

Influence of Schottky Diode Modelling Under Flat-Band Conditions on the Simulation of Submillimeter-Wave Mixers

José V. Siles¹, Jesús Grajal¹ and A. di Carlo²

¹Dep. de Señales, Sistemas y Radiocomunicaciones, Universidad Politécnica de Madrid, E.T.S.I. Telecomunicación, Ciudad Universitaria s/n, 28040 Madrid, Spain, e-mail: {jovi, jesus}@gmr.ssr.upm.es, tel: +34 91.336.73.58

²Dip. di Ingegneria Elettronica, Università degli Studi di Roma “Tor Vergata”, Via del Politecnico 1, 00133 Roma, Italy e-mail: aldo.dicarlo@uniroma2.it

Abstract — Flat-band conditions are usually reached in submillimeter-wave Schottky diode-based mixer operation. Numerical drift-diffusion (DD) models with conventional boundary conditions, which are based on the thermionic emission theory, do not correctly predict the behaviour of Schottky diodes under flat-band conditions so mixers performance cannot be accurately estimated. We employ a Monte Carlo simulator to analyze the performance of GaAs Schottky diodes in this operation regime. The results are employed for the refinement of DD model in the epitaxial layer. This new model is able to accurately predict the performance of submillimeter-wave mixers.

I. INTRODUCTION

Harmonic balance simulators employing numerical physics-based models for Schottky diodes have shown very good results for the analysis and optimization of submillimeter-wave multipliers [1] and they might represent the best alternative for the design and optimization of Schottky mixers at millimeter and submillimeter-wave bands. These mixers usually reach the flat-band operation regime. Thus, an accurate modelling of the diodes under these conditions [2] is required.

When employing traditional drift-diffusion diode models to simulate Schottky mixers at and beyond flat-band voltages, important discrepancies appear between measurements and simulations. These discrepancies consist of an anomalous increase in the simulated conversion loss when flat-band voltages are reached (Fig. 1). Thus, physics-based drift-diffusion Schottky models must be refined in order to correctly simulate submillimeter-wave mixers. For this task, a deeper understanding of the transport phenomena through the Schottky barrier is required.

We have analyzed the response of typical Schottky diodes employed for submillimeter-wave applications by means of a Monte Carlo (MC) simulator [3]. We have found an excellent agreement between drift-diffusion results and Monte Carlo results below flat band conditions for different physical parameters as the charge concentration, the electric field and the electron velocities. However, beyond flat-band voltages, important differences appear due to non-local transport phenomena [4]. Monte Carlo results will be employed for the refinement of the DD model for GaAs Schottky diodes under flat-band conditions. The aim of this work is to provide an accurate

numerical modelling for Schottky diodes beyond flat-band. This is a key point for an accurate analysis of the performance of Schottky diode-based mixers at millimeter and submillimeter-wave bands.

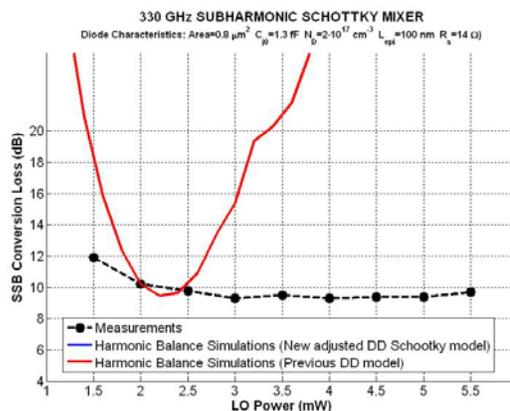


Fig. 1: Comparison between measurements and simulations (including drift-diffusion Schottky diode models) for a 330 GHz SHP mixer fabricated at the Observatory of Paris [5].

II. DESCRIPTION OF THE SIMULATION TOOLS

a. Mixer CAD Tool

The numerical CAD tool employed in this work couples a external circuit simulator with a physics-based drift-diffusion (DD) model of the Schottky diode by means of multi-tone Harmonic Balance (HB) techniques [6]. The Almost Periodic Fourier Transform (APFT) is utilized to perform the time-to-frequency transforms. Thus, no assumptions are made regarding the LO and RF power levels.

