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Monte Carlo Simulation of Electronic Noise in Semiconductor Materials and Devices Operating under Cyclostationary Conditions

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Abstract. To qualify the feasibility of standard semiconductor materials and Schottky-barrier diodes (SBDs) for THz high-order harmonics generation and extraction, the noise-to-signal ratio is calculated by the Monte Carlo method. Heavily doped GaAs SBDs are found to exhibit conditions for frequency mixing and harmonics extraction which are definitively superior to those of bulk materials.

Keywords: Monte Carlo simulation, hot-carrier noise, cyclostationary conditions

1. Introduction

To extend power generation within the submillimeter and THz frequency range starting from available sources of fundamental signal in the frequency range $f = 0.1$–0.3 THz [1], significant attention is recently paid to high-order harmonics generation in bulk semiconductors [2,3] and various semiconductor structures [1,4]. The generation is originated by the nonlinearity of velocity/current response when a strong microwave electric field/voltage is applied to the semiconductor/device. However, the extraction of these harmonics is limited by the intrinsic high-frequency noise of the nonlinear medium, which can mask the generated high-order harmonics. The aim of this work is to qualify the feasibility of standard semiconductor materials and Schottky-barrier diodes for THz radiation generation due to high-order harmonics generation and extraction. For this sake, the harmonics intensity, the spectral density of fluctuations and the noise-to-signal ratio are calculated by means of Monte Carlo (MC) simulations when a microwave electric field or voltage is applied to the nonlinear medium or diode.

2. Theoretical Background

The main steps of the calculation procedure are similar to those described in [3]. Accordingly, under cyclostationary conditions the spectra of the regular response $\langle q(t)\rangle$ and of the instantaneous fluctuations $\delta q(t) = q(t) - \langle q(t)\rangle$ of a given physical quantity $q(t)$ (carrier velocity, total current, etc.) can overlap in the whole frequency range of interest. The most direct comparison of these spectra is based on the finite Fourier transform (FT) of $q(t)$ performed in the time interval $0 \leq t \leq T = NT_f$ which is usually taken as a large integer number N of the applied signal periods T_f [3]. For this sake a sufficiently long history of $q(t)$ simulated by the MC method is subdivided into a set of time intervals of duration T and the spectral density of the total response is then defined as:

$$S_{qq}(v_n) = 2T\langle g(v_n)g^*(v_n)\rangle, \qquad (1)$$

where $v_n = n/T$, with $n = 0, 1, 2, \ldots$, brackets $\langle \cdots \rangle$ denote the averaging over an ensemble of different realizations of $q(t)$ histories during time intervals T, and the Fourier coefficients are given by:

$$g(v_n) = \frac{1}{T}\int_0^T q(t)\exp(-i2\pi v_n t)\,dt. \qquad (2)$$

Typically, to perform the finite Fourier transform, the simulated history calculated with time step $\Delta t = 1-10$ *fs* is subdivided into $10^2 - 10^3$ T-intervals with 10^5 points in each.

The advantage of this approach is that both the regular response and noise are present in the spectrum. However, their contributions depend on the sampling time T. Therefore, by supposing the additivity of these contributions, the spectral density of the total response can be represented as [3]:

$$S_{qq}(v) = \bar{S}_{\delta q\delta q}(v) + 2T|q_m|^2\delta_{vv_m}, \qquad (3)$$

where $v_m = mf$ and $|q_m|$ are the frequency and amplitude of the m-th harmonic ($m = 1, 2, 3, \ldots$) of the total response $q(t)$ to the applied electric-field or voltage with frequency f, $\bar{S}_{\delta q\delta q}(v)$ is the mean spectral density of the fluctuations of the quantity $q(t)$ with respect to its regular time-dependent response $\langle q(t)\rangle$, δ_{vv_m} is the Kroneker symbol, and T is the time interval used to perform the finite FT, which determines the frequency resolution $\Delta v = 1/T$. As shown in [3], such a representation of $S_{qq}(v)$ allows one to express the signal-to-noise ratio in terms of the threshold bandwidth:

$$\Delta v_{th} = 2|q_m|^2/\bar{S}_{\delta q\delta q}(v_m), \qquad (4)$$

in which the net intensity of the intrinsic noise is set equal to the intensity of the m-th harmonic of the regular response, and thus harmonic extraction from the noise level becomes impossible. From Eq. (3) one can also obtain a somewhat different representation of the noise-to-signal ratio as:

$$Q_m \equiv f/\Delta v_{th} = \bar{S}_{\delta q\delta q}(v_m)f/(2|q_m|^2), \qquad (5)$$

which gives the ratio between the noise power and the power of the generated m-th harmonic assuming that the bandwidth used for harmonic extraction takes the maximum possible value $\Delta v = f$.

