

Monte Carlo Calculation of Voltage-Current Nonlinearity and High-Order Harmonic Generation in GaAs Microstructures

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INTRODUCTION

The use of semiconductor systems for broadband telecommunication stimulates a more accurate knowledge of both their low and high frequency electric response. Recent advances in electronics pushes the devices to achieve higher output power and efficiency at very high frequencies around the THz region. The miniaturization of integrated circuits implies that even at moderate applied voltages these systems are typically exposed to very intense electric fields.

For these reasons, nonlinear processes involving dynamical effects and high-order harmonic generation in semiconductor structures exposed to intense radiation are attracting increasing attention. Furthermore, the understanding of such processes in semiconductors exposed to far-infrared radiation can be fruitfully exploited for implementing coherent sources in the THz region. Both experimental and theoretical analysis have shown high conversion efficiency for the third and fifth harmonics in low-doped Si, GaAs and InP crystals in the frequency range 30-500 GHz and temperature range 80-400 K, due to the nonlinearity of the velocity-field relation [1-4]. The problem of nonlinear processes in the sub-terahertz region has been recently investigated by considering the nonlinearity of the I-V characteristic, the harmonic generation and the electronic noise behavior in a nanometric n+n metal GaAs Schottky-barrier diode [3]. In the Schottky diode the behavior of high-order harmonic intensity is similar to that exhibited by bulk materials. The hysteresis-like behavior of the curve $\langle I(V) \rangle$ is accompanied by a rapid increase

with the frequency f of the amplitude of the higher order harmonics.

The aim of this work is to study and discuss the dependence of the voltage-current hysteresis cycle and the high-order harmonic efficiency in GaAs n+nn+ structures operating under sub-terahertz signals by the frequency and the intensity of the excitation signal. These structures have been chosen because they form the basis for various high-frequency semiconductor devices.

MODEL AND CALCULATIONS

Using a multiparticles Monte Carlo (MC) code, self-consistently coupled with a one-dimensional Poisson solver, we simulate the nonlinear carrier dynamics in GaAs n+nn+ structures operating under large-amplitude periodic signals. In order to compare the results with those obtained in a previous analysis of GaAs bulk [4], we analyse a symmetric GaAs n+nn+ structure with doping levels of $n+=10^{17} \text{ cm}^{-3}$ and $n=10^{15} \text{ cm}^{-3}$. The spatial length of the n+ region is $0.15 \mu\text{m}$ and $1 \mu\text{m}$ for the n region. All calculations are performed at lattice temperature $T=300 \text{ K}$. We simulate electronic transport in the structure driven by a periodic voltage $V(t)=V_0\sin(2\pi ft)$, with amplitude V_0 and frequency f . To solve the Poisson equation the self-consistent electric field is updated every 10 fs and the structure is meshed by cells of 10^{-8} m length. The total simulated history duration is greater than 100 periods of the frequency of the applied voltage. We set 10^3 particles in the whole diode.

The algorithm of MC simulation of the electron motion in the alternating electric field used involves the nonparabolicity of the band structure and the

intervalley and intravalley scattering of electrons in multiple energy valleys. We assume field-independent scattering probabilities; accordingly, the external fields may alter them only indirectly through the field-modified electron velocities [2]. Electron scatterings due to ionized impurities, acoustic and polar optical phonons in each valley as well as all intervalley transitions between the equivalent and non-equivalent valleys are taken into account. The parameters of the band structure and the modelling for harmonic generation are taken from Ref. [3]. The adopted impurity concentration is 10^{13} cm^{-3} .

NUMERICAL RESULTS

At sufficiently low frequencies dynamical relations recover those of the static case. However, when the applied signal frequency increases the inertia of carrier transport and the heating/cooling processes significantly modify the static J-V relation. Figure 1 presents the instantaneous total current density $\langle J \rangle$ as a function of the instantaneous periodic voltage $V(t)$ applied to the diode, with $V_0=4 \text{ V}$ and different frequencies. The inertia effect into the current response is nearly absent up to $f \approx 20 \text{ GHz}$. Here the $\langle J(V) \rangle$ diagram follows practically the static J-V relation. For $f > 20 \text{ GHz}$, the instantaneous $\langle J(V) \rangle$ characteristic begins to be significantly different with respect to the static case. In figure 2 we show the harmonic spectra of the current density obtained for some values of frequency. A strong reduction of harmonic emission is clearly evident for $f=62.5 \text{ GHz}$, which is the frequency value in which the J-V curve changes its shape.

CONCLUSION

We have studied the nonlinear behavior of a n+nn+ junction. Our results show that: (i) for $f > 100 \text{ GHz}$, the hysteresis-like behaviour of $\langle J(V) \rangle$ produces a similar increasing of the amplitude of the high order harmonics with f observed in bulk samples. This increasing ends only for very high values of frequency ($f > 600 \text{ GHz}$); (ii) in the n+nn+ structure some peculiar mechanism is present and produces a significant reduction in the harmonic emission rate in a very low frequency range. This is a very interesting result, not expected in bulk or in other structures, as the Schottky diode, and remains an open problem.