The Schottky diode DD model accounts for the most important transport phenomena at the interface: barrier lowering, tunnelling, velocity saturation.

b. Monte Carlo simulator for Schottky diodes

Our Monte Carlo (MC) simulator has been developed at the “Tor Vergata” University in Rome (Italy) [3]. It consists of a band structure with three valleys at the conduction band (the central valley ‘T’ and the two

satellite valleys ‘L’ and ‘X’), and three valence bands (heavy-holes, light-holes and spin-orbit). Spherical constant-energy surfaces are assumed and non-parabolicity correction factors are applied for the calculations [3].

The following scattering events are included in the MC simulator: acoustic phonon interaction, polar-optical phonon interaction, electron-plasmon interaction, impurity scattering, electron-hole scattering, intervalley scattering and impact ionization.

III. SCHOTTKY DIODE MODELLING UNDER FLAT-BAND CONDITIONS

a. Focusing the problem

In order to focus the problem concerning the anomalous increase of the simulated conversion loss of Schottky mixers, we firstly compared the I-V curves obtained with DD simulation and MC simulation for a Schottky diodes with similar characteristics to the one employed in the 330 GHz mixer [5]. The Schottky diodes analysed in this section has the following parameters: A 90 nm epilayer with doping concentrations varying from $1 \cdot 10^{16} \text{ cm}^{-3}$ to $1 \cdot 10^{18} \text{ cm}^{-3}$, anode area of $0.9 \mu\text{m}^2$, and a $4 \cdot 10^{18} \text{ cm}^{-3}$ doping in the substrate (the length of the substrate has been reduced to 30 nm to speed up the MC simulations).

It can be appreciated in Fig. 2 that an early saturation of DC current occurs according to DD results when compared to MC results. However, for DC voltages below flatband ($\sim 0.95 \text{ V}$) both simulation results agree very well. It has been also checked that the increase in the simulated conversion loss of the 330 GHz mixer (Fig. 1) starts at the LO power for which the peaks of the voltage swing in the diodes reach flat band voltages.

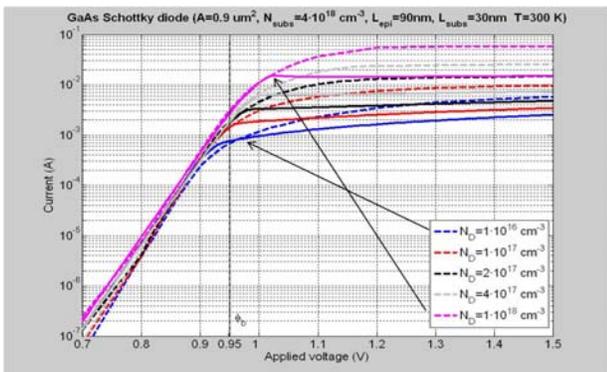


Fig. 2: Schottky diode I-V curves as a function of epilayer doping obtained by Monte Carlo simulation (dashed lines) and drift-diffusion simulation (solid lines). ϕ_b represents the ideal Schottky barrier height.

The DD results for the internal distributions of the Schottky diodes are also in a big disagreement with MC results beyond flat band voltages. In Fig. 3 it can be noticed that an important increment in the electron concentration is predicted by MC in the vicinity of the

Schottky contact under flatband conditions. On the contrary, DD predicts a homogeneous increment of the electron concentration throughout the epilayer. Discrepancies between MC and DD can be also appreciated in Fig. 4 for the electric field profiles.

