

Monte Carlo Simulation of Threshold Bandwidth for High-Order Harmonic Extraction

P. Shiktorov, E. Starikov, V. Gružinskis, S. Pérez, T. González, L. Reggiani, L. Varani, and J. C. Vaissière

Abstract—The feasibility of bulk semiconductors subjected to strong periodic electric fields for terahertz radiation generation due to the high-order harmonic extraction is analyzed by using Monte Carlo simulations. The high-order harmonic intensity and the spectral density of velocity fluctuations are calculated for GaAs, InP, and InN. By comparing the harmonic intensity with the noise level the threshold bandwidth for high-order harmonic extraction determined by their ratio is introduced and evaluated for the above materials. The results show that semiconductor materials with a high value of the threshold field for the Gunn-effect are characterized by a high value of the threshold bandwidth under high-order harmonic generation and, hence, they are promising materials for microwave generation in the THz frequency range by high-order harmonic extraction.

Index Terms—Frequency multiplication, Monte Carlo simulation, terahertz generation.

I. INTRODUCTION

THE CHALLENGE of extending power generation within the submillimeter and terahertz frequency range is a persistent issue of advanced solid-state electronics since several decades [1]. By recalling that the maximum generation frequency f_M of today Gunn-devices and IMPATT-diodes is restricted to the short millimeter wave range ($f_M = 100 \div 300$ GHz) [1], the typical method to achieve the THz region is frequency multiplication. Historically, for this purpose, the exponential current–voltage I – V characteristics of Schottky barrier diodes under forward bias, the variable capacitance under reverse bias of varactors, etc. are commonly used [2]–[5]. In general, the frequency multiplication is performed by using second or third harmonics of the fundamental signal. In such a case to achieve the terahertz region starting from the available sources of fundamental signal a multicascade multiplication is performed [1] so that the obtained second or third harmonics

are further used as a fundamental signal for next multiplication step. The efficiency of multicascade multiplication is rather low, therefore, the usage of the fifth- and higher-order harmonics of the primary signal can be sometimes preferable. In recent years, significant attention has been paid to the method of high harmonic generation from bulk materials, such as Si, GaAs, InP, GaN, etc. [6]–[8]. Here, for the generation of high-order (odd) harmonics induced by a periodic electric field of sufficiently large amplitude one takes advantage of the nonlinearity of the velocity-field characteristic originated by the threshold character of some microscopic scattering mechanisms (optical phonon emission, carrier transfer to upper valleys, etc.). From the theoretical point of view, the response spectrum of a nonlinear medium subjected to a microwave electric field can include harmonics of arbitrary high order. However the extraction of these harmonics is restricted by the intrinsic high-frequency noise which can mask the generated high-order harmonics.

In the case of carrier heating under a static field, the intrinsic noise can be described as velocity fluctuations, $\delta v(t) = v(t) - \langle v \rangle$, of the instantaneous velocity $v(t)$ with respect to the average value (regular part) $\langle v \rangle$. Since $\langle v \rangle$ is independent of time, the regular and noise components are separated in the spectral representation. Indeed, the regular part has contribution only at zero frequency, while the noise manifests itself in the whole frequency range up to the cut-off value determined by the rate of momentum relaxation. By contrast, under an alternating electric field the regular response, $\langle v(t) \rangle$, is a time-periodic function which, because of the nonlinearity of the velocity-field relation can contain all high order harmonics of the fundamental signal. As a consequence, the spectra of the regular and of the noise part overlap in the whole frequency range. Therefore, to verify the possibility of extracting high-order harmonics it is necessary to compare the spectral power of both: the regular and the noise contributions. This comparison is especially important for the case of harmonic generation in bulk materials, since the same scattering mechanisms are responsible for both harmonic generation and noise.

The aim of this paper is to address this issue by presenting an original Monte Carlo (MC) calculation of the intrinsic noise level of a semiconductor sample in the presence of high-order harmonic generation. At the present time, the MC procedure [9], [10] based on a numerical solution of the Boltzmann transport equation by stochastic methods is recognized as the most powerful tool for the study of hot carrier transport and noise in bulk semiconductors and semiconductor devices (see, for example, [6]–[16] and references therein). On the one hand, this approach provides a complete microscopic picture of carrier

Manuscript received October 22, 2002. This work was supported by a NATO Collaborative-Linkage Grant PST.CLG.977520, the Spanish *Secretaría de Estado de Educación y Universidades* through the Grant SAB2000-0164, the *Dirección General de Investigación (MCyT)* through Project TIC2001-1754, and the French-Lithuanian bilateral cooperation n. 12864 of French CNRS. The review of this paper was arranged by Editor M. Anwar.

P. Shiktorov, E. Starikov, and V. Gružinskis are with the Semiconductor Physics Institute, Lithuanian Academy of Sciences, 2600 Vilnius, Lithuania (e-mail: pavel@pav.pfi.lt).

S. Pérez and T. González are with the Departamento de Física Aplicada, Universidad de Salamanca, 37008 Salamanca, Spain.

L. Reggiani is with INFN - National Nanotechnology Laboratory, Dipartimento di Ingegneria dell' Innovazione, Università di Lecce, 73100 Lecce, Italy.

L. Varani and J. C. Vaissière are with the Centre d'Electronique et de Microoptoelectronique de Montpellier, (CNRS UMR 5507) Université Montpellier II, 34095 Montpellier Cedex 5, France.

Digital Object Identifier 10.1109/TED.2003.813461

transport taking into account details of the band structure, scattering mechanisms, peculiarities of carrier dynamics in external and self-consistent internal fields, device design, etc. On the other hand, it contains in a natural way the source of fluctuations caused by the stochastic nature of the quantum-mechanical description of various interactions. Thus, the MC approach allows one to simulate at once both the regular and the noise behavior of carrier response under various biasing conditions.

