Analysis of the transient spectral density of velocity fluctuations
in GaAs and InP

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Using a multiparticle Monte Carlo method, a theoretical analysis of the spectral density of velocity fluctuations in semiconductors has been performed, under both stationary and transient conditions (when the electric field applied to a semiconductor changes). In the case of the transient analysis a general method has been developed and applied to N-type GaAs and InP. The results obtained are interpreted in terms of the microscopic processes occurring during the transient. Significant differences between these materials have been observed. The following results were found: (i) The main source of noise is the presence of carriers in the Γ valley subject to the action of high fields, and the velocity-disorienting effect of the intervalley mechanisms; (ii) the maximum in the spectral density is essentially due to the presence of intervalley mechanisms; (iii) the dominant frequencies in the spectral density are strongly affected by the duration of the free flights; (iv) for long times, the transient spectral density converges on the steady-state one of the final field.

I. INTRODUCTION

Many phenomena leading to the appearance of noise that may mask the output signal occur during the functioning of a semiconductor device. Among the possible sources of this noise is that inherent to the bulk material with which the device has been constructed. The Monte Carlo method is a powerful tool for the analysis of such problems, since it affords a microscopic simulation of the dynamics of the carriers in a semiconductor, providing the magnitudes required for their interpretation. Using this method, different studies have been carried out to analyze the velocity fluctuations under stationary conditions, and to calculate their spectral density in different semiconductor materials and in some devices. In recent years, exhaustive work has also been performed on current spectral density, considering several phenomena in the semiconductor (carrier-carrier scattering, generation-recombination processes). Frequency analysis is done following a simple method, applying the Wiener-Kintchine theorem, by calculating spectral density as the Fourier transform of the autocorrelation function.

However, owing to the high functioning frequencies of such devices, and especially when these work under switching conditions, the semiconductor is not usually in a stationary situation. Among the different factors that may lead to noise in the signal during a transient, the contribution of the processes inherent to the bulk material of the device has received little attention, and even less its frequency analysis. Up to now, Monte Carlo simulations have been performed to analyze the evolution in the transient of velocity, energy, diffusion coefficient, and valley population; some studies have even analyzed velocity fluctuations through transient autocorrelation functions. Despite this, the spectral density in the transient has not been calculated. The main problem underlying this calculation is that since the study of velocity fluctuations is performed over finite times in the transient, the Wiener-Kintchine theorem cannot be applied, and the spectral density cannot be obtained as the Fourier transform of the autocorrelation function; although, it can be calculated in the way we present here, and that was briefly described in Ref. 18.

In the present work we report on a method for obtaining the spectral density of velocity fluctuations of electrons for several times in the transient, starting from the instantaneous velocity values obtained from a multiparticle Monte Carlo simulation. The method has been applied to N-type GaAs and InP, the two III-V semiconductors currently most employed in the construction of rapid devices, with the finding of interesting differences between them.

The article is organized as follows: Section II presents the theoretical analysis of the method developed, and Sec. III describes the multiparticle Monte Carlo procedure used to simulate GaAs and InP. Section IV reports the results, and is divided in two parts: (a) the results corresponding to stationary conditions, of great interest for later interpretation of the transient results, and (b) those relating to transient conditions. The main conclusions are presented in Sec. V.

II. THEORETICAL ANALYSIS

Let us consider an ensemble of carriers subject to the action of an electric field which at \( t=0 \) undergoes a change from a value \( E_1 \) to another \( E_2 \). Let \( \tau \) be the time in the transient up to which we wish to analyze the fluctuations in the longitudinal component of velocity. The function that represents the variations in the velocity of one carrier during the transient up to a time \( \tau \) will be
\[ \delta v_r(t) = \begin{cases} 0, & \text{for } t < 0, \\ \delta v(t), & \text{for } 0 < t < \tau, \\ 0, & \text{for } t > \tau \end{cases} \] (1)

with \( \delta v(t) = \langle v(t) \rangle - \langle v(t) \rangle \), where the angular brackets indicate ensemble average.

The origin of these fluctuations in velocity, that will determine their evolution, is due to essentially three facts: (a) the action of the electric field during the free flights; (b) the effect of scattering mechanisms, mainly isotropic (intervalley), that to a large extent delocalize velocity orientation; and (c) the different effective masses of each of the valleys in which the carrier may remain, leading the evolution of the velocity in the free flights to be faster or slower.

