Monte Carlo analysis of noise spectra in Schottky-barrier diodes

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We present a microscopic analysis of current fluctuations in a GaAs Schottky-barrier diode under forward-bias conditions. The calculations are performed by employing a one-dimensional Poisson solver coupled self-consistently with an ensemble Monte Carlo simulator. Results support and complement previous findings of M. Trippe, G. Bosman, and A. van der Ziel [IEEE Trans. Microwave Theory Tech. **MTT-34**, 1183 (1986)] based on phenomenological models. In particular, the coupling between fluctuations in carrier velocity and self-consistent field is found to be essential in determining the noise spectra as a function of applied voltages.

The excellent high-frequency behavior of the Schottky-barrier diodes (SBDs) has made them increasingly employed for several applications, such as mixers and detectors of signals up to frequencies of some hundred gigahertz. The current-voltage characteristics of these devices have been extensively treated in the literature,[1–3] and several models for their simulation have been developed.[4–6] Also some Monte Carlo simulations of the behavior of this structure under forward-bias conditions have been performed.[5,7,8] In recent years special attention has been paid to the characterization of the noise performances in SBDs.[9–13] However, the use of phenomenological approaches makes an unambiguous identification of the noise sources responsible of current fluctuations difficult. The purpose of this letter is to present the results of a theoretical study of the noise spectra in a GaAs SBD under forward-bias conditions, employing for the calculations an ensemble Monte Carlo simulator coupled with a one-dimensional Poisson solver (PS). This method has the great advantage of providing a full microscopic analysis without relying on *ad hoc* assumptions and/or simplifications. Therefore, it can offer a reliable test for the physical interpretation of noise performances in SBD and more generally in semiconductor devices.

The simulated SBD is modeled as a one-dimensional GaAs n^+-n-metal structure. The doping of the n^+ region is 10^{17} cm^{-3} and it is 0.35 μm long. At its left side an ohmic contact is simulated, where the carriers are injected into the device, updating the number of electrons considered. The n region is 0.35 μm long and its doping is 10^{16} cm^{-3}. At its end it is the Schottky barrier with the metal contact acting as a perfect absorbing boundary. The height of the barrier considered in the simulation is 0.735 V, which leads to an effective built-in voltage at equilibrium V_{bi} of 0.640 V between the n region of the semiconductor and the metal. The GaAs microscopic model is the same of Ref. 14. The Monte Carlo simulation follows the standard scheme.[15] The device is divided into equal cells of 100 Å each, and the electric field is updated each 10 fs by employing a one-dimensional PS. The cross sectional area adopted for the device is 2×10^{-13} m^2, which means an average number of simulated carriers around 7600 depending on the bias. The simulation is performed at 300 K.

Here we make use of current noise operation:[16] The voltage at the terminals of the device is kept constant in time and the current fluctuations are analyzed. Under this condition, and considering that the length of the device is small compared to its lateral dimensions, the total instantaneous current is given by[16]

$$I(t)=\frac{q}{L}\sum_{i=1}^{N_T(t)} v_i(t), \tag{1}$$

where q is the absolute value of the electron charge, L the total length of the device, $v_i(t)$ the instantaneous value of the velocity component in the field direction of the ith carrier, and $N_T(t)$ the number of carriers which are instantaneously present in the device. The mathematical quantity employed for the characterization of the current fluctuations is the autocorrelation function of current fluctuations, $C_I(t)$, defined as

$$C_I(t)=\overline{\delta I(0)\delta I(t)}, \tag{2}$$

where $\delta I(t)=I(t)-\bar{I}$ is the total current fluctuation around the average value $\bar{I}$ and the bar indicates time average. By the Wiener–Kintchine theorem the autocorrelation function is related to the spectra density, $S_I(f)$, as

$$S_I(f)=2\int_{-\infty}^{\infty} C_I(t)e^{i2\pi ft}dt$$
$$=4\int_0^{\infty} C_I(t)\cos(2\pi ft)dt. \tag{3}$$

Once the stationary situation is reached, the value of $I(t)$ is recorded each time step, for thereafter calculating $C_I(t)$. The simulation must be long enough to get a good convergence of the autocorrelation function. To this end the carrier kinetics is simulated for 750 ps after a transient of 20 ps to obtain an autocorrelation function which is found to vanish around 2.0 ps within a resolution of at most 2%.