In the present paper, the fluctuating instantaneous drift velocity is simulated by the single-particle MC method [9], [10] when a harmonic electric field is applied to a bulk semiconductor. Then, the generated high-order harmonics of the velocity response and the hot-carrier noise characteristics are calculated by an averaging of relevant quantities over the simulated trajectory. The results obtained for the regular response are presented in Section II. Section III is devoted to the calculation of the spectral density of velocity fluctuations within the correlation function approach. The analysis of the regular and the noise contributions into the spectrum of the velocity response is performed in Section IV. Here, a comparison between the spectra obtained within the correlation function and the finite Fourier transform of the fluctuating signal is carried out. On this basis, we introduce in Section V the concept of the threshold bandwidth for harmonic extraction and provide the prescription to verify the possibility of extracting the high-order harmonics. The main conclusions are drawn in Section VI.

II. REGULAR VELOCITY RESPONSE

The general objective of the regular response calculation is to determine the magnitude of the fundamental and high-order harmonic generated by the nonlinear medium when a harmonic electric field $E(t) = E_1 \cos(2\pi ft)$ at frequency f and with an amplitude E_1 sufficiently large for nonlinear velocity field characteristics to set in, is applied to a bulk material. For this sake, in the framework of the single-particle MC procedure, the time dependence of the average drift velocity (i.e., the regular response) during a period of the harmonic electric field $T_f = 1/f$ is determined by averaging over a large number M of such periods in accordance with

$$\langle v(\theta) \rangle = \frac{1}{M} \sum_{l=0}^{M-1} v(t = \theta + lT_f) \quad (1)$$

where θ belongs to the time interval $0 \leq \theta \leq T_f$ and $v(t)$ is the velocity component of the single-carrier in the applied field direction. Then, the Fourier coefficients of the fundamental and high-order harmonics are calculated as

$$v_m = \frac{1}{T_f} \int_0^{T_f} \langle v(\theta) \rangle \exp(-i2\pi mf\theta) d\theta \quad (2)$$

where $m = 0, \pm 1, \pm 2, \pm 3$ is the harmonic order. In the general case, the Fourier coefficients are complex, and the m th harmonic intensity is characterized by the quantity $|v_m|^2$. By averaging over a sufficiently large number of periods in (1), the regular velocity response and the harmonic intensities can be calculated with sufficiently high accuracy. In other words, in such

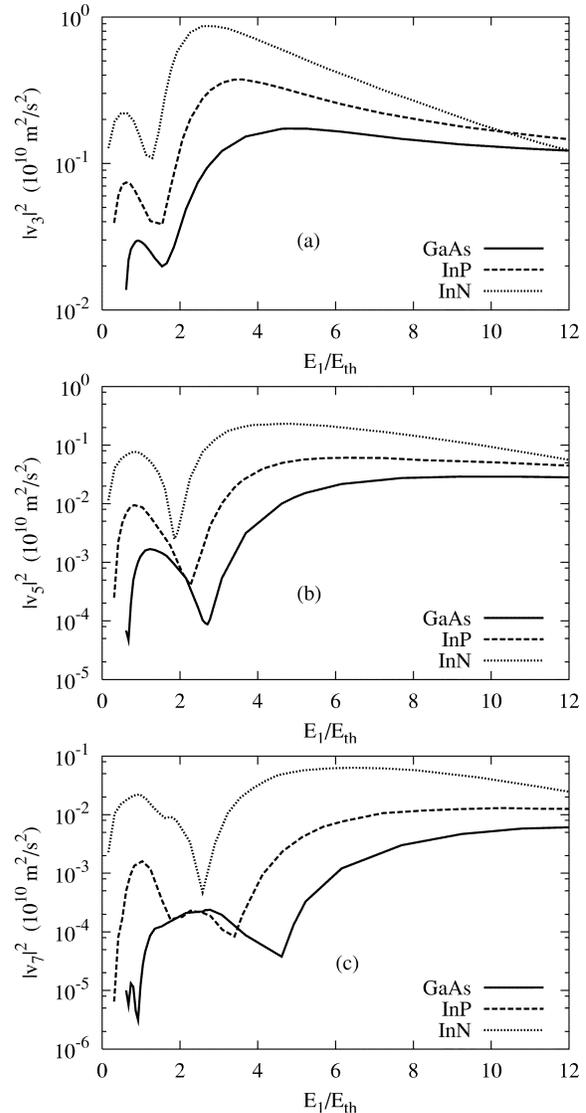


Fig. 1. Fourier coefficient squares for: (a) third, (b) fifth, and (c) seventh harmonics calculated by the MC method for GaAs, InP, and InN at $T_0 = 80$ K and the harmonic field frequency $f = 200$ GHz.

calculations of the regular response characteristics any physical noise of the nonlinear medium is excluded from consideration.

Fig. 1(a)–(c) reports the intensities of, respectively, the third, fifth, and seventh harmonic calculated by the MC method for n-type GaAs, InP, and InN at $T_0 = 80$ K as function of the electric field amplitude E_1 for the same fundamental frequency $f = 200$ GHz (due to symmetry reasons, all even harmonics are absent). Here, the field amplitude E_1 is normalized to the value of the threshold static field for Gunn-effect, $E_{th} = 3.25, 9.7, 62$ kV/cm for, respectively, n-GaAs, n-InP, and n-InN at 80 K. Electron scatterings due to ionized impurity, acoustic, and polar optical phonon in each valley, as well as all intervalley transitions between the equivalent and nonequivalent valleys are accounted for in the usual way [9], [10]. The parameters of the band structure and scattering mechanisms are taken from [11] (GaAs and InP with impurity concentration 10^{13} cm^{-3}) and from [12] (InN with 10^{16} cm^{-3}).