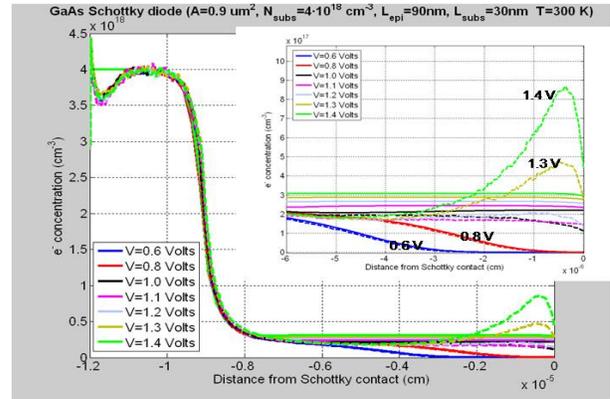


Fig. 3: Doping concentration as a function of the distance to the Schottky contact at different bias voltages. Monte Carlo simulations (dashed lines) and drift-diffusion simulations (solid lines). Epilayer doping is $N_D = 2 \cdot 10^{17} \text{ cm}^{-3}$.

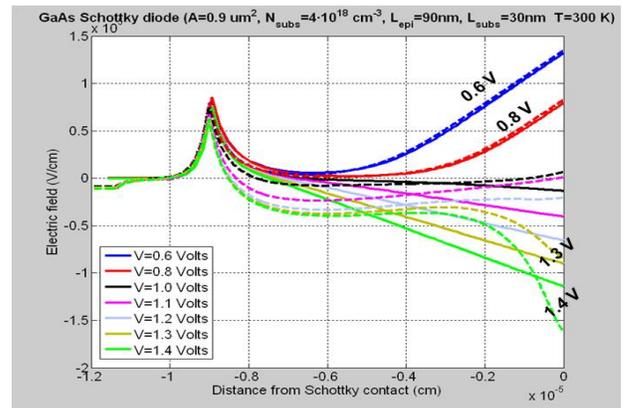


Fig. 4: Electric field as a function of the distance to the Schottky contact at different bias voltages. Monte Carlo simulations (dashed lines) and drift-diffusion simulations (solid lines). Epilayer doping is $N_D = 2 \cdot 10^{17} \text{ cm}^{-3}$.

b. Analysing the problem

The study of the internal distributions (electron velocities, electron distributions, populations of different valleys, electric field profiles, etc.) by means of MC simulation give us a physical insight on the limitations of DD and the modifications to be included in the DD formulation to overcome some of these limitations, especially at the Schottky contact.

Figure 5 shows a peak in the velocities predicted by the MC simulator just after reaching flat-band conditions. This peak does not appear in DD simulations.

The physical justification of this velocity overshoot can be deduced from Monte Carlo simulations (M. Lundstrom in [4]): When flatband voltages are reached, electron

population in the Γ valley grows as the electric field increases and electrons gain energy rapidly. The maximum occupation in the Γ valley corresponds to the peak of velocity (Figs. 5 and 6), and the dominant scattering mechanism is the optical phonon scattering. However, when electrons exceed a certain energy (0.3 eV for GaAs), intervalley scattering starts to dominate and the occupation in the satellite valleys (L and X) rises. Hence, velocity drops because of the higher effective mass of electrons in these valleys.

An analogous effect occurs for the recombination velocity at the Schottky contact. MC results showed a recombination velocity twice higher than that shown in Fig. 5. This is due to the hemi-maxwellian velocity distribution in the vicinity of the Schottky junction [7]. The classical formula for the recombination velocity given by Crowell and Sze [8], typically used in drift-diffusion models, does not predict either the increment of the electron velocity by a factor of 2, or the existence of the velocity peak.

The last analysis performed consisted of comparing the mobility curves obtained with both MC and DD models. Fig. 7 shows the mobility near the Schottky junction for different doping levels. It can be noticed that MC and DD results agree well below flatband voltages (corresponding to positive electric fields in Fig. 7). However, beyond flatband, the MC mobility drops at higher electron fields due to the peak in the average electron velocity. Furthermore, the field-dependent mobility depends on the distance to the Schottky junction as shown in Fig. 8.