The Fourier transform of \( \delta v_r(t) \), \( \delta V_r(\omega) \), is

\[ \delta V_r(\omega) = \int_{-\infty}^{\infty} \delta v_r(t) e^{i\omega t} dt = \int_{0}^{\tau} \delta v(t) e^{i\omega t} dt. \] (2)

The mean value up to a time \( \tau \) of the square of the velocity fluctuations, \( \overline{\delta v_r^2} \), is given by

\[ \overline{\delta v_r^2} = \frac{1}{\tau} \left( \int_{0}^{\tau} \delta v^2(t) dt \right). \] (3)

According to Parseval’s theorem, and since \( \delta v(t) \) is real, one has that

\[ \int_{-\infty}^{\infty} \delta v^2(t) dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\delta V_r(\omega)|^2 d\omega, \] (4)

such that

\[ \overline{\delta v_r^2} = \frac{1}{\tau} \left( \frac{1}{2\pi} \int_{-\infty}^{\infty} |\delta V_r(\omega)|^2 d\omega \right), \] (5)

Defining the transient spectral density (TSD) up to a time \( \tau \), \( S_r(\omega) \), with \( \omega = \omega / 2\pi \), as

\[ \overline{\delta v_r^2} = \int_{-\infty}^{\infty} S_r(\omega) d\omega, \] (6)

and comparing Eq. (5) and Eq. (6), one obtains

\[ S_r(\omega) = \frac{1}{\tau} \left( \frac{1}{2\pi} \int_{-\infty}^{\infty} |\delta v(t) e^{i\omega t} dt| \right)^2. \] (7)

Thus the value of \( S_r(\omega) \) has two influences: one from the stationary state of the first field \( (\tau_1) \), and another coming from the effect of the transient \( (\tau_2) \). In this way, and varying \( \tau_2 \), it is possible to observe more clearly the transition from the initial stationary state towards the final situation after applying the new field, and how the processes taking place in the transient modify that initial stationary state. The results for both types of analysis will be shown in Sec. IV.

With these elements, one is able to study the behavior of the velocity fluctuations in the transient in a semiconductor material, in both the time and frequency domains.

### III. MONTE CARLO PROCEDURE

To perform the above-described analysis we have used a standard multiparticle Monte Carlo method. The simulation was carried out at 300 K for the III-V semiconductors most used today: GaAs and InP. The materials considered are N-type \( (N_D = 10^{15} \text{cm}^{-3}) \), homogeneous, and infinite. In the simulation, 100 000 particles were used; this number is sufficient to achieve stability in the results. We consider the conduction band formed of three nonparabolic spherical valleys \( (\Gamma, L, X) \), that are the only ones populated for the fields analyzed. The scattering mechanisms considered in both materials are: intervalley (equivalent and nonequivalent), polar optical, nonpolar optical, acoustic, piezoelectric, and interaction with ionized impurities.

The physical parameters employed in the simulation for GaAs and for InP are the same as those used for the valleys of the first conduction band in earlier works, some of which have already been used by other authors. The main novelty is the inclusion of the value \( \Delta E_{\Gamma \rightarrow L} = 0.86 \text{ eV} \) for the InP. This is the value calculated in the most recent theoretical works, \( \Delta E_{\Gamma \rightarrow L} \) higher than that calculated previously, and permits a better fitting of the velocity characteristics to the experimental ones. This value is of great importance in calculating noise since it implies a greater presence of carriers in the \( \Gamma \) valley for high fields.

At the beginning of the simulation the 100 000 electrons are placed in the \( \Gamma \) valley, with the thermic energy corresponding to a temperature of 300 K. The carriers evolve under the action of a first electric field \( E_1 \) for sufficient time for the stationary situation to be reached. When this time has elapsed, an instantaneous change in the electric field occurs to another value \( E_2 \), the moment at which the time origin is taken up again \( (t = 0) \), thereby recording the value of the velocity of each of the particles at different intervals of time \( dt \). This interval must be small enough to permit later analysis of very high frequencies. In general, a \( dt \) value was taken that is at least ten times smaller than the period of the highest frequency to be studied.

During the transient, the evolution of different magnitudes is also recorded; these are of great use in the microscopic interpretation of the calculated TSD, and are: mean velocity, mean energy, population of the valleys, and velocity distribution functions. Such calculations are made
for as long as one wishes to analyze the transient, $\tau$. After the actual simulation, the operations indicated in Eq. (7) are performed, which are those requiring the longest computation time.

IV. RESULTS

A. Stationary conditions

In this section we show some results corresponding to spectral densities in stationary conditions (SSD) of velocity fluctuations, both in InP and in GaAs. These are of great interest for later correct interpretation of the results corresponding to transients. Additionally, as will be seen later, the transient spectral densities converge towards the stationary ones for sufficiently long times $\tau$.