The earlier figures evidence quite similar behavior of harmonic intensities in the compound semiconductors considered

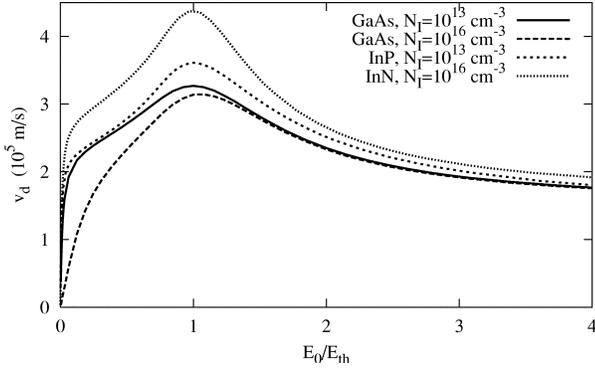


Fig. 2. Steady-state drift velocity of electrons in bulk materials as function of the static electric field E_0 normalized to the Gunn-effect threshold field equal to $E_{th} = 3.25, 9.7, \text{ and } 62 \text{ kV/cm}$ for, respectively, GaAs, InP, and InN at $T = 80 \text{ K}$.

here. In all cases there exist two main regions where the harmonic intensity takes maximum values. To understand their origin it is worthwhile to compare Fig. 1(a)–(c) with the static velocity-field relation $v_d(E_0/E_{th})$ presented in Fig. 2. It is evident that the similarity in the field dependence of the harmonic intensity reproduces the similarity of the $v_d(E_0/E_{th})$ characteristics, which exhibit two main kinks. The first takes place in the low field region and marks the transition from an Ohmic to a sub-Ohmic behavior. The transition is associated with the onset of an intensive polar-optical phonon emission, which controls carrier heating in the Γ -valley and reduces considerably the initial slope of $v_d(E_0/E_{th})$. This nonlinearity originates the first narrow maximum of the harmonic intensity in the low-field region $E_1/E_{th} \approx 0.5 \div 1$. The second kink corresponds to the maximum of the drift velocity and occurs in the intermediate field region at the threshold value for the Gunn effect, i.e., in concomitance with the appearance of the negative differential mobility. This nonlinearity is responsible for the second wide region of the harmonic intensity maximum which occurs at amplitudes well above E_{th} . By comparing the curves of different materials, we conclude that the higher the E_{th} the higher the maximum intensity of generated harmonics.

III. SPECTRUM OF VELOCITY FLUCTUATIONS

To calculate the intrinsic noise associated with velocity fluctuations, we use the approach based on the correlation functions (CF) implemented to the case of periodic processes. The CF approach is based on the assumption that the correlation between fluctuating quantities taken at two different time moments t and t' tends to zero when $s = |t - t'| \rightarrow \infty$ [17]. Since in the general case the average value of the instantaneous velocity $\langle v(t) \rangle$, differs from zero, this requirement can be fulfilled for the CF constructed only for velocity fluctuations $\delta v(t) = v(t) - \langle v(t) \rangle$. Therefore, in the general case of a nonstationary process, the CF of velocity fluctuations is defined as

$$C_{\delta v \delta v}(t, t') = \langle v(t)v(t') \rangle - \langle v(t) \rangle \langle v(t') \rangle \quad (3)$$

where brackets $\langle \dots \rangle$ mean averaging over an ensemble of different realizations of $v(t)$ histories. The mutual independence of the $\delta v(t)$ belonging to each history at long correlation

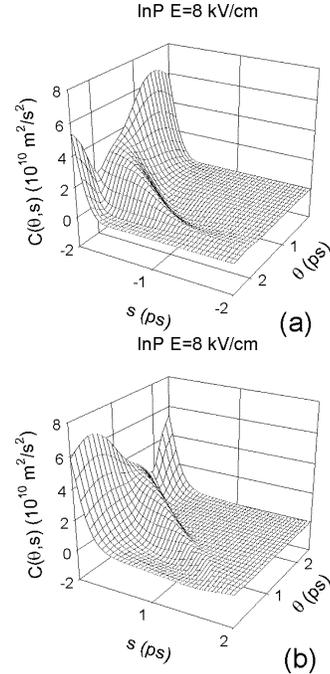


Fig. 3. Correlation function of velocity fluctuations in bulk InP at 80 K subjected to a periodic electric field with amplitude $E_1 = 8 \text{ kV/cm}$ and frequency $f = 200 \text{ GHz}$ calculated at different time moments θ for: (a) negative and (b) positive values of the correlation time s .

times $s = t - t'$ is the condition which guarantees the necessary convergence to zero of the CF. In accordance with the Wiener–Khintchine theorem, only under this condition the corresponding spectral densities will take finite values. Thus, the CF approach allows one to describe only the fluctuating part of the response, not providing any information on the regular part. Since the process considered here is nonstationary, the two-time CF defined by (3) can not be transformed into a single-time CF, which depends on the correlation time $s = t - t'$ only, as it takes place in the case of stationary processes. Nevertheless, because of the periodical property of the process considered here, the following simplifications are possible.

Owing to the periodicity of the applied field and thus of the regular velocity response, i.e., $\langle v(t + lT_f) \rangle = \langle v(t) \rangle$, where $l = 0, \pm 1, \pm 2, \dots$, in full analogy with (1), the ensemble average in (3) can be replaced by the average over the sequence of equivalent time moments $t = \theta + lT_f$, where θ belongs to the time interval $[0, T_f]$. As a consequence, the CF is conveniently represented as a function of the two relevant times, namely, θ and $s = t - t'$, as [17]

$$C_{\delta v \delta v}(\theta, s) = \langle v(\theta)v(\theta + s) \rangle - \langle v(\theta) \rangle \langle v(\theta + s) \rangle. \quad (4)$$

The CF of velocity fluctuations calculated for bulk InP at $E_1 = 8 \text{ kV/cm}$ and fundamental frequency $f = 200 \text{ GHz}$ is shown in Fig. 3 separately for the negative and positive values of the correlation time s [(a) and (b), respectively]. As clearly evidenced by Fig. 3, such a CF is an asymmetric function of the correlation time s due to the physical inequivalence of times $\theta - s$ and $\theta + s$ with respect to the time θ , i.e., due to different conditions for carrier dynamics and heating at various phases of the microwave field. Due to symmetry reasons, $C_{\delta v \delta v}(\theta, s) =$

$C_{\delta v \delta v}(\theta + T_f/2, s)$, therefore only the part of the CF corresponding to times $\theta = 0 \div T_f/2$ is shown in Fig. 3. The curve for $s = 0$ gives the variance of velocity fluctuations, $\langle \delta v(\theta) \delta v(\theta) \rangle$ as function of θ . As expected, the variance reaches the maximum near the maximum values of the instantaneous microwave field $|E(\theta)|$, i.e., near times $\theta = 0$ and $T_f/2$ being slightly shifted due to the inertia of carrier heating. Here the shortest relaxation of the CF is usually achieved (see Fig. 3). The variance passes the region of minimum values near $E(\theta) = 0$ (i.e., at $\theta = T_f/4$) that corresponds to the longest relaxation time of the CF.

