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Monte Carlo modelling of Schottky diode for rectenna simulation

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ABSTRACT

Before designing a detector circuit, the electrical parameters extraction of the Schottky diode is a critical step. This article is based on a Monte-Carlo (MC) solver of the Boltzmann Transport Equation (BTE) including different transport mechanisms at the metal-semiconductor contact such as image force effect or tunneling. The weight of tunneling and thermionic current is quantified according to different degrees of tunneling modelling. The I-V characteristic highlights the dependence of the ideality factor and the current saturation with bias. Harmonic Balance (HB) simulation on a rectifier circuit within Advanced Design System (ADS) software shows that considering non-linear ideality factor and saturation current for the electrical model of the Schottky diode does not seem essential. Indeed, bias independent values extracted in forward regime on I-V curve are sufficient. However, the non-linear series resistance extracted from a small signal analysis (SSA) strongly influences the conversion efficiency at low input powers.

1. Introduction

The Schottky diode is the cornerstone of rectifying and mixing circuits to perform non-linear behavior. The efficiency of a detector or a mixer depends mainly on this device and a correct modelling is required to effectively predict the performance of the circuit.

The voltage-current characteristic of the Schottky diode based on the metal/semiconductor (SC) junction depends on the nature of electron conduction mechanisms (tunneling and thermionic) through the barrier, that it could be simulated with a Monte-Carlo (MC) modelling.

The usual parameters of the diode such as the ideality factor, the saturation current and the series resistance are often extracted from the measured I-V characteristic in a limited voltage region where forward current density is far over small leakage current components around 0 V. By including several physical effects in a MC modelling along the vertical layer stack of the diode, this limitation is overcome, and the ideality factor, the saturation current and the series resistance can be extracted from different voltage range. Therefore, we propose an original model which takes into account the entire I-V curve including the bias dependence of the parameters (ideality factor and saturation current) for a Schottky diode on Gallium Arsenide (GaAs). The bias dependence of the series resistance is obtained with a small signal analysis. A comparison is done on the conversion efficiency of a rectifying circuit depending on the voltage range used to perform the parameters extraction.

This circuit works at 2.45 GHz like most of rectennas reported in the literature [1,2]. Schottky barrier on GaAs are probably not appropriate at this frequency because of high barrier height between metal and semiconductor making them less sensitive to very small signals. Indeed, Schottky diodes designed for detection applications are generally fabricated with n-type or p-type silicon according to the barrier height [3]. However, GaAs Schottky diode can also be used at higher frequencies up to THz frequencies, due to higher electron mobility than in silicon [4]. The final target of the present work, starting in the usual 2.45 GHz dedicated to industrial applications, is to design THz circuits.

This article is organized as follows. In Section 2, we present the structure investigated and the Monte-Carlo simulator used for the study, by describing four models to treat the electron current at the rectifying contact and quantifying tunneling and thermionic current for each model. Next, in Section 3, three sets of diode parameters are exposed and extracted from the current-voltage characteristic calculated from MC results: one set considers only the forward bias regime, another one is focused around zero and reverse bias and the last one includes the full characteristic with bias dependent parameters, excepted for the series resistance which is considered constant and identical for each set. In addition, an extraction of the series resistance based on a small signal analysis is proposed to show its variation with bias voltage, which

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cannot be carried out from the I-V curve. The Section 4 shows the comparison between these different extractions on a typical rectifying circuit working at 2.45 GHz. Finally, in Section 5, the main conclusions are presented.

2. Studied structure and Monte-Carlo simulator descriptions

The simulated device is a one dimension (1D) N-N$^+$ structure on GaAs. The doping level of the N$^+$ and N region is 10^{17} cm^{-3} and 10^{16} cm^{-3}, and the thickness is 100 nm and 400 nm, respectively. At the end of the N$^+$ region, the behavior of an ideal ohmic contact is reproduced: the carrier concentration in the cell close to the contact is constant and equal to the doping density. For each time step, this condition is satisfied by injecting particles at thermal equilibrium with a random velocity according to a particular distribution: a velocity-weighted Maxwellian distribution for the component parallel to the diode axis and a Maxwellian distribution for the other two directions [5]. At the Schottky contact on the N region side, the barrier height is 0.735 V [6] and is assumed constant with the applied voltage. The 1D MC simulator takes into account three isotropic and non-parabolic bands (Γ, L and X for GaAs band structure) and the considered interactions are phonons and ionized impurities. The device is divided into cells of 2.5 nm and the time step considered to self-consistently solve the Poisson equation is 2 fs. The low number of carriers close to the Schottky contact can artificially introduce noise on numerical results. To overcome this difficulty, an expansion/compression algorithm has been implemented to keep a quasi-constant number of carriers in each cell [7].

