Analysis of the THz Responsivity of AlGaN/GaN HEMTs by means of Monte Carlo Simulations

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Abstract—In this work, by means of Monte Carlo (MC) simulations, the current responsivity of AlGaN/GaN HEMTs operating as zero-bias detectors is analyzed, reaching the THz frequency range. Two approaches are used for the calculation of the responsivity, trying to get physical information on the detection mechanisms from the comparison of their respective results. First, we determine the responsivity directly from the MC values of DC drain current shift originated by an input AC drain voltage excitation. As second approach, the responsivity is estimated from a closed-form expression involving the MC calculation of both the DC I-V curves of the transistor (to determine Taylor expansion coefficients) and the AC response in terms of the Y-parameters (to be converted into S-parameters). Both approaches coincide at low frequency, but the closed-form expression starts to deviate from the correct result at frequencies around 1 THz. Moreover, a modest plasma resonance is visible in the 2-5 THz range.

Index Terms—Monte Carlo Simulations, Analytical model, High-electron mobility transistor (HEMT), GaN, Microwave detector, Power detector, Terahertz (THz) detectors, Responsivity model

I. INTRODUCTION

The field of Terahertz science and technology is gaining international interest due to its broad potential applications, ranging from ultra-high speed wireless communication systems to sensing and imaging for medical diagnostic, industrial quality control, security-screening tools, THz astronomy or pharmacology. As described in the detailed snapshot of the 2017 state-of-the-art THz technologies made in Ref. [1] photonic and electronic approaches compete for conquering the “THz gap” but optical approaches often need for bulky and expensive equipment. Detectors based on different technologies (bolometers, pyroelectric detectors, Golay cells, Josephson junctions, etc.) are available [2], [3], but due to its simplicity, compactness and speed of response, Schottky barrier diodes (SBDs) are presently the benchmarking reference for THz detection [4], even if their sensitivity is not the best (with values of Noise Equivalent Power, NEP, around 250 pW/√Hz in the 1.5 THz range, as compared with the tens of pW/√Hz provided by bolometers). However, the large value of its input impedance when using them as zero-bias detectors poses significant complications for their design, so that other approaches, such as 3-terminal Field-Effect Transistors (FETs), are being explored in the recent years. In fact, apart from their “classical” operation as amplifiers and digital switches, they have demonstrated to provide good performances as THz detectors well above their typical cut-off frequencies \( f_t \) and \( f_{max} \). This is coherent with the fact that, by definition, those cut-off frequencies indicate the limit of operation of transistors as amplifiers (used as a 2 port circuit) under different loads, while when used as THz detectors, the operating conditions are completely different (as well explained in Refs. [5] and [6]), since they act as a one-port circuit, with just one AC input (RF or THz) and one DC output.

At low frequencies, the physical origin of the detection with FETs is a resistive self-mixing mechanism [7], [8], given by the nonlinearity of the \( I_d-V_{ds} \) curves. The frequency dependence can be described using the well-established voltage dependent lumped element modelling by means of a Small-Signal Equivalent Circuit (SSEC). This kind of approach is able to correctly explain the results obtained in graphene FETs up to almost 1 THz [6], and has been helpful for the optimization of the design of the detectors [7]. However, for higher frequencies, the consideration of more complex models is necessary. For example, resonant plasma waves can have a contribution to the detection at THz frequencies, but only to a limited extent (much lower than expected by the Dyakonov–Shur theory) due to the high-frequency dependence of the channel impedance [7], not considered in the ideal plasma-wave models [9]. Another mechanism suggested to be significant at intermediate and high frequencies is the hot-carrier thermoemission process [10], in which thermoelectric emission of electrons above the barrier imposed by the gate potential is able to provide a non-zero drain current, and thus allows for RF detection with FETs. Taking advantage of the better understanding of the FET detection mechanisms and making use of circuit models, the fabrication of THz detectors based on FETs with specific designs (and often with integrated antennae for an improved free-space coupling) have been achieved in the last times [5], [6], [7], [11].