The Fourier transform of $C_{\delta v \delta v}(\theta, s)$ with respect to s determines the so-called *instantaneous* [17] spectral density of velocity fluctuations at time moment θ

$$S_{\delta v \delta v}(\theta, \nu) = \int_{-\infty}^{\infty} C_{\delta v \delta v}(\theta, s) \exp(i2\pi\nu s) ds \quad (5)$$

which is a complex quantity due to the asymmetric time dependence of the CF. Due to symmetry reasons [$C_{\delta v \delta v}(\theta, s) = C_{\delta v \delta v}(\theta + s, -s)$], the imaginary part of the spectral density of the CF gives no contribution to the mean spectral density that is obtained by averaging over the whole set of values of θ during the period T_f of the regular response

$$\bar{S}_{\delta v \delta v}(\nu) = \frac{1}{T_f} \int_0^{T_f} S_{\delta v \delta v}(\theta, \nu) d\theta. \quad (6)$$

The mean spectral density given by (6) is a real quantity that describes the intrinsic noise intensity of the nonlinear medium. As we shall see later, this spectral density coincides with the spectral density of velocity fluctuations calculated within the finite Fourier transformation approach. Thus, (5) and (6) can be considered as an extension of the Wiener–Khinchine theorem to the case of a periodic process.

Fig. 4 shows the mean spectral densities of velocity fluctuations calculated by using the CF approach at different values of E_1 and with the same field frequency $f = 200$ GHz. Fig. 4(a)–(c) refers, respectively, to n-GaAs, n-InP, and n-InN. The general behavior of $\bar{S}_{\delta v \delta v}(\nu)$ is analogous to that obtained for the case of a static applied field [13]–[15], [18]. For the lowest field, just below E_{th} , the spectral density exhibits the usual Lorentzian shape (solid lines in Fig. 4). At increasing fields, above E_{th} , the electron transfer to upper valleys starts to play a predominant role. This leads to a systematic increase of $\bar{S}_{\delta v \delta v}(\nu)$ in the whole frequency range (see dashed curves in Fig. 4) and in the formation of a peak due to hot-carriers that takes the maximum value when $E_1 \approx 2E_{th}$ [see curves for $E_1 = 7$ kV/cm in GaAs, Fig. 4(a); $E_1 = 20$ kV/cm in InP, Fig. 4(b); and $E_1 = 120$ kV/cm in InN, Fig. 4(c)]. With a further increase of E_1 , the value of this peak decreases and shifts to higher frequencies. By comparing the spectra of different materials we find that the spectral density of velocity fluctuations in InN is smaller than in GaAs and InP for a factor of about 2~3, mainly due to the shorter relaxation time of velocity fluctuations.

To evidence the difference between the cases of static and periodic fields, it is worthwhile to compare the mean spectral density of velocity fluctuations by keeping similar conditions for the various materials. Accordingly, we have

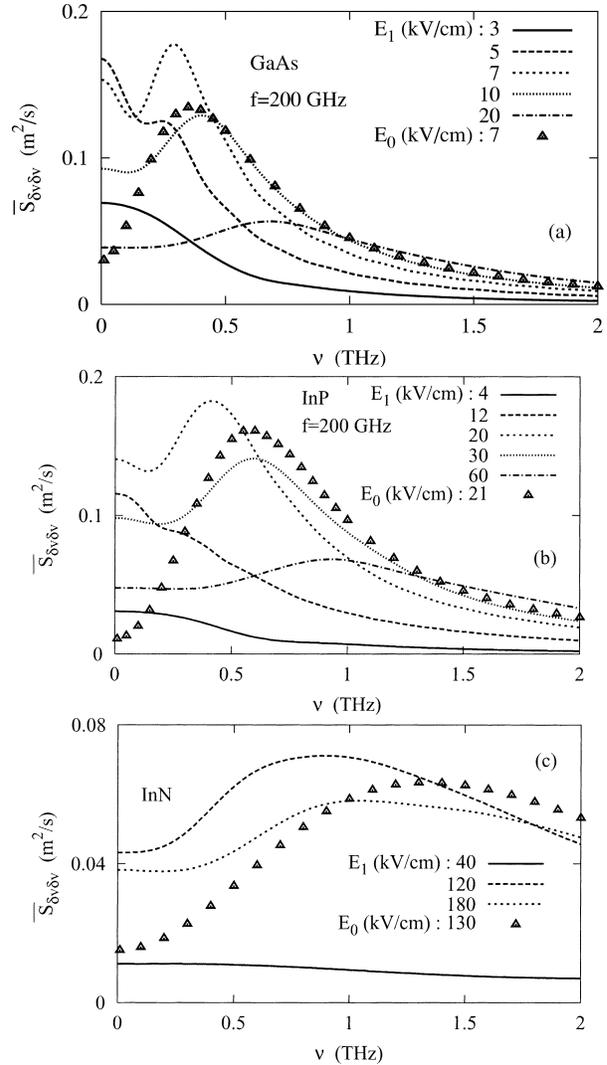


Fig. 4. Mean spectral density of velocity fluctuations in bulk materials: (a) GaAs, (b) InP, and (c) InN at 80 K subjected to a periodic electric field with frequency $f = 200$ GHz and different amplitudes E_1 calculated by the CF approach. For comparison, symbols show $S_{\delta v \delta v}(\nu)$ calculated at a static applied field $E_0 \approx 3E_{th}/\sqrt{2}$.

considered the curves calculated at harmonic field amplitudes of $E_1 = 10, 30$, and 180 kV/cm for, respectively, GaAs, InP, and InN, i.e., at the same normalized field value $E_1/E_{th} = 3$. Since similar conditions of carrier heating under periodic and static fields occur when $E_1 = E_0\sqrt{2}$, the spectral densities of velocity fluctuations for the static case have been calculated at static field values of $E_0 = 7, 21$, and 130 kV/cm for, respectively, GaAs, InP, and InN. The results are presented in Fig. 4(a)–(c) by full triangles. In the high-frequency region these spectra agree very well with those obtained under periodic conditions, as expected. However, in the low-frequency region the static spectra are significantly suppressed with respect to those corresponding to periodic conditions. This significant reduction of the static spectrum is caused by the energy relaxation due to electron transfer to upper valleys which gives negative contribution to $S_{\delta v \delta v}(\nu)$ [18]. Therefore, the enhancement of the low-frequency noise spectrum under the harmonic field conditions is mainly due to the partial

cutoff of intervalley transitions that occurs in the presence of a high-frequency periodic field.