Figures 1(a) and 1(b) show the SSD of velocity fluctuations for different values of the electric field in GaAs and InP, respectively. They were obtained by the above-described method [Eq. (7)], without changing the electric field and for a sufficiently large $\tau$. The results are seen to coincide with those obtained employing the method normally used: the Fourier transform of the autocorrelation function of velocity fluctuations.

For low-electric-field values, 1 kV/cm, when all the carriers are in the $\Gamma$ valley (Fig. 2), the maximum in the spectral density appears for low frequencies, and is higher for GaAs than for InP. This is due to the fact that in GaAs the effective mass in the bottom of the $\Gamma$ valley (0.063) and its nonparabolicity coefficient (0.7) are lower than for InP (0.078 and 0.83, respectively); the duration of the free flights also being longer in GaAs. This leads to the occurrence of greater deviations in the velocity in GaAs than in InP during the free flights due to its lower effective mass, and because the interaction with optical polar phonons—which are those limiting velocity for these fields—is more frequent in InP, since the time elapsed between two successive interactions is shorter.

As the electric field increases, a maximum appears in the SSD for higher frequencies in both materials; this is essentially due to two factors: the passage of carriers towards the higher valleys (Fig. 2), with greater mean effective mass than the $\Gamma$ valley, where they evolve with a slower velocity, this causing greater deviations from the mean; and the appearance of (isotropic) inter-valley mechanisms, that delocalize the orientation of the carrier's velocity.

The frequency at which this maximum occurs is governed by the combination of frequencies characteristic of the transitions among the different valleys, which are the
mechanisms which cause the strongest deviations in velocity. As the electric field increases, the maximum occurs at higher frequencies because the free flights are shorter, such that the intervalley transitions responsible for the noise occur at shorter and shorter time intervals.

Regarding the amplitude of the spectral power of the noise and of its maximum value, it is governed by the greater or lesser magnitude of the deviations of the velocity from the mean value. Figure 3 shows velocity distribution functions in stationary conditions for several electric fields. The maximum values in the spectral density are seen to coincide with situations in which the value of the electric field (6 kV/cm for GaAs and 15 kV/cm for InP) and the occupation of the valleys lead to considerable dispersion in velocity distribution, almost always due to the high presence of carriers in the \( \Gamma \) valley subjected to a high field. Thus, for 25 kV/cm, when the occupation of the \( \Gamma \) valley is much higher for InP than for GaAs (Fig. 2), there is a higher proportion of carriers with very high velocities in InP (Fig. 3); this means that the noise for this field is much greater than in GaAs (Fig. 1). For higher fields (50 kV/cm) the presence of carriers in the \( \Gamma \) valley in InP is lower, such that the noise and deviations decrease.

In the light of the foregoing, the differences observed in the SSD between GaAs and InP are mainly governed by the two following factors.

The first is the higher degree of population in the \( \Gamma \) valley in InP within the range of the electric field studied, owing to the fact that \( \Delta \varepsilon_{\Gamma - L} = 0.86 \text{ eV} \), whereas \( \Delta \varepsilon_{\Gamma - L} = 0.32 \text{ eV} \) in GaAs. This causes the highest values of noise in InP for high fields, when intervalley mechanisms are present.

The second is the shorter duration of the free flights in GaAs than in InP for the same values of the electric field (higher than 4 kV/cm). This causes the appearance of the maxima for higher frequencies in GaAs.

Accordingly, regarding the noise inherent to the material, and under stationary conditions, it seems wiser to use InP for low fields (1–10 kV/cm), while for higher fields GaAs presents less noise.

B. Transient conditions

In this subsection we present the results obtained for the TSD in several instantaneous changes in the electric field both in GaAs and InP. We also show the evolution of different magnitudes during the transient that are of great interest for understanding and explaining the evolution of the TSD.