However, a clear understanding of the detection mechanisms in FETs in the whole frequency range is still lacking. Monte Carlo (MC) simulations, containing all the ingredients to tackle...
this problem, have been scarcely exploited so far; only a first attempt to qualitatively study the THz rectification capabilities of InGaAs HEMTs was made by some of the authors in Ref. [12]. In this paper, by means of detailed MC simulations, we will provide a physics-based description of the detection with GaN HEMTs, from low frequency (several GHz) to the THz range, thus allowing to determine up to which frequency the resistive-mixing concept is valid and to which extent the celebrated resonant plasma-wave (together with hot-carrier thermoemission process) enhancement of THz detection is feasible with present technologies. We will make use of the closed-form model developed in Ref. [13] for the case of resistive-mixing detection in order to identify the contribution of this specific detection mechanism. In this way we will be able to compare results on ideal models of a same device simulated in transient and harmonic representation, without focusing on the fitting of experimental results and avoiding discrepancies associated with experimental errors or electrical models used in the measurements.

The organization of this paper is as follows: firstly, the information about the MC simulator and the details of the device under test are provided. Following this, it delves into the description and comparison of the two approaches used for the calculation of the AC responsivity, a direct MC simulation and a closed-form expression based on the $I_d$-$V_{ds}$ curves and the values of the S-parameters of the device. Finally, the paper summarizes the main conclusions drawn from the analysis.

II. MONTE CARLO SIMULATOR AND DEVICE DETAILS

For the simulation, we will use a two-dimensional (2D) semi-classical ensemble MC model self-consistently coupled with the solution of the Poisson equation [14]. The microscopic dynamics of the electron transport is simulated in time steps of $\Delta t=1.0$ fs, where free flights are truncated by scattering mechanisms (considered instantaneous) which change the trajectory and energy of electrons. The scattering mechanisms included in the simulator are: intervalley, acoustic and optical (polar and non-polar) phonons and piezoelectric [15], [16]. At the end of each time step $\Delta t$, the Poisson equation is solved using a mesh size ranging between 0.5 and 5 nm (depending on the electron concentration level), providing the electric field to be taken into account in the next time step in each cell. The Poisson solver makes use of the LU decomposition algorithm [17] in a finite differences approach suitable for non uniform meshes and complicated geometries. In order to correctly take into account the quantum behaviour of the electrons within the 2DEG it would be necessary to solve the Schrödinger equation self-consistently with Poisson equation, and then calculate the sub-bands energy levels and the 2D scattering rates for electrons. The electron confinement also gives rise to other quantum effects such as degeneracy and tunneling from the channel to the gate. However, in order to keep the calculation time at an acceptable level we will make use of a semiclassical MC model which locally takes into account the effect of the degeneracy by using the rejection technique [18], and the rest of quantum effects are not considered. This assumption does not introduce a significant error at room temperature.

Ohmic boundary conditions (following the model presented in Ref. [19]) are considered in the source and drain contacts, which are simulated in vertical position, adjacent to the different material layers. Accordingly, nonuniform potential and concentration profiles are considered along these contacts: those that would be obtained if real top electrodes were simulated [20], [21]. These profiles are calculated from a separated simulation at equilibrium and are applied for every biasing. The Schottky gate is simulated as a non-injecting, perfectly absorbing contact. The conduction band of GaN (Wurtzite crystal structure), AlGaN and AlN are modelled by three non-parabolic spherical valleys ($\Gamma_1$, $U$ and $\Gamma_3$). The classical laws of conservation of total energy and momentum perpendicular to the heterojunctions are used for modelling the electron transfer at the heterolayers. If the normal energy is enough to jump over the barrier, the carrier has a transmission coefficient of 1, in other case it is specularly reflected; quantum reflection and tunneling are not considered. In this kind of processes it is assumed that the electron does not change
of valley, since the important variation of momentum which implies an intervalley transition becomes improbable. The conduction band discontinuities imposed at the AlN/GaN, AlGaN/AlN, and GaN/AlGaN heterojunctions are, 1.57 eV, 1.1 eV and 0.47 eV, respectively. More details about the model and the parameters used in the MC simulations can be found in Refs. [15], [22], [23].

The topology of simulation domain, depicted in Fig. 1(a), reproduces that of the real device as closely as possible. However, in order to optimize the computation time the source and drain contacts are simulated as vertical interfaces with adequate injection and potential profiles [24], [25], and the simulated source-gate region has been reduced to 300 nm instead of 600 nm (it is just an ohmic region, whose influence can be analytically included in a post-processing stage). The mesh to solve the Poisson equation consists of 56 rows and 240 columns, having a total number of 13,440 cells. Finally, in order to reproduce electron mobility in the channel (1800 cm² V⁻¹ s⁻¹), dislocation and roughness scattering at the AlGaN/GaN heterointerface have also been considered [16], [26].