IV. SPECTRUM OF VELOCITY RESPONSE

In the previous two sections, we have presented the results of an independent analysis of the regular and fluctuating parts of the instantaneous drift velocity of free carriers under the action of a strong harmonic electric field of high frequency. However, for the description of the generated harmonics and noise, different mathematical frameworks have been used. The intensity of harmonics was characterized by the square modulus of their amplitudes $|v_m|^2$, while the noise intensity was described by the spectral density of velocity fluctuations $\overline{S}_{\delta v \delta v}(\nu)$. The aim of this section is to present a way to compare the spectral power of the generated harmonics with that of the noise, using the results of the previous sections, i.e., in terms of $|v_m|^2$ and $\overline{S}_{\delta v \delta v}(\nu)$. For this sake we use the finite Fourier transform (FT) of the fluctuating signal which allows one to determine the spectral density of the instantaneous drift response $S_{vv}(\nu)$ thus, avoiding its decomposition into the regular and noise parts.

In the framework of the finite FT [17], the fluctuating velocity response during the finite time interval $0 \leq t \leq T$ is represented by the Fourier series as

$$v(t) = \sum_{n=-\infty}^{\infty} g(\nu_n) \exp(i2\pi\nu_n t) \quad (7)$$

where $\nu_n = n/T$, with $n = 0, \pm 1, \pm 2, \dots$, and with the Fourier coefficients given by

$$g(\nu_n) = \frac{1}{T} \int_0^T v(t) \exp(-i2\pi\nu_n t) dt. \quad (8)$$

The spectral density of the velocity response is then defined as

$$S_{vv}(\nu) = \lim_{T \rightarrow \infty} S_{vv}^T(\nu_n) \quad (9)$$

where $S_{vv}^T(\nu_n)$ is the spectral density in the finite time interval T given by

$$S_{vv}^T(\nu_n) = 2T \langle g(\nu_n) g^*(\nu_n) \rangle \quad (10)$$

where brackets $\langle \dots \rangle$ mean averaging over an ensemble of different realizations of the random $v(t)$ history. To implement such an averaging in the framework of the single-particle MC procedure the whole single-particle history $v(t)$ simulated by the MC method is subdivided into a set of subhistories of duration T . The calculation of $S_{vv}^T(\nu_n)$ is then performed in accordance with (8) and (10).

It should be underlined that the spectral density $S_{vv}(\nu)$ given by (9) becomes a continuous function of the frequency ν only after having performed the limit $T \rightarrow \infty$. However, in practical calculations the time duration T takes always a finite value. Therefore, the calculated $S_{vv}^T(\nu_n)$ is determined over a discrete set of frequency values $\nu_n = n/T$ and, hence, it can be considered as an average value inside the bandwidth $\Delta\nu_{\min} = 1/T$ corresponding to the minimum frequency separation at a given T .

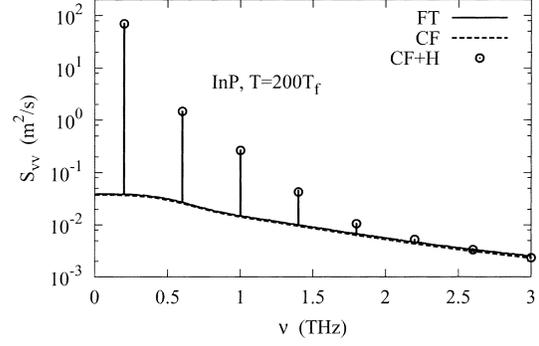


Fig. 5. Spectral density of velocity response calculated for InP by the FT approach (FT-curve) at $T = NT_f$ with $N = 200$. $\overline{S}_{\delta v \delta v}$ obtained by the CF approach is shown by the CF-curve, which practically coincides with the FT-curve outside the spike points. Open circles are values of S_{vv} recalculated from $\overline{S}_{\delta v \delta v}$ with the harmonic amplitudes in accordance with (11).

Since the finite FT approach implies that $S_{vv}^T(\nu_n)$ becomes independent of the time interval T only in the limit $T \rightarrow \infty$, different sequences of $T_{N+1} > T_N$ can be used to reach this limit. In numerical calculations it is convenient to choose T as an integer multiple of the fundamental period T_f , i.e., as $T_N = NT_f$ with N an integer sufficiently large. In this case, only the Fourier coefficient $g(\nu_n)$ for which the ratio n/N is an integer number m will contain the contribution of the regular part $\langle v(t) \rangle$ at the frequency of the m th harmonic. All other Fourier coefficients $g(\nu_n)$, by corresponding to fractional values of n/N , will contain only the noise part.

