG), captured at low temperatures are released when increasing T, thus indicating a thermal activation of the surface traps. According to the electrical measurements of SSDs with different channel widths (W), the value of W_d at equilibrium at 300 K is 18 nm [2], so it is quite reasonable to assume an almost closed channel for the lower temperatures. Another noteworthy point is the sign change in the bowing coefficient ($\gamma=R\cdot\partial^2I/\partial V^2$), represented in the inset of Fig. 2, reflecting the evolution of the *I-V* curve from a concave shape ($\gamma < 0$) to a convex one ($\gamma > 0$) for T above 150 K.

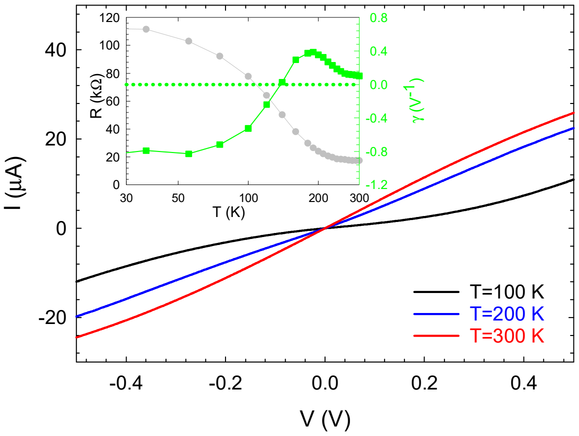

Fig. 2. *I-V* curves of the SSD under test for different temperatures. The inset shows the zero-bias resistance, R, and the bowing coefficient, γ, obtained with the QS model [3].

To get more insight into the experimental results, MC simulations using the CCM for the surface charge have been carried out to reproduce the measurements. As a starting point, the above-mentioned SSD was simulated at room temperature by adjusting the surface charge to the experimental value of $\sigma/q= 18\cdot10^{14}$ m^{-2}. The result was very consistent with the measurements, thus verifying the validity of our approach, see Fig. 3(a). Then, we simulated the diode using different values of the constant surface charge density for each temperature. Circles in Fig. 3 correspond to the simulations using the values of σ which correctly reproduce the zero-bias resistance (σ/q=18, 35 and 39.4×10^{14} m^{-2} for 300, 200 and 100 K, respectively). A fairly good agreement between such MC simulations and the experiments is found in the whole bias range under analysis for T above 220 K, indicating that a constant value of σ is able to correctly reproduce the behaviour of the device. By contrast, for T<220 K, when the channel is nearly closed, a good agreement can only be achieved if a bias-dependent surface charge density is employed. Therefore, a more advanced algorithm reflecting the complex nature of traps occupancy is required. In this case, we fit the value of σ for each applied bias and temperature, i.e. $\sigma = f(V,T)$, which is computed by comparing the experimental *I-V* curve with the simulations made with varying values of $\sigma(V)$ at each T. Therefore, a series of MC simulations with constant σ have been compared with the measured *I-V* curves, so as to straightforwardly estimate the required value of σ to fit the current values at every bias point. The so obtained values of $\sigma(V, T)$ providing the good agreement with the experiments are plotted on the