The GaN HEMT studied in this paper is based on a AlGaN/GaN heterostructure with a 14 nm thick Al₀.₂₅Ga₀.₇₅N layer, a 1.0 nm AlN spacer and a 0.5 nm GaN cap, the same used in [16], [27], whose fabrication was explained in [16], [28]. The material parameters used in the simulation of the GaN cap are the same as those used for the channel, even if some deviation is expected due to its small thickness. In any case this layer is completely depleted, so that its influence is not significant. The C-doping used in the bottom GaN layer in order to provide a better confinement of electrons near the heterojunction [27] has been included in the simulations by considering a p-type doping with N_A=10¹⁷ cm⁻³. To ensure an accurate simulation of such epitaxial structure, we add surface charges reproducing the effect of spontaneous and piezoelectric polarization at every heterojunction [29], [30], [31], denoted as P_A, P_B and P_C (located at the GaN/AlGaN, AlGaN/AlN and AlN/GaN heterojunctions with values of -2, -2 and 15×10¹² cm⁻², respectively, see Fig. 1(a)). Additionally, a surface charge density \( \sigma = -1 \times 10^{12} \, \text{cm}^{-2} \) is added at the top of the cap GaN layer. As a consequence, the charge-neutrality condition at equilibrium \( P_A + P_B + P_C + \sigma - n_s = 0 \) provides the experimental value for the electron sheet charge density in the 2DEG \( n_s = 10^{13} \, \text{cm}^{-2} \).

MC simulations of the intrinsic device shown in Fig. 1(a) are able to very closely reproduce the extrinsic \( I_d-V_{ds} \) curves of a real 150 nm-gate GaN HEMT with \( 2 \times 25 \, \mu \text{m} \) width, Fig. 1(b), by analytically including the effect of the extrinsic resistances and the Schottky barrier height [32]. In the following we will present the results of the simulations of the intrinsic device (the inset of Fig. 1(b) shows the intrinsic \( I_d-V_{ds} \) curves), since the effect of the parasitic resistances and capacitances, which are quite significant, should be studied separately.

## III. RESULTS AND DISCUSSION

### A. AC Power Detection: Direct Monte Carlo Simulations

Time-domain MC simulations allow to directly reproduce the AC power detection experiments by applying a sinusoidal voltage signal with frequency \( f \) to the gate or drain terminals (leading to gate-injection, GI, or drain-injection, DI, modes, respectively) and taking the short-circuited drain current as output signal. This zero-bias detection conditions (in absence of drain bias) are the optimum ones for improving the low-noise operation of the detectors, and therefore their sensitivity, due to the suppression of the low frequency (mainly 1/f) noise appearing when the drain is biased. In this paper we will focus on DI in order to avoid the low-frequency dependence displayed by the GI case [27]. Fig. 1(a) shows a sketch of such simulation scheme.

The responsivity within this DI zero-bias current-mode detection scheme, \( \beta_{d, opt} \), is calculated directly using MC simulations by computing the DC average of the drain current, \( \bar{i}_d \), when a single tone voltage signal \( v_{AC}(f) \) with amplitude 0.25 V is applied to the drain terminal, see Fig. 1(a), as:

\[
\beta_{d, opt}(f) = \frac{\bar{i}_d(f)}{P_{AC}(f)}, \quad (1)
\]

where \( P_{AC} \) is the AC power absorbed by the device. \( \bar{i}_d(\Gamma) \) is computed within the time domain MC simulation as the instantaneous drain current provided by the MC simulation).