To include quantum tunneling processes, we propose to calculate the transmission coefficient (TC) following four models. The first model does not consider tunneling effects close to the barrier: it is the classical model of the thermionic (TH) emission. In this case, TC is equal to one if the particle energy is greater than the barrier energy and equal to zero otherwise. The second model takes into account tunneling only for electrons which have energy lower than the barrier energy. This model comes from the Wentzel-Kramers-Brillouin (WKB) approximation for a triangular barrier. The third model is based on the exact solution of the Schrödinger equation, in the frame of the effective mass and the envelope function approximation for a triangular barrier involving Airy functions (AIRY model). In this quantum approach, the effective particles can pass through the barrier by tunneling, but also be reflected if their energy is greater than the barrier energy. The last and more complete model includes Airy function but also considers the barrier lowering with the image force (IF) phenomena. The expression of the barrier lowering along the distance x is given by [8]:

$$\Delta\phi(x) = -\frac{q^2}{16\pi\varepsilon_{sc}x} \tag{1}$$

where q is the electron charge, ε_{sc} the permittivity of the semiconductor and x the position with $x = 0$ corresponding to the metal-semiconductor (M-SC) interface. The IF plays a role close to this interface. By taking into account IF effect, the maximum potential corresponds to a location x_m. According to Eq. (1), the potential tends to infinity when x is close to zero. Thus, an effective potential has been used in the MC solver. This potential is assumed to be nearly constant between the M-SC interface and x_m as the authors did in [9]. Due to the particular potential shape, TC was calculated from the transfer matrix with the Airy functions by assuming a linear variation of the potential between two successive meshes [10]. Tunneling is considered only over several tens of nanometers close to the Schottky contact and the mesh size is 1 nm in this region. Fig. 1 shows the transmission coefficient (TC) for each model as a function of the energy in eV for a bias V_S of 0.2 V. The WKB model overestimates the value of TC for energies near and over the barrier energy. The behavior of the TC for AIRY and FI models are very close. TC of the AIRY model is slightly shifted to lower energies by 0.01 eV due to the barrier lowering.

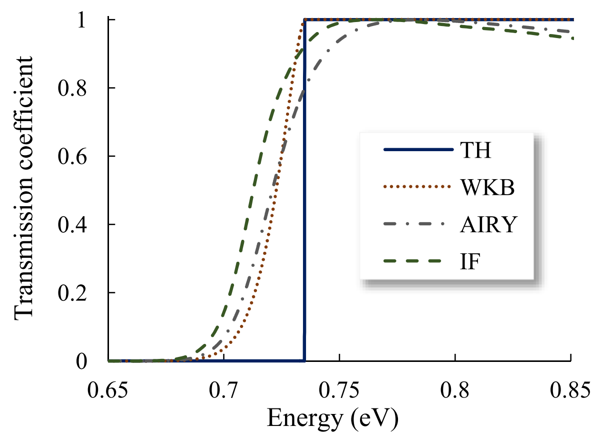

Fig. 1. Transmission coefficient (TC) as a function of energy (eV) for the four models (TH, WKB, AIRY, IF) at 0.2 V.

For particles that could exit the device at the Schottky contact by reaching the turning point in the region where tunneling is considered, a rejection technique involving TC has been implemented to decide if the particle is absorbed by the metal or reflected [11]. To determine the number of carriers to be injected from the metal to the semiconductor at each time step, Eq. (2) giving the injected current density is used, in the same way as [12]:

$$J_{m\to s} = \frac{A^*T}{k_B}\int_0^\infty TC(E)f_m(E)(1-f_s(E))dE \tag{2}$$

where A^* is a pseudo Richardson's constant, T the temperature, k_B the Boltzmann's constant, E the electron energy, TC the transmission coefficient, f_m and f_s the Fermi-Dirac energy distribution function in the metal and in the semiconductor. The injected particles are placed inside the device at the turning point according to their incident energy. Under equilibrium conditions, the current absorbed from the semiconductor to the metal must be the same that the current injected from the metal to the semiconductor. In order to verify this condition, the pseudo Richardson's constant, which depends on the model used, is adjusted by making equal to zero the total current at zero bias [13].

The MC code used here is at the state of the art of the Schottky diode modelling with a MC solver in forward and reverse regime. Only impact ionization involved in Zener effect has not been included.

3. Results from MC simulation and parameters extraction

Fig. 2 shows the current-voltage characteristic obtained for each model discussed in the previous section, implemented in the Monte Carlo simulator. The current can be calculated in different ways: from the particle velocity throughout the structure using the Ramo-Shockley theorem [14,15] or by counting the number of particles leaving the Schottky contact. Both methods give similar results after averaging over a time's period. We chose a diode area equal to 2.6×10^{-6} cm^{-2} in order to reach diode parameters (capacitance at $V_S = 0$ V, saturation current I_s, etc.) comparable to commercial diodes [16]. In reverse regime, when increasing the reverse bias, one can observe a slight increase of the current for almost all the models except the thermionic one. It originates in the reduction of the potential barrier width due to an increasing