The spectrum of $S_{vv}^T(\nu_n)$ calculated for bulk InP by using the FT approach at $T_N = NT_f$ with $N = 200$ is reported as the FT-curve in Fig. 5 for the harmonic field amplitude $E_1 = 8$ kV/cm and the corresponding frequency $f = 200$ GHz. The spikes in the spectrum correspond to the contribution of the harmonics of the regular response $\langle v(t) \rangle$, while the smooth part gives the noise level associated with velocity fluctuations, i.e., $\overline{S}_{\delta v \delta v}(\nu_n)$. For comparison, Fig. 5 also reports the results of the CF approach (CF-curve), which practically coincide with the FT-curve corresponding to the noise level. In the same figure, open circles refer to the velocity response spectrum at the harmonic frequencies calculated in accordance with

$$S_{vv}^T(\nu_m) = \overline{S}_{\delta v \delta v}(\nu_m) + 2T|v_m|^2 \quad (11)$$

where $\overline{S}_{\delta v \delta v}(\nu_m)$ is obtained with the CF approach and $|v_m|$ is the amplitude of the m th Fourier harmonic of $\langle v(t) \rangle$ calculated in accordance with (1) and (2). The coincidence of the open circles with the spike tops demonstrates the additivity of the two components at the discrete set of frequencies ν_n . As follows from (11), the amplitude of a spike with respect to the noise level is equal to $2T|v_m|^2$ and tends to infinity when $T \rightarrow \infty$ keeping the same spike area within the minimum bandwidth $\Delta\nu_{\min} = 1/T$. This dependence of the harmonics on the discrete set of frequencies ν_n when going to the continuous frequency spectrum as $T = \infty$ is usually described by a δ -function. Accordingly, for $T = \infty$ the spectral density of the velocity response can be written as

$$S_{vv}(\nu) = \overline{S}_{\delta v \delta v}(\nu) + 2 \sum_{m=-\infty}^{\infty} |v_m|^2 \delta(\nu - \nu_m). \quad (12)$$

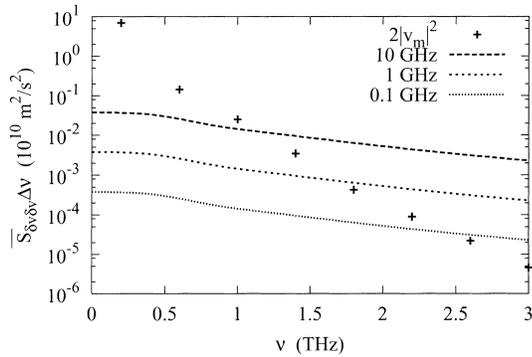


Fig. 6. Comparison of the regular and noise contributions into the velocity response spectrum calculated for InP at $E_1 = 8$ kV/cm and $f = 200$ GHz. Symbols refer to $2|v_m|^2$ while continuous curves presents $\overline{S}_{\delta v \delta v} \Delta \nu$ at three different values of the frequency bandwidth $\Delta \nu = 10, 1, \text{ and } 0.1$ GHz.

The presence of δ -functions in (12) means that the regular and the noise contributions can be compared only as net powers inside a certain bandwidth $\Delta \nu$. Such a comparison will be considered in next section.

V. THRESHOLD BANDWIDTH

The regular contribution to the velocity response spectrum represented by the quantity $2|v_m|^2$ calculated for InP at $E_1 = 8$ kV/cm and $f = 200$ GHz as a function of the frequency of odd harmonics $\nu_m = mf$ with $m = 1, 3, 5, \text{ etc.}$ is shown in Fig. 6 by symbols. For comparison, the continuous curves show the noise contribution represented by the quantity $\overline{S}_{\delta v \delta v} \Delta \nu$ at three different values of the frequency bandwidth $\Delta \nu = 10, 1, \text{ and } 0.1$ GHz.

As follows from Fig. 6, the number of harmonics that can be extracted and thus observed by an external receiver depends crucially on the frequency bandwidth $\Delta \nu$ used to extract the harmonics. For example, for the case of $\Delta \nu = 1$ GHz, only first, third, fifth, and seventh harmonics are above the noise level. This is the reason why only these harmonics are well separated from the noise level in Fig. 5. In this context, the results presented in Fig. 5 by the FT-curve play the role of the signal-to-noise ratio for a receiver with $\Delta \nu_{\text{rec}} = 1$ GHz which corresponds to the minimum resolution $\Delta \nu_{\text{min}} = 1/T$ used in numerical calculations of $S_{vv}^T(\nu_m)$. Of course, the narrower is the frequency bandwidth used to extract harmonics, the better are the conditions for harmonic extraction and a larger number of harmonics can be observed.

Therefore, to characterize the conditions for harmonic extraction it is worthwhile to introduce a threshold bandwidth defined as that for which the levels of the regular and noise contributions are the same. Integration of the right-hand side (RHS) of (12) around the frequency $\nu = \nu_m$ allows one to define the frequency bandwidth

$$\Delta \nu_{th} = 2|v_m|^2 / \overline{S}_{\delta v \delta v}(\nu_m) \quad (13)$$

in which the net intensity of the noise equals the m th harmonic intensity. Such a bandwidth, which is a function of the intensity and frequency of the applied harmonic field, is an intrinsic characteristic of the material and plays the role of a threshold below which it is impossible to extract the m th harmonic from

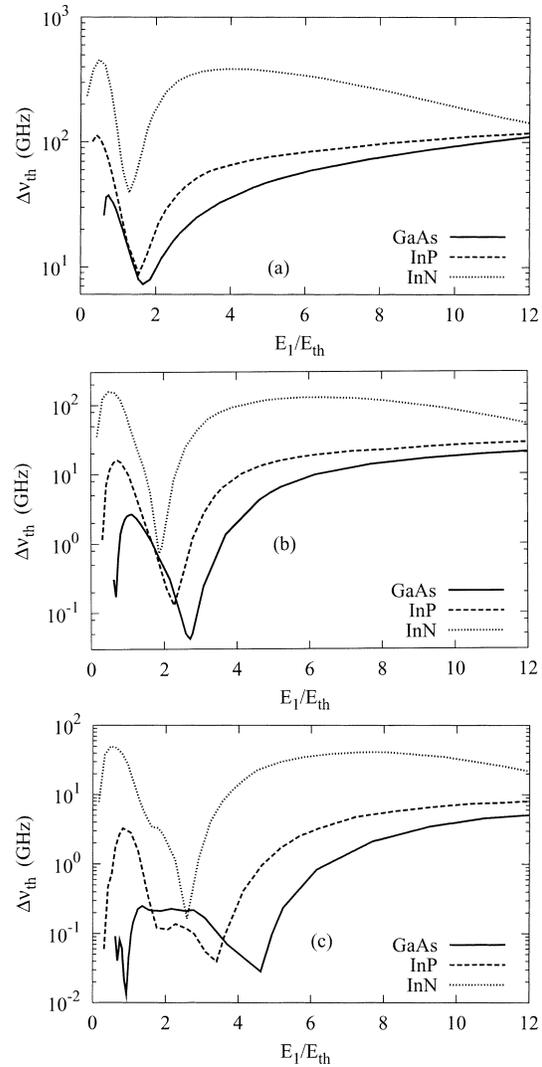


Fig. 7. Threshold bandwidth calculated by (13) for: (a) the third, (b) the fifth, and (c) the seventh harmonic of the harmonic field applied to bulk semiconductors at frequency $f = 200$ GHz as function of the normalized field amplitude E_1/E_{th} .

the noise background. In practice, to detect the m th harmonic over the noise level, the bandwidth resolution of the receiver $\Delta \nu_{\text{rec}}$ must be considerably lower than $\Delta \nu_{th}$.