The previous calculation provides the optimum responsivity of the detector assuming a perfect impedance matching with the AC power source. However, in real-world experiments the impedance of the source, \( R_0 \), is significantly lower than that of the transistor (mainly for \( V_{gs} \) near pinch-off). As a result, in order to extract the practical value of the responsivity we have to take into account the reflection coefficient at the input port (i.e. the drain, since DI is considered here), \( \Gamma_d(f) \). The expression for this mismatched value of the DI responsivity, \( \beta_d \), is given by:

\[
\beta_d(f) = \beta_{d, opt}(f) \left( 1 - |\Gamma_d(f)|^2 \right) \quad (2)
\]

where \( \Gamma_d \) is not just the \( S_{22} \) parameter of the transistor, but depends on both the S-parameters of the device and the load connected to the gate terminal [33], since

\[
\Gamma_d(f) = \frac{S_{22} - \Delta S \Gamma_L}{1 - S_{11} \Gamma_L}, \quad (3)
\]

being \( \Gamma_L \) the reflection coefficient of the load, and \( \Delta S = S_{22} S_{11} - S_{21} S_{12} \). In the case when the gate is connected to a \( R_0 \) load, \( \Gamma_L = 0 \) and simply \( \Gamma_d = S_{22} \), but for a short-circuited gate (as in MC simulations), \( \Gamma_L = -1 \) and \( \Gamma_d \neq S_{22} \). Thus, the direct calculation of the responsivity using MC simulations, \( \beta_{d, MC} \), is the following:

\[
\beta_{d, MC}(f) = \beta_{d, opt}(f) \left( 1 - \frac{S_{22} - S_{12} S_{21}}{1 + S_{11}} \right)^2 \quad (4)
\]

The S-parameters can be obtained from MC simulations (as explained later) using the well-known two-port conversion...
From now on we will focus on the $V_{gs}$ range where maximum responsivity is achieved, between -4.5 and -3.5 V, the gray shaded region in Figs. 2(a) and (b). The frequency dependence of $\beta_d^{MC}$, shown in the inset of Fig. 2(a), displays a low-frequency plateau up to around 100 GHz followed by steep roll-off, regardless of the gate bias. At THz frequencies a sign change, with a relatively significant peak at around 4-5 THz (visible mainly at intermediate values of $V_{gs}$) may indicate the presence of a plasma resonance [12].

**B. AC Power Detection: Analytic Formalism Based on $I_d$-$V_{ds}$ Curves and S-parameters**

If one defines the Taylor coefficients, $g_{ij}$, of the $I_d$-$V_{ds}$ curves as:

$$g_{ij} = \frac{\partial^{(i+j)} I_d}{\partial V_{gs}^i \partial V_{ds}^j} ,$$

whose values are shown in Fig. 2(b), one can easily obtain the expected value for $\beta_d$ at low frequency [27] using eq. (2) and knowing that $\beta_{d,opt}(0)=g_{02}/2g_{01}$, and using $\Gamma_d(0)=R/(R+R_0)$, being $R$ the resistance of the device (note that $g_{01}=g_{d1}/R$, with $g_d$ the drain dynamic conductance). As observed in Fig. 2(a), the prediction of such simple quasi-static (QS) model for the detection based on the nonlinearity of the $I_d$-$V_{ds}$ curves perfectly agrees with the low frequency value of $\beta_d$ obtained directly with the time-domain MC simulations.

In order to generalize the previously used quasi-static model for AC power detection and analytically obtain the frequency dependent value of $\beta_d(f)$, we have recently developed (see Ref. [13]) a formalism which provides its value taking as a base the second order Taylor coefficients, $g_{ij}$ (assumed to be frequency independent), where the frequency dependence is included by means of the two-port $S_{ij}(f)$ parameters. The closed-form (CF) expression for the DI current responsivity $\beta_d^C(f)$ in A/W is given by:

$$\beta_d^C(f) = \frac{R_0}{2} \left( g_{20} S_{12}(f)^2 + g_{02} |1 + S_{22}(f)|^2 \right) + 2g_{11} R \left[ S_{12}(f)[1 + S_{22}(f)] \right] \left[ \beta_{DP}(f) \right],$$

being $R_0$ the characteristic impedance of the transmission line, typically 50 Ω. This CF expression for the responsivity was obtained in [13] assuming that both drain and gate ports are connected to $R_0$ loads, as happens in the experiments. However, if the gate is connected to a different load, the $S$-parameters to be included in the CF expression are those corresponding to the association of the device with its termination ($S$-matrix) [33].