Figure 1 shows the current-voltage characteristic of the SBD simulated. Only the forward-bias range leading to

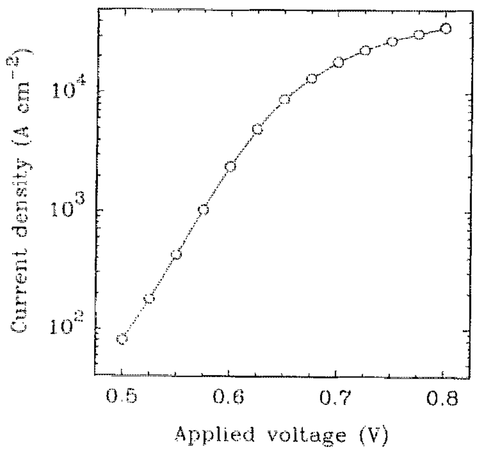

FIG. 1. Current-voltage characteristic under forward-bias conditions for the Schottky-barrier diode simulated.

a built-in voltage lower than $5K_BT/q$ can be reliably simulated with the present method. In agreement with expectations, two different regions can be clearly observed in this characteristic according to the conditions $V<V_{\mathrm{bi}}$ and $V>V_{\mathrm{bi}}$. In the former, the current exhibits an exponential behavior which is determined by the thermionic emission of carriers over the metal-semiconductor barrier. In the latter, the current tends to assume a linear behavior due to the disappearance of the barrier, and it is the semiconductor series resistance which controls the current in the device. As shown in Fig. 2, in the former range all the potential drop is localized in the depletion region close to the barrier, while in the latter range the voltage drop is distributed along the whole device. This difference in the voltage profile, by controlling the current through the diode, is responsible for two limiting behaviors of the spectral density at low frequency $S_I(0)$.

Figure 3 presents the results for $S_I(0)$. The uncertainty of the calculations is estimated to be within 20% due to the spread in the time resolution of $C_I(t)$. This value is well justified being comparable to the experimental counterpart. In the low-current region (corresponding to

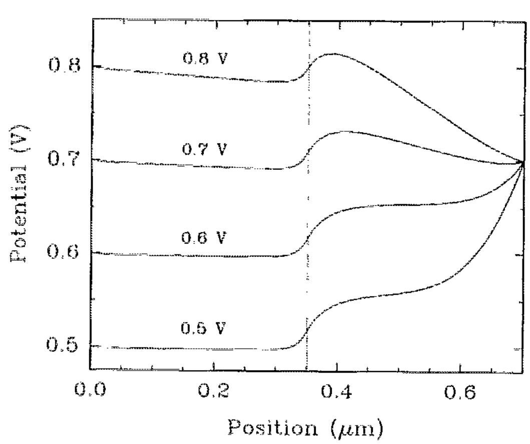

FIG. 2. Profile of the potential as a function of the position in the Schottky-barrier diode under study for different forward applied voltages.

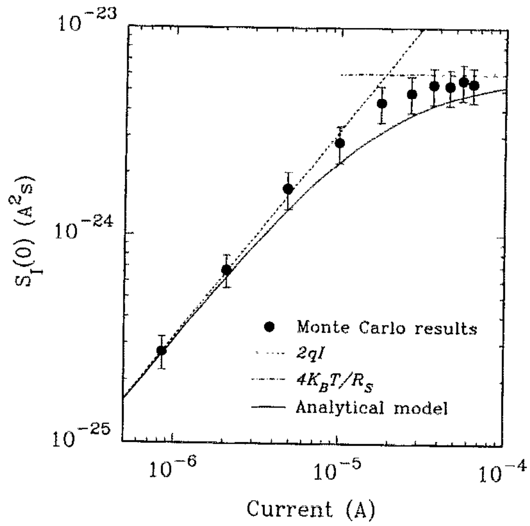

FIG. 3. Low-frequency value of the spectral density of current fluctuations as a function of the current flowing through the structure. Symbols refer to Monte Carlo calculations, the continuous line to the analytical model from Ref. 11.