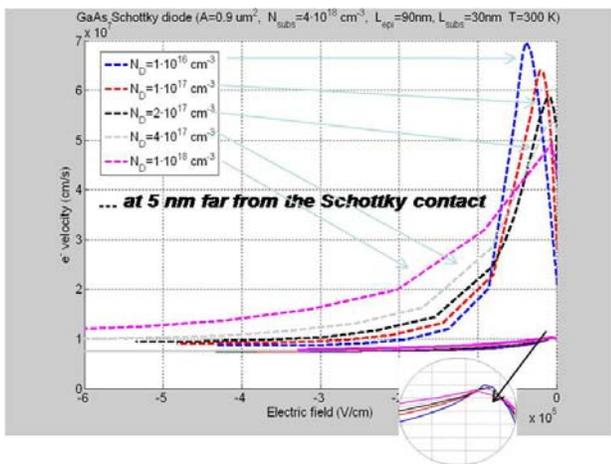


Fig. 5: Electron velocity as a function of the electric field for different epilayer dopings. Monte Carlo simulations (dashed lines) and drift-diffusion simulations (solid lines). Electric field is negative beyond flatband.

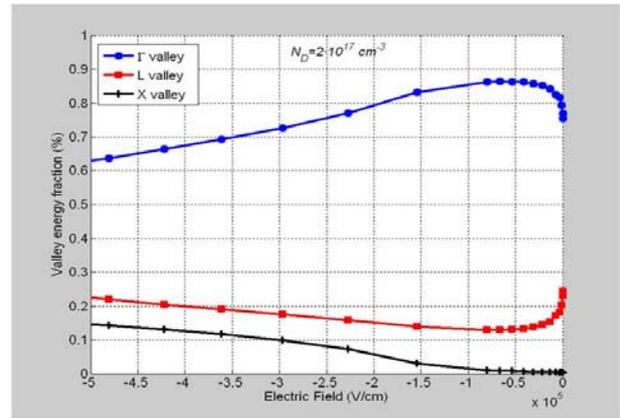


Fig. 6: Valley population (obtained by Monte Carlo simulations) as a function of the electric field. Epilayer doping is $N_D=2 \cdot 10^{17} \text{ cm}^{-3}$.

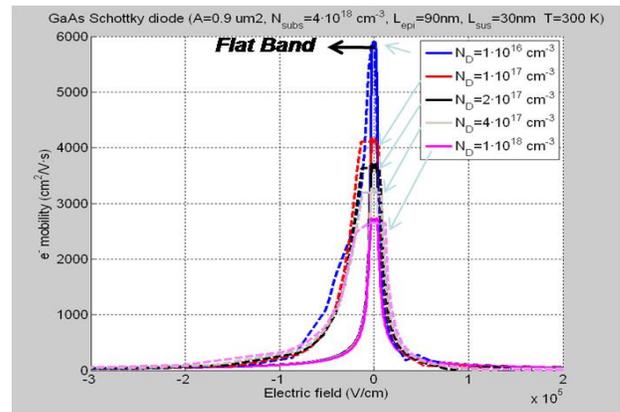


Fig. 7: Electron mobility as a function of the electric field for different epilayer dopings. Monte Carlo simulations (dashed lines) and drift-diffusion simulations (solid lines). Electric field is negative beyond flatband.

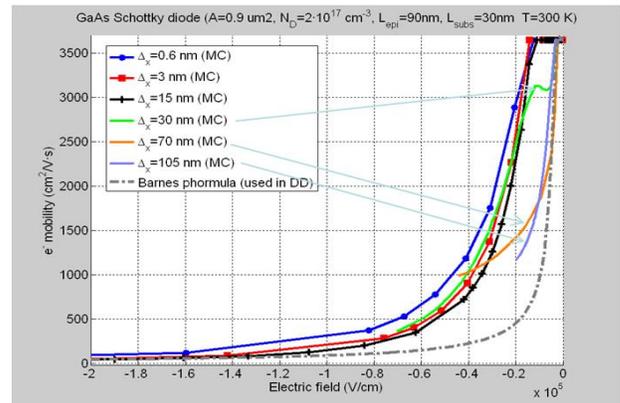


Fig. 8: Monte Carlo electron mobility as a function of the electric field and the distance to the Schottky contact. Results are compared with the traditional DD mobility (Barnes phormula [9]).