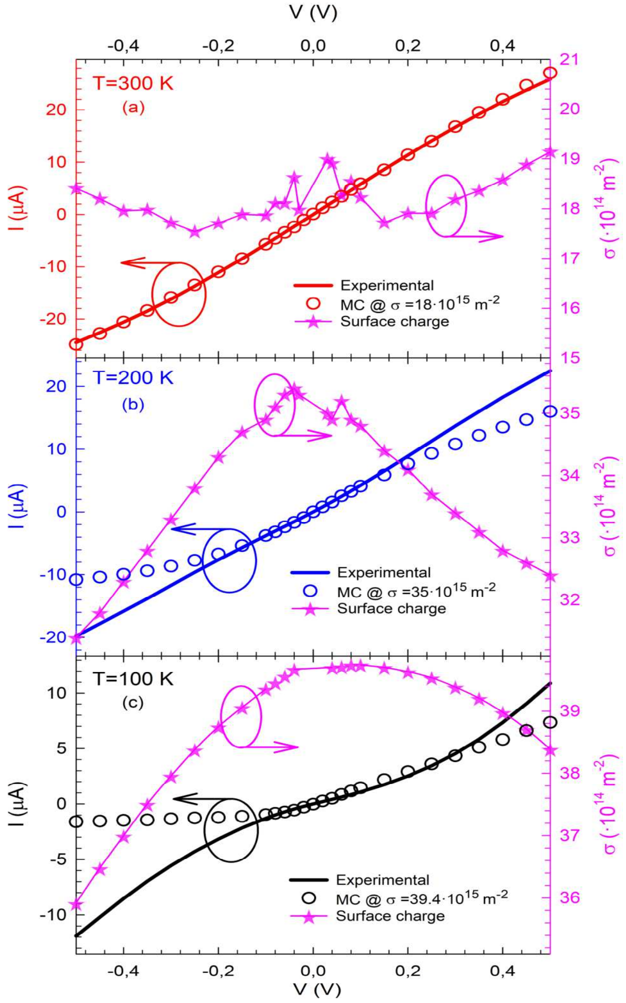

Fig. 3. Comparison of the measured (lines) and MC simulated (circles) *I-V* curves (left axis) for three temperatures (a) 100 K, (b) 200 K and (c) 300 K. Stars (right axis) represent the obtained values of surface charge density as a function of the bias.

right axis of Fig. 3. The surface charge density at equilibrium significantly increases when lowering *T*, additionally exhibiting a parabolic behavior with the applied voltage. These facts again indicate that the occupancy of the surface states depends not only on thermal activation, but also on the applied bias.

To better understand the dependence $\sigma(V,T)$, Fig. 4 shows it in a color map. As expected, $\sigma(V)$ is practically constant for 300 K, for then showing a maximum around zero-bias for lower *T*. It is also remarkable that $\sigma(V)$ is very asymmetric for 100 K (much lower for negative values of the applied voltage, thus making the reverse bias current to be higher than that for forward bias). In fact, this behaviour is at the origin of the change of sign in the responsivity shown in Fig. 1, since it makes the bowing coefficient (inset of Fig. 2) of the *I-V* curve to be negative at low *T* (the curve becomes concave, instead of the typical rectifying convex shape).

IV. CONCLUSIONS

By means of a semi-classical MC simulator, an asymmetric GaN diode, 1 μm long and 80 nm wide, where the presence

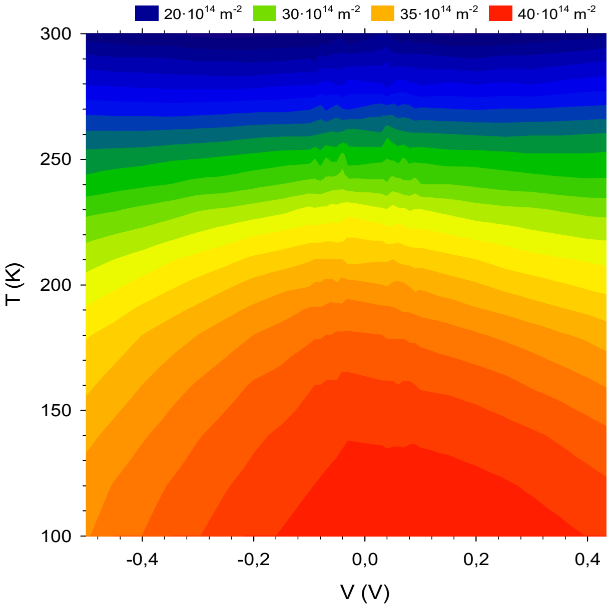

Fig. 4. Surface charge density color map as a function of temperature and applied bias. The lower the temperature the higher the surface charge values.

of surface traps has been proved to play a major role, has been analyzed. Particularly, we have provided an explanation of its *I-V* curves at different temperatures in terms of the evolution of the surface charge density. For *T* above 220 K, a qualitative agreement has been found between the experimental measurements and the simulations obtained with the CCM model. However, for lower temperatures, a new model taking into account the variation of σ with the applied bias is needed, proving that the occupancy of the surface states is temperature and bias dependent. Finally, we have correlated the change of sign in the responsivity and bowing coefficient with the bias dependence of the surface traps.

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