3. Bulk Semiconductors

In the case of bulk materials, the generation of high-order harmonics of the velocity response in the presence of a strong microwave electric field, $E(t) = E_1\cos(2\pi ft)$, with amplitude E_1 and frequency f, is caused by the nonlinearity of the static velocity-field characteristic, $v_d(E_1)$, originated by the threshold character of some scattering mechanisms (low-temperature optical phonon emission, carrier transfer to upper valleys, etc.). The additivity of the regular response with the noise spectra in this case is illustrated by Fig. 1, which refers to bulk InP at 80 K. Here, curve 1 is calculated by using the finite FT of fluctuating histories during the time interval $T = 200T_f$, where $T_f = 1/f$ is the microwave field period. The spikes in the spectrum correspond to the contribution of the harmonics of the regular response $\langle v(t)\rangle$, while the smooth part practically coincides with the mean spectral density of velocity fluctuations, $\bar{S}_{\delta v\delta v}(v)$, calculated with the correlation function (CF) approach (curve 2) as described in [3]. The top of the spikes

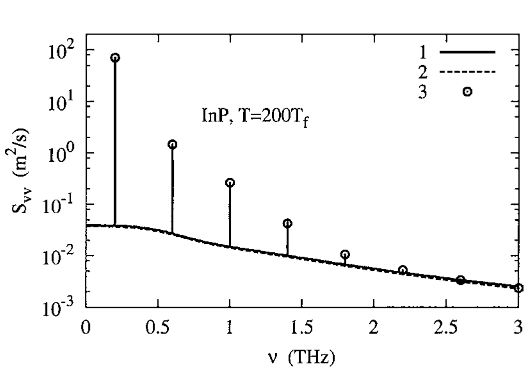

Figure 1. Spectral density of velocity response calculated for InP at 80 K by the finite FT approach (curve 1) at $T = N\,T_f$ with $N = 200$. $\bar{S}_{\delta v\delta v}$ obtained by the CF approach is shown by curve 2, which practically coincides with the FT-curve outside the spike points. Open circles are values of S_{vv} recalculated from $\bar{S}_{\delta v\delta v}$ with the harmonic amplitudes in accordance with Eq. (3). $E_1 = 8$ kV/cm, $f = 200$ GHz.

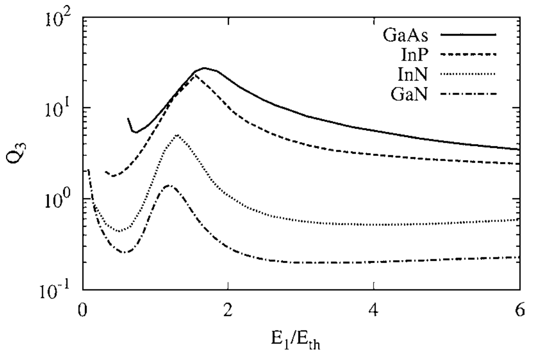

Figure 2. Noise-to-signal ratio calculated from Eq. (5) for the 3rd harmonic of the velocity response to the electric field applied to bulk semiconductors at frequency $f = 200$ GHz as function of the normalized field amplitude E_1/E_{th}.

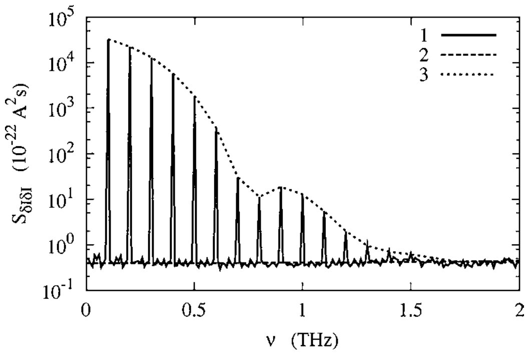

Figure 3. Comparison between the spectral densities of current fluctuations calculated for the SBD with three different approaches based on: (i) finite FT of fluctuating current at time interval $T = 100$ ps; (ii) CF of current fluctuations; (iii) in accordance with Eq. (3) with $T = 100$ ps; curves 1 to 3, respectively.