The first term in eq. (6) is null, because $g_{20}=0$ for zero-biased drain (since $\forall V_{gs}, I_d(V_{gs}, V_{ds}=0) \approx 0$), so that it can be discarded. The third contribution to $\beta_d^C(f)$, proportional to $g_{11}$, $\beta_{DG}$, is associated to the gate-drain coupling and therefore is null at $f=0$, so that the QS case explained before is recovered, since, regardless of the value of $\Gamma_d$, $S_{12}=S_{21}=0$ for a FET at low frequency, and the equality $R_0[1+\Gamma_d(0)]^2=R[1-\Gamma_d(0)^2]$ holds [13]. Indeed, the QS equation from Y to S matrix considering a load impedance of $R_0=50\Omega$ [34].

Fig. 2(a) shows the dependencies on frequency and $V_{gs}$ of the simulated responsivity of the GaN HEMT obtained directly from MC simulations by applying eq. (2). As expected, $\beta_d^{MC}$ shows always negative values with a maximum in $V_{gs}$ (of about -2.3 A/W) located just above the threshold voltage (with an intrinsic value of around -4.6 V), following the behaviour typically obtained in the detection experiments realized with a wide variety of FETs [7], [9], [10], [27], [13]. Using these values of responsivity one can extract the optimum value of the intrinsic NEP, which is around 4.3 pW/√Hz. The intrinsic value of $\beta_d^{MC}$ obtained with the MC simulations is significantly higher than that obtained in the experiments made with a real device (with maximum values around 1.5 A/W, see [27]), while that of the intrinsic NEP is only slightly lower (minimum of 4.5 pW/√Hz). This happens because the extrinsic contact resistances lead to a significant decrease of the device nonlinearity, which is in part counteracted by a larger resistance (thus providing a lower noise power).
model is just a particular case of this general frequency-dependent formalism.

The frequency dependent S-parameter matrix of the device to be included in eqs. (4) and (6) can be straightforwardly obtained from MC simulations by computing its complex Y-parameters, $Y_{ij}$, defined as:

$$
\tilde{i}_1 = Y_{11} \tilde{v}_1 + Y_{12} \tilde{v}_2 \tag{7}
$$

$$
\tilde{i}_2 = Y_{21} \tilde{v}_1 + Y_{22} \tilde{v}_2
$$

being $\tilde{i}_1$ and $\tilde{i}_2$ ($\tilde{v}_1$ and $\tilde{v}_2$) the gate and drain complex representation of the AC currents (voltages), respectively. This is the natural outcome in the case of MC simulations, where voltage sources are used and the current is the output magnitude. In order to compute the values of $Y_{ij}(f)$, a single-tone voltage signal with varying frequency is first applied to the gate terminal (port 1) and the drain and gate currents are recorded in order to extract the complex values of $Y_{11}(f)$ and $Y_{21}(f)$. The same is done for $Y_{12}(f)$ and $Y_{22}(f)$ by applying an AC voltage to the drain contact. The values of the real and imaginary parts of $Y_{ij}(f)$ for different values of $V_{gs}$ are shown in Fig. 3 (note that $Y_{21}(f)=Y_{12}(f)$ in unbiased-drain conditions, as in any passive network). As expected, at low frequency a purely capacitive value is obtained for the gate admittance $Y_{11}$ (related to the gate-source and gate-drain capacitances, $C_{gs}$ and $C_{gd}$, respectively), while the drain admittance $Y_{22}$ displays a plateau in the real part (corresponding to $g_d=g_{02}$). At higher frequencies, above 100 GHz, the capacitive effects are predominant. Finally, at THz frequencies the well known plasma effects [12] are evident, providing resonances in all the Y parameters at around 1-2 THz (leading to a maximum in the real part and a zero-crossing in the imaginary part).

In order to analyze the frequency dependence of the responsivity according to eq. (6), the values of the factors $DD(f)=|1 + S_{22}|^2$ and $DG(f)=\Re[S_{12}^*(1 + S_{22})]$, involved in the formula providing the direct-drain, $\beta_{DD}$, and drain-gate coupling, $\beta_{DG}$, detection terms (proportional to $g_{02}$ and $g_{11}$, respectively) are plotted in Fig. 4. The first, $\beta_{DD}(f)$, displays a low-frequency plateau followed by a roll-off starting at frequencies below 100 GHz. On the other hand, $\beta_{DG}(f)$ is null at low frequency and increases in parallel to the decrease of $\beta_{DD}(f)$, peaking at about 200 GHz for low $V_{gs}$, while...
it monotonically increases up to THz frequencies for high $V_{gs}$. Since $g_{02}$ takes always negative values while $g_{11}$ is positive, both frequency dependencies add up to produce a significant decay in the DI responsivity already evident below 100 GHz, as observed in the symbols of Fig. 5(a). Moreover, since parasitic effects are not considered in these simulations, this cutoff frequency is much higher than that found in the measurements, which is below 10-20 GHz [13].