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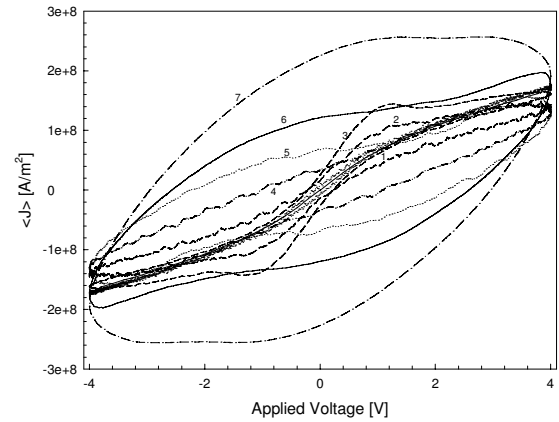


Fig.1 Instantaneous total current density $\langle J \rangle$ as a function of the instantaneous periodic voltage $V(t)$ applied to the n+nn+ junction and frequencies $f=10, 20, 50, 62.5, 100, 200, 400 \text{ GHz}$ (curves 1 to 7, respectively). The thick solid line shows the dc behaviour of the structure, drawn for comparison.

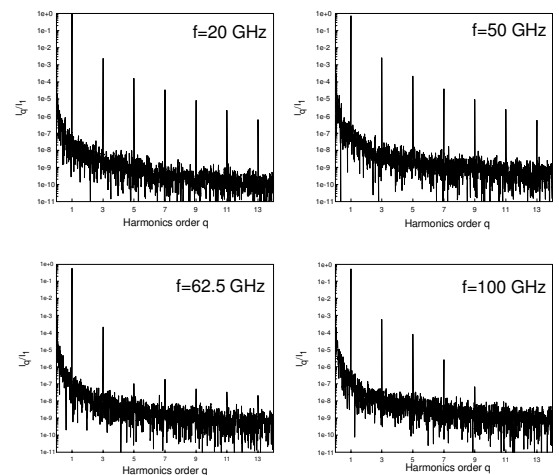


Fig.2 Harmonics generation efficiency versus their order. $V_0=4 \text{ V}$ and $f=20, 50, 62.5$ and 100 GHz .

Static-Electric-Field Effects on Harmonic Generation in Gallium Arsenide Bulk Exposed to Intense Sub-THz Radiation

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INTRODUCTION

The process of high order harmonic generation in semiconductors driven by intense radiation fields having sub-terahertz frequencies has been widely investigated in recent years [1-3]. This field of research represents a useful mean for the general understanding of several features of the highly non linear processes of carrier transport in doped semiconductors. Moreover a possible way to achieve high-power and high-frequency radiation sources is given by the efficient frequency conversion of high-power gyrotron radiation in nonlinear materials.

Harmonics generation in the presence of an additional static field has been addressed by several authors [4-5]. Among others, Bao and Starace have experimentally found that in H⁻ and in Ar the addition of a static field, having an amplitude less than 2% of that of the laser field, produces very intense even harmonics. Furthermore, they have shown that the intensities of odd harmonics near the low-order end of the plateau increase by orders of magnitude. A static field thus appears to have a very sensitive role for controlling the emission rates of both even and odd high harmonics [4].

In this paper we report and discuss the static-electric-field effects on harmonic generation in a GaAs bulk driven by an intense alternating field. To the best of our knowledge this subject in semiconductors has never been addressed before.

PHYSICAL MODEL AND CALCULATIONS

We assume that our GaAs sample is acted by an oscillating electric field and a static field having the components:

$$\begin{aligned} E_x &= E_0 + E_1 \cos \varphi \cos (2\pi\nu_1 t - k_1 z) \\ E_y &= E_1 \sin \varphi \cos (2\pi\nu_1 t - k_1 z) \end{aligned}$$

where φ is the angle between the polarization of the static field E_0 and the oscillating field E_1 .

The theory of harmonic generation in semiconductors has been derived in a previous paper [2] and it is based on the Maxwell equation for the propagation of an electromagnetic wave in a medium along a given direction. Our analysis is referred to a thin sample and for this reason we do not consider the complex form of the dielectric function $\epsilon(\nu)$ in our calculations and neglect the field-dependent absorption. Within these assumptions, the efficiency of the harmonic generation at frequency ν , normalized to the fundamental one (ν_1), is given by:

$$\eta_\nu = \frac{I_\nu}{I_{\nu_1}} = \frac{V_1^2 u_\nu^2}{\nu^2 u_{\nu_1}^2} \quad (1)$$

where u_ν is the Fourier transform of the electron drift velocity, obtained via a multiparticles Monte Carlo (MC) simulation of the electron motion in the semiconductor. The spectra of emitted radiation are reconstructed by the analysis of the velocity Fourier components. The algorithm for MC simulation of the electron motion in the alternating electric field used in this work follows the standard procedure. It takes into account the nonparabolicity of the band structure and the intervalley and intravalley scattering of electrons in multiple energy valleys. Since the far-infrared frequencies are below the absorption threshold, in our model we consider the