fully coincides with the velocity response spectrum at the harmonic frequencies (open circles) calculated in accordance with Eq. (3). This result validates the use of Eq. (3) and, hence of Eqs. (4) and (5) in this case. As an example,Fig. 2 reports the noise-to-signal ratio Q_3 calculated for the 3rd harmonic in accordance with Eq. (5) as function of the applied field amplitude E_1 normalized to the threshold static field for Gunn-effect $E_{th} = 3.25$, 9.7, 62, 132 kV/cm for, respectively, n-GaAs, n-InP, n-InN and n-GaN at 80 K. The curves show two main regions of field amplitudes where Q_3 is minimum, and thus appropriate for harmonic extraction. The first region is a narrow one at amplitudes just below E_{th}. Here, the nonlinearity is originated by the threshold character of optical phonon emission by electrons in the Γ-valley. The second region is a wider one at amplitudes well above E_{th}. Here, the nonlinearity is caused by intense transfer of electrons into upper valleys. As follows from Fig. 2, materials with higher values of E_{th} are characterized by lower noise-to-signal ratio value and, thus, they are preferable for the purposes of high-order harmonic extraction. In this respect we notice that a high value of Q_3 implies that for harmonic extraction from the noise level the resolution bandwidth must be sufficiently narrow. Of course, the increase of the harmonic order leads to an additional deterioration of the harmonic extraction.

4. Schottky-Barrier Diodes

Let us compare now the results obtained for bulk semiconductors with those calculated by the Monte Carlo method for a Schottky-barrier diode (SBD) operating under periodic large-signal conditions in the THz-frequency region typical of modern mixers and multipliers. For this sake, we consider the room temperature operation of an heavily doped GaAs 0.02–0.03 μm n^+n-Schottky-barrier structure similar to that of Gelmont *et al.* [4], with barrier height $U_b = 1.03$ V, cross-sectional area $A = 4.5 \times 10^{-14}$ m^2, and carrier concentrations $n^+ = 8 \times 10^{18}$ cm^{-3} and $n = 1.1 \times 10^{18}$ cm^{-3}. Here harmonic generation is caused mainly by the nonlinearity of the current-voltage and capacitance-voltage characteristics. Figure 3 reports the comparison between the spectra of the regular response and the noise obtained by various procedures for a voltage $U(t) = U_0 + U_1 \cos(2\pi f t)$, with $U_0 = 0.7$ V, $U_1 = 0.3$ V and frequency $f = 100$ GHz. Curve 1 refers to the spectral density of the current response $S_{II}(v)$ calculated by finite FT of the fluctuating current $I(t)$ at the finite time interval $T = 100\,ps$ corresponding to a frequency resolution $\Delta v = 1/T = 10$ GHz. In full analogy with the case of bulk materials (see Fig. 1), $S_{II}(v)$ exhibits δ-like spikes at the fundamental and high-order harmonics of the applied voltage which are superimposed to the noise level. This level (curve 2) fully coincides with $\bar{S}_{\delta I \delta I}(v)$ calculated by using the CF approach. The envelope function, reported as curve 3, is calculated from Eq. (3). The excellent fit of curve 3 with the top of the spikes confirms the additivity of the current noise with the regular response of the current at the fundamental and higher order harmonics of the large-signal. In full analogy with the case of bulk materials, Fig. 4 reports the noise-to-signal ratio for 2nd, 3rd, 4th and 5th harmonics (curves 1 to 4) as function of the amplitude U_1

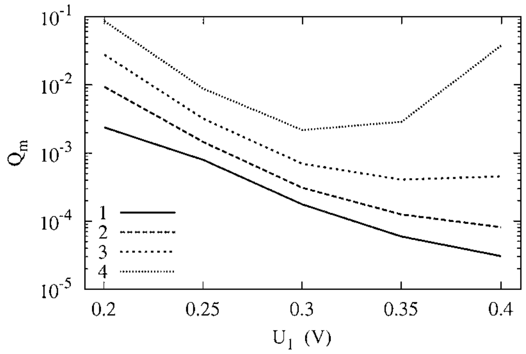

Figure 4. Noise-to-signal ratio calculated for the 2nd, 3rd, 4th and 5th harmonics (curves 1 to 4, respectively) generated by the SBD as function of the microwave voltage amplitude U_1, with $U_0 = 0.7$ V and $f = 100$ GHz.

of the microwave voltage applied to the SBD under test at $U_0 = 0.7$ V and $f = 100$ GHz. When comparing the noise-to-signal ratio obtained in SBD (see Fig. 4) with that obtained in bulk materials (see Fig. 2), we conclude that heavily doped GaAs SBDs exhibit conditions for frequency mixing and harmonics extraction which are much better than those of bulk materials.

Acknowledgments

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