$V<V_{\mathrm{bi}}$) $S_I(0)$ exhibits a $2qI$ dependence typical of a full shot noise behavior caused by the carriers crossing the barrier individually and at random.[11] When going to the high current region the effect of the series resistance becomes increasingly important (since the built-in potential tends to disappear), and $S_I(0)$ deviates from the shot noise behavior. In this region $S_I(0)$ approaches ultimately a value close to $4K_BT/R_s$, where K_B is the Boltzmann constant and T is the lattice temperature, corresponding to the thermal noise associated to the series resistance R_s (due to the n and n^+ regions in the device). This result is what expected by assuming that the carriers are in thermal equilibrium with the lattice. By considering these two behaviors, $S_I(0)$ can be expressed in the whole range of current considered as[11]

$$S_I(0)=\frac{2qIR_j^2}{(R_s+R_j)^2}+\frac{4K_BTR_s}{(R_s+R_j)^2}, \tag{4}$$

where R_j is the junction space-charge differential resistance. Equation (4) predicts that for low currents, when $R_j \gg R_s$, the behavior of S_I is $2qI$, while for high currents, when $R_s \gg R_j$, it is $4K_BT/R_s$. These two limit behaviors are reported in Fig. 3 where the results obtained from the simulations are compared with those of Eq. (4). The value adopted for R_j is obtained from the exponential region of the I-V characteristic while that for R_s is calculated from the slope of the linear region, and it is about 2750 Ω. The discrepancies between the Monte Carlo results and the analytical model can be attributed to the constant value assigned to the series resistance, whose determination involves some difficulties due to the fact that it is expected to be voltage dependent.[10]

Figure 4 shows the spectral density in the whole frequency range for an applied voltage of 0.575 V, which corresponds to a current of 2.07×10^{-6} A. Two peaks are clearly evidenced. The first one at about 500 GHz is attributed to the carriers that have insufficient kinetic energy to

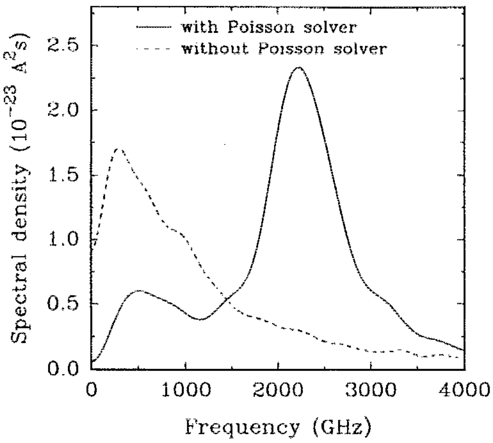

FIG. 4. Spectral density of current fluctuations as a function of frequency for an applied voltage of 0.575 V, corresponding to a current of 2.07×10^{-6} A. The continuous (dashed) lines refer to the case in which the instantaneous fluctuations of the self-consistent field are considered (neglected) in the simulation.

surpass the barrier and return to the neutral semiconductor, as was originally proposed in Ref. 11. The second one at about 2100 GHz is associated with the coupling between the fluctuations in carrier velocity and in the self-consistent field originated by the inhomogeneity introduced by the n^+-n homojunction,[17] and is mostly related to the plasma frequency of the n^+ region. Its magnitude and frequency are found to depend on the characteristics (doping and length) of the n and n^+ regions. This dependence will be the subject of a later publication.

To emphasize the necessity of including the PS when studying noise spectra in SBDs, and more generally in nonhomogeneous devices,[17,18] in Fig. 4 we present the spectrum obtained under the same bias condition but with a fixed field profile (therefore not including the field fluctuations). The result, which is reported as a dashed curve, shows that at low frequencies the spectral density takes significantly higher values with respect to the case in which fluctuations in the field are considered; the result including PS being in much better agreement with the analytical model. Furthermore, the second peak completely disappears, thus corroborating our interpretation about it.

In conclusion, we have presented a microscopic analysis of noise spectra in a GaAs Schottky-barrier diode. By using a Monte Carlo simulator coupled with a Poisson solver we have avoided any *a priori* assumptions on the noise sources responsible for current fluctuations. Results support the reliability of previous phenomenological findings of Ref. 11 and evidence the presence of a peak in the spectral density related to the n^+-n homojunction. Furthermore, we prove the essential role played by the coupling between fluctuations in carrier velocity and self-consistent electric field in determining the noise spectra in whole range of applied voltages.

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