To compare different materials, Fig. 7 reports the threshold spectral resolution calculated in accordance with (13) for n-GaAs, n-InP, and n-InN at 80 K. Fig. 7(a)–(c) refer to the third, fifth, and seventh harmonics, respectively. As usually, the field amplitude E_1 is normalized to the threshold static field for Gunn-effect E_{th} . Again, the curves show two main regions of field amplitudes where $\Delta \nu_{th}$ is maximum, and thus appropriate for the harmonic extraction. By comparing Figs. 7 and 3 we conclude that the structure so found is caused mainly by the field dependence of the harmonic intensity $|v_m|^2$ and, in turn, is originated by the existence of two main regions of nonlinearity. Due to the relatively weak level of the noise in the low-field region $E_1 \leq E_{th}$, the value of the threshold bandwidth around the first maximum increases additionally with respect to that in the second region. Furthermore, an additional increase of $\Delta \nu_{th}$ is obtained in the case of InN due to a smaller value of

the spectral density of velocity fluctuations in comparison with the cases of GaAs and InP. Thus, materials with high values of E_{th} are preferable for the purposes of high-order harmonic extraction.

VI. CONCLUSION

We have presented a general method to calculate the intrinsic noise of a semiconductor sample in the presence of high-order harmonic generation. By using the approach based on the two-time correlation functions and their spectral densities, the time and frequency behavior of hot-carrier velocity fluctuations in bulk semiconductors subject to strong periodic electric fields is analyzed. The obtained spectral densities of velocity fluctuations and the generated high-order harmonic intensities are compared with direct calculations of the velocity response spectrum by the finite Fourier transform of the fluctuating signal. On this basis, the threshold frequency resolution which qualifies the material feasibility for high-order harmonic extraction is introduced and calculated for relevant III–V and nitride semiconductors. The results indicate that n-InN is significantly better than InP and GaAs. Moreover, the general approach developed here can be applied (with minor modifications) to the analysis of high-order harmonic extraction in more complex semiconductor structures and devices such as Schottky barrier diodes, heterostructure barrier varactor multipliers, etc.

REFERENCES

- [1] R. E. Miles, P. Harrison, and D. Lippens, Eds., *Terahertz Sources and Systems*. ser. NATO Science Series: II. Mathematics, Physics and Chemistry. Dordrecht, The Netherlands: Kluwer Academic, 2001, vol. 27, p. 349.
- [2] N. R. Erickson, "Low-noise submillimeter receivers using single-diode harmonic mixers," *Proc. IEEE*, vol. 80, pp. 1721–1728, 1992.
- [3] A. Jelenski, A. Grub, V. Krozer, and H. L. Hartnagel, "New approach to the design and the fabrication of THz Schottky barrier diodes," *IEEE Trans. Microwave Theory Tech.*, vol. 41, pp. 549–557, 1993.
- [4] B. L. Gelmont, D. L. Woolard, J. L. Hesler, and T. W. Crowe, "A degenerately-doped GaAs Schottky diode model applicable for terahertz frequency regime operation," *IEEE Trans. Electron Devices*, vol. 45, pp. 2521–2527, Dec. 1998.
- [5] T. W. Crowe, J. L. Hesler, R. W. Weikle, and S. H. Jones, "GaAs devices and circuits for terahertz applications," *Infrared Phys. Technol.*, vol. 40, pp. 175–189, 1999.
- [6] R. Brazis, R. Ragoutis, and M. R. Siegrist, "Suitability of drift nonlinearity in Si, GaAs, and InP for high-power frequency converters with a 1 THz radiation output," *J. Appl. Phys.*, vol. 84, no. 7, pp. 3474–3482, 1998.
- [7] R. Brazis, R. Raguotis, Ph. Moreau, and M. R. Siegrist, "Enhanced third-order nonlinearity in semiconductors give rise to 1 THz radiation," *Int. J. Infrared Millimeter Waves*, vol. 21, no. 4, pp. 593–602, 2000.
- [8] D. Persano Adorno, M. Zarcone, and G. Ferrante, "High order harmonic generation efficiency in n-type Silicon and InP," *Laser Phys.*, vol. 11, pp. 291–295, 2000.
- [9] W. Fawcett, A. D. Boardman, and S. Swain, "Monte Carlo determination of electron transport properties in gallium arsenide," *J. Phys. Chem. Solids*, vol. 31, pp. 1963–1990, 1970.
- [10] C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*. ser. Springer Series in Computational Micro Electronics, S. Selberherr, Ed. Berlin, Germany: Springer, 1989.
- [11] K. Brennan and K. Hess, "High field transport in GaAs, InP and InAs," *Solid-State Electron.*, vol. 27, no. 4, pp. 347–357, 1984.
- [12] B. E. Foutz, S. K. O'Leary, M. S. Shur, and L. F. Eastman, "Transient electron transport in wurtzite GaN, InN, and AlN," *J. Appl. Phys.*, vol. 85, no. 11, pp. 7727–7734, 1999.
- [13] G. Hill, P. N. Robson, and W. Fawcett, "Diffusion and power spectral density of velocity fluctuations for electrons in InP by Monte Carlo methods," *J. Appl. Phys.*, vol. 50, no. 1, pp. 356–360, 1979.
- [14] R. Fauquemberdud, J. Zimmermann, A. Kaszynski, and E. Constant, "Diffusion and the power spectral density and correlation function of velocity fluctuation for electrons in Si and GaAs by Monte Carlo methods," *J. Appl. Phys.*, vol. 51, no. 2, pp. 1065–1071, 1980.
- [15] T. Gonzalez Sanchez, J. E. Velazquez Perez, P. M. Gutierrez Conde, and D. Pardo Collantes, "Analysis of the transient spectral density of velocity fluctuations in GaAs and InP," *J. Appl. Phys.*, vol. 72, no. 6, pp. 2322–2330, 1992.
- [16] E. Starikov, P. Shiktorov, V. Gružinskis, J. P. Nougier, J. C. Vaissiere, L. Varani, and L. Reggiani, "Monte Carlo calculation of noise and small-signal impedance spectra in submicrometer GaAs n^+nn^+ diodes," *J. Appl. Phys.*, vol. 79, no. 1, pp. 242–252, 1996.
- [17] J. S. Bendat and A. G. Piersol, *Random Data*. New York: Wiley, 1986.
- [18] L. Varani, P. Houlet, J. C. Vaissiere, J. P. Nougier, E. Starikov, V. Gružinskis, P. Shiktorov, L. Reggiani, and L. Hlou, "A model noise temperature for nonlinear transport in semiconductors," *J. Appl. Phys.*, vol. 80, no. 9, pp. 5067–5075, 1996.