c. Solving the problem

The last step of this work was to refine our DD Schottky diode model by using the MC results previously discussed. A new recombination velocity at the Schottky contact, obtained from MC simulations, was defined in order to take into account that effect of the intervalley transitions. Also, a new field-dependent mobility characteristic as a function of the doping level, the distance to the Schottky contact and the epilayer length has to be set in the DD model. The most accurate modeling should define a different mobility at each position in the Schottky diode. However, it is enough to define two regions in the epilayer. The regions are indicated in Fig. 9. The first region is characterized by an almost constant electric field for a given voltage, and therefore, the mobility in this region can be assumed to be constant. In the second region close to the Schottky contact, the mobility predicted by MC is far from the mobility expression given by Barnes [9] (see Fig. 8). The field-dependent mobility characteristic to be used in DD is derived from MC results by assuming a negligible effect of diffusion (that is, drift velocity is dominant and velocity can be written as the product of mobility and electric field). Next, this mobility is slightly tuned to improve the agreement between MC and DD internal distributions.

Further analyses are being carried out to obtain a general rule for automatic segmentation of the epilayer for which different mobility characteristics are employed.

The results after the corrections on the DD model are shown in Figs. 9 and 10. The early saturation of the current that was shown in Fig. 2 is also corrected and the new I-V curves obtained with the adjusted DD model match pretty well the MC results.

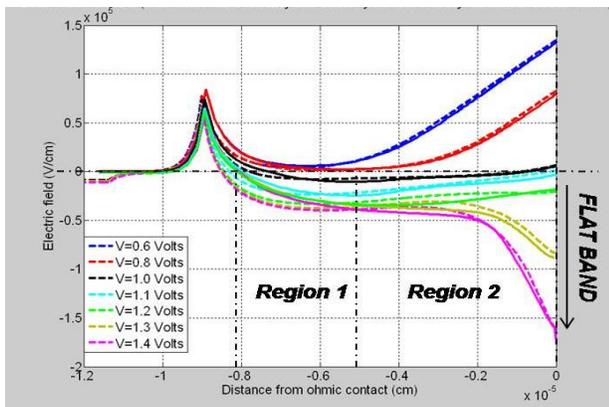


Fig. 9: Electric field as a function of the distance to the Schottky contact at different bias voltages. Monte Carlo simulations (dashed lines) and drift-diffusion simulations (solid lines). Epilayer doping is $N_D=2 \cdot 10^{17} \text{ cm}^{-3}$.

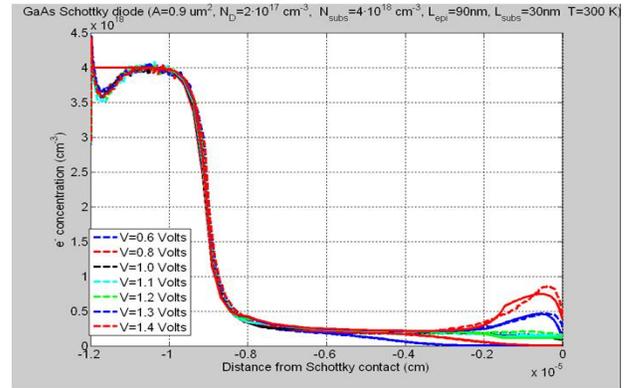


Fig. 10: Doping concentration as a function of the distance to the Schottky contact at different bias voltages. Monte Carlo simulations (dashed lines) and drift-diffusion simulations (solid lines). Epilayer doping is $N_D=2 \cdot 10^{17} \text{ cm}^{-3}$.