In Fig. 5(a) we compare the results obtained for $\beta_d^{CF}(f)$ using the analytic expression of eq. (6) (symbols) based on the DC curves and $S$-parameters of the device and those computed directly with MC simulations (lines) using the averaged DC drain current, $\beta_d^{MC}(f)$ of eq. (4). The first interesting observation is that the low-frequency roll-off is much different due to the fact that MC simulations of the detection do not account for the drain-gate coupling mechanism, as the gate terminal is RF grounded (the electric potential of the gate terminal is fixed to the static value of $V_{gs}$). As such, the correct quantity to compare with the direct result of the simulations is the value of the CF expression of eq. (6) but using the $S'$-matrix of the device terminated with a short-circuited gate, $S^{'N}$. In this case, $S_{12}^{sh} = 0$ (so that the term on $g_{11}$ vanishes) and $S_{22}^{sh} = S_{22} - S_{12}S_{21}/(1 + S_{11})$, see eq. (3), thus providing the responsivity with short-circuited gate $\beta_d^{CFsh}(f)$ as:

$$\beta_d^{CFsh}(f) = \frac{R_0}{2} g_{02} \left| \frac{1}{1 + S_{22}^{sh}} \right|^2 = \frac{R_0}{2} g_{02} \left| \frac{S_{12}S_{21}}{1 + S_{11}} \right|^2.$$  

(8)

Figs. 5(b) and (c) show a very good agreement in the low frequency region (below 1 THz, approximately) between the MC results and the values of $\beta_d^{CFsh}(f)$.

Another very significant conclusion of this comparison is that, even if eq. (6) predicts an important enhancement of the responsivity at THz frequencies due to plasma effects, direct MC simulations show that it is very small, and the expected resonant plasma detection almost vanishes (even if a slight increase is observed in the 4-5 THz range, surprisingly taking positive values). These results also indicate that the resistive self-mixing mechanism described by the closed-form expression of eq. (6) appears to be at the origin of the detection at frequencies even approaching 1 THz, while plasma/thermoemission effects, clearly visible in the $Y$ parameters of Fig. 3, have a significant influence at frequencies above that range. We attribute the discrepancy between the MC results and the prediction of the closed-form expression to the assumption of real and frequency-independent values of the $g_{ij}$ coefficients. The frequency dependent nonlinearity and the possible phase shift between the voltage excitation and the current response should be taken into account in the model through complex frequency dependent $g_{ij}$ coefficients.

IV. Conclusion

We have performed MC simulations of AC power detection by AlGaN/GaN HEMTs in drain injection configuration. The simulator has been calibrated by comparison with measurements, achieving a very good fitting of the output characteristics of a 150 nm-gate transistor with $2 \times 25 \mu m$ width. Direct MC calculations of the zero-bias drain current responsivity of the device to AC power reaching the THz range $\beta_d(f)$ have been compared to an estimation obtained by means of a closeform model based on a second-order Taylor series expansion of the output current, with static coefficients calculated from the DC curves and the frequency dependence included by means of the $S$-parameters (obtained from the MC simulation of the $Y$-parameters). This last approach allows identifying the direct-drain and drain-gate coupling contributions to the responsivity and its frequency dependence.

The agreement between the direct MC calculation of the responsivity and the Taylor-based estimation using constant $g_{ij}$ coefficients is remarkable up to frequencies reaching 1 THz. At frequencies beyond that range, the calculated $Y$ and $S$ parameters exhibit plasma resonances which, been present in the values of $\beta_d^{CF}(f)$ estimated with the closed-form model, do not appear in the direct MC calculations $\beta_d^{MC}(f)$, what
indicates that the static approach used for the calculation of the Taylor coefficients is not valid at such high frequencies.

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