P. Shiktorov was born in Vilnius, Lithuania, in 1954. He received the Ph.D. degree (i.e., Candidate of physical-mathematical sciences) in semiconductor physics from Vilnius State University in 1986.

From 1976 to 1986, he was a Junior Research Associate with the Laboratory of Plasma Phenomena, Semiconductor Physics Institute (SPI), Lithuanian Academy of Sciences. Since 1989, he has been a Senior Research Associate in SPI. His present interests include device physics and submicron device modeling by the Monte Carlo and hydrodynamic approaches, where he is involved in noise phenomena and terahertz radiation generation. He is the author and coauthor of approximately 160 scientific articles in refereed journals.

E. Starikov was born in Krasnoyarsk, Russia, in 1953. He received the Ph.D. degree (i.e., Candidate of physical-mathematical sciences) in semiconductor physics from Vilnius State University, Vilnius, Lithuania, in 1982.

Since 1986, he has been a Senior Research Associate with Semiconductor Physics Institute (SPI), Lithuanian Academy of Sciences. He investigated the inverted distributions of hot carriers in bulk semiconductors by the Monte Carlo method. His present interests include device physics and mathematical simulation of hot carrier transport, noise, and terahertz radiation generation in bulk materials and submicron semiconductor devices by the Monte Carlo and hydrodynamic approaches. He is the author and coauthor of approximately 160 scientific articles in refereed journals.

V. Gružinskis was born in Klaipeda, Lithuania, in 1950. He received the Ph.D. degree (i.e., Candidate of physical-mathematical sciences) in semiconductor physics from Vilnius State University, Vilnius, Lithuania, in 1983.

Since graduation, he has been with the Semiconductor Physics Institute (SPI), the Lithuanian Academy of Sciences. Since 1989, he has been a Senior Research Associate with SPI. His present interests include device physics and mathematical simulation of hot carrier transport, noise and terahertz radiation generation in submicron semiconductor devices by the Monte Carlo and hydrodynamic approaches. He is the author and coauthor of approximately 150 scientific articles in refereed journals.

S. Pérez was born in Salamanca, Spain, in 1970. She graduated in physics in 1993 and received the Ph.D. degree in physics in 1999 from the University of Salamanca. Her graduate work focused on low-phase noise and high-frequency oscillator circuit design.

Since 1994, she has been an Assistant Professor with the Science Faculty of Salamanca University. She was a Visiting Researcher during one year in the LCR of Thomson-CSF, Orsay, France, and during half a year in the IRCOM, Limoges, France. Her current research interest is in the field of numerical simulation of electronic transport and noise in submicron semiconductor devices.

T. González was born in Salamanca, Spain, in 1967. He graduated in physics from the University of Salamanca in 1990, where he also received the Ph.D. degree in physics in 1994.

In 1991, he joined the Electronics Group, Department of Applied Physics, University of Salamanca, with a Grant from the Spanish Education Ministry. Since 1996, he has been an Associate Professor. His main research activity is in the field of electronic transport in semiconductor materials, electronic devices and mesoscopic structures, with special application to the modeling of electronic noise by microscopic approaches.

L. Reggiani was born in Modena, Italy, in 1941. He received the Dr. degree in physics in 1968 and the Diploma di Perfezionamento degree in physics in 1972 from Modena University.

From 1972 to 1982, he was an Assistant Professor and later an Associate Professor with the Science Faculty of Modena University. Since 1994, he has been full Professor with the Engineering Faculty, Lecce University/ Lecce, Italy. His main research activity is in the field of electron transport and fluctuations in semiconductors where he is also an expert of Monte Carlo simulations. He has authored or coauthored more than 300 scientific works. He is the editor of *Hot-Electron Transport in Semiconductors* (New York: Springer-Verlag, 1985).

Prof. Reggiani is a member of the Italian Physical Society.

L. Varani was born in Carpi, Italy, in 1963. He graduated in physics in 1989 from the University of Modena. He received the Ph.D. degree in physics from the University of Modena, Modena, Italy, in 1993 and the Ph.D. degree in electronics in 1996, from the University of Montpellier II, Montpellier, France.

He is now in charge of research at the French National Centre for Scientific Research (CNRS) and responsible of the modeling group in the Centre for Electronics and Micro-optoelectronics, University of Montpellier II. His current research interest is in numerical simulation of transport and noise properties of semiconductor devices. He is author and coauthor of approximately 180 scientific articles in refereed journals.

J. C. Vaisière was born in Castelnaudary, France, in 1946. He graduated in physics in 1971 from the University of Montpellier II, Montpellier, France, where he also received the Doctorat d'état in electronics in 1986.

From 1971 to 1976, he was Assistant Professor with the Science Faculty of Libreville. Since 1976, he has been with the Centre for Electronics and Micro-optoelectronics, University Montpellier II, where he is full Professor. His present activity is in the field of the simulation of electronic transport and noise in semiconductor materials and devices by microscopic approaches.