III. 330 GHz SHP MIXER SIMULATION

Harmonic Balance simulations of the 330 GHz SHP Schottky mixer described in [5] were performed with the new DD model for the Schottky diode. The Schottky diode employed in the design and fabrication of the mixer is the *SDIT7-D20* from the University of Virginia. The characteristics of this diode (provided by the University of Virginia) can be found in [5]: An epitaxial layer of 100 nm, an anode area of $0.9 \mu\text{m}^2$, an epilayer doping of $2 \cdot 10^{17} \text{ cm}^{-3}$, a built-in potential of 0.72 Volts, a zero junction capacitance of 1.3 fF and a series resistance of 11-15 Ω .

The DC analysis of the diode showed a series resistance of 14 Ω and a 1.3 fF zero junction capacitance, C_{j0} , that are in good agreement with the nominal values specified by the University of Virginia. The optimum impedances employed in the simulation were optimized at a 1.5 mW LO power in absence of parasitics: $Z_{RF}=77+j \cdot 138 \Omega$ and $Z_{LO}=142+j \cdot 238 \Omega$. These values are very close to those considered in [5]: $Z_{RF}=83+j \cdot 53 \Omega$ and $Z_{LO}=147+j \cdot 207 \Omega$. A 100 Ω IF output impedance has been considered in both the fabrication and the simulation of the 330 GHz mixer. This value is optimum for the antiparallel-diode pair according to [5], and agrees with the result provided by the IF impedance optimization performed with our CAD tool. The parasitic capacitance of the fabricated mixer is 5 fF according to [5]. The optimum impedances (when C_p is considered) that are predicted by our CAD tool ($Z_{RF}=5+j \cdot 56 \Omega$ and $Z_{LO}=4+j \cdot 120 \Omega$) are very different to those employed in the fabrication of the 330 GHz mixer so we have considered that the parasitic capacitance was not tuned out in the results presented in [5]. In order to make possible the comparison, the quasi-optical losses (0.7 dB) and the losses in the IF circuit and SMA connectors (2.5 dB) predicted in [5] have been added to the simulation results.

Taking into account all these considerations, the new results are provided in Fig. 11. The adjusted DD model eliminates the anomalous increase in the conversion loss that occurred with the previous model when flatband

voltages were reached. As a consequence, new simulation results are in a very good agreement with measurements, certifying the validity of the correction done.

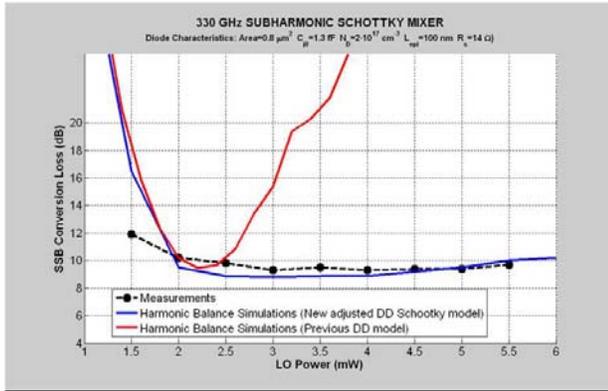


Fig. 11: Comparison between measurements and HB simulations with the new adjusted DD Schottky model for the 330 GHz SHP mixer.

IV. CONCLUSION

Limitations of present DD models for Schottky diodes operating above flatband voltages have been presented in this work. Mixer designs based on these models are not accurate enough, and, therefore, a refinement of DD models is necessary.

Monte Carlo models can be used for a better understanding of the physics inside Schottky diodes. However, mixer design including MC models is not viable due to the high computational cost. Hence, circuit simulation with refined DD models offers a very good trade-off between accuracy and computation time for submillimeter-wave mixer design, as the agreement between measurements and simulations for a 330 GHz SHP mixer shows.

This work is part of an effort to establish a numerical CAD tool for the design and optimization of millimetre-wave and submillimeter-wave circuits based on Schottky diodes and HBV diodes including accurate physical models for the semiconductor devices.

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