Initially, we shall analyze the transient from 1 to 25 kV/cm in both materials, that display very different kinds of behavior for this field change. In GaAs the TSD (Fig. 4) begins by taking low values (0.15 and 0.30 ps); thereafter it increases until it reaches a maximum value for 0.75 ps, then decreasing for longer times, and converging towards the SSD value of 25 kV/cm. Additionally, the value of the frequency for which the maximum is produced decreases as the transient occurs. By contrast, in InP (Fig. 5) the evolution is very different. Also starting from low values, the TSD increases progressively for longer times towards the stationary values corresponding to 25 kV/cm, although it never exceeds this. Also, the SSD is much higher than that of GaAs. The evolution of the maximum towards lower frequencies is similar in both materials.
When the field change in GaAs occurs, the carriers remain for some time (0.2 ps) in the $\Gamma$ valley [Fig. 6(a)], subject to a field of 25 kV/cm, such that their velocities evolve rapidly and uniformly toward higher values [Figs. 6(b) and 7] in long free flights. This causes the TSD to adopt small values and to exhibit its maximum for low frequencies in this range (0.15 and 0.3 ps). For longer times (0.3-0.75 ps) the carriers acquire high energy in the $\Gamma$ valley, leading to the appearance of intervalley mechanisms, transporting them to the $L$ and $X$ valleys. At this moment, the velocity of the carriers evolves under the effect of two very different effective masses, as shown by the two maxima of the velocity distribution functions of Fig. 7 for times of 0.3 and 0.4 ps. This, together with the velocity-disorienting effect of the intervalley mechanisms (isotropic), causes a maximum in the dispersion of the velocity [Fig. 6(b)] for these times, such that noise increases and the TSD acquires very high values, the maximum characteristic of the intervalley transitions appearing in it. Later, as the population of the valleys becomes more and more stabilized, all the magnitudes reach the stationary value for 25 kV/cm. Dispersion in velocity decreases because the proportion of carriers remaining in the $\Gamma$ valley is low, causing only a small zone of high velocities in the distribution function. Thus, for times longer than 1 ps the noise inherent to the material decreases progressively and the TSD converges towards the stationary value of the final field as $\tau$ increases, because the effect of the transient at those times becomes increasingly smaller. Throughout the process, the mean kinetic energy of the carriers, which regulates the total probability of interaction and hence the duration of the free flights, evolves as shown in Fig. 6(c), passing through a maximum and thereafter decreasing. This type of evolution strongly influences the behavior over time of the dominant frequencies of the spectral density, causing them to start by increasing, and thereafter decreasing.

In InP the carriers remain in the $\Gamma$ valley longer (0.5 ps) [Fig. 8(a)] from the moment at which the field
changes, owing to the greater $\Gamma$-$L$ energy gap. The velocity dispersion in this material [Fig. 8(b)] increases continuously as time progresses without showing any maximum, until it becomes saturated with a value far higher than the stationary value of GaAs; noise is therefore greater. This is because, unlike what happens in the case of GaAs, the effect of the $\Gamma$ valley does not disappear as the transient occurs, as shown in Fig. 9. Accordingly, under stationary conditions for 25 kV/cm there is a much more pronounced zone of high velocities owing to the high presence of carriers in this valley. All these factors mean that the TSD increases progressively and that it is always lower than the stationary value for 25 kV/cm, which it approaches for high values of $\tau$.

As may be seen, the behavior of both materials is very different during this transition. However, owing to the different band structure of InP, this material shows a similar response to that of GaAs in this transition for field changes to higher values, such as from 1 to 50 kV/cm.

To study a transition from a high to a lower field, we present the results corresponding to a change in the field from 25 to 1 kV/cm in GaAs. In this case, the duration of the transient is much longer than in the previous ones because it is not the high value of the electric field that governs the evolution of the carriers, but rather the relaxation effect of the different scattering mechanisms, which is much slower. In this case, the TSD (Fig. 10) does not show a maximum except that of the low frequencies, because the intervalley mechanisms are only produced to make the carriers descend to lower valleys, until all of them remain in the $\Gamma$ valley, whereas in the previous transitions they were produced continuously to maintain valley population balanced.

![FIG. 10. Transient spectral density of electron velocity fluctuations in the direction of the electric field as a function of frequency at several times in the transient from 25 to 1 kV/cm in GaAs.](image)

![FIG. 9. Velocity distribution functions for the longitudinal component at different times in the transient from 1 to 25 kV/cm in InP.](image)
FIG. 11. Evolution of several magnitudes in the transient as a function of the time elapsed from the change in the electric field from 25 to 1 kV/cm in GaAs: (a) valley occupation; (b) (—) average drift velocity in the electric-field direction and (—) its standard deviation; (c) (—) average total energy and (—) average kinetic energy.

Starting from the stationary situation for 25 kV/cm, when the field changes to 1 kV/cm the carriers begin to leave the L and X valleys, passing on to the Γ valley [Fig. 11(a)]. The velocity-disorienting effect of the intervalley mechanisms causes the component of the velocity in the direction of the electric field to diminish rapidly; at the same time as its dispersion increases [Fig. 11(b)]. Thus, as the carriers increasingly occupy the Γ valley, and evolve in it with a lower effective mass, velocity increases and dispersion decreases progressively, until they reach their stationary values. The evolution of the TSD is governed by the temporal behavior of the previous magnitudes. It begins by taking small values (0.4–1.4 ps) and increases due to the effect of the high dispersion zone (up to 4 ps), and then decreases towards the stationary value as dispersion becomes smaller, because the zone of high deviations has little effect for longer times (10 ps). The kinetic energy of the carriers decreases during the transient [Fig. 11(c)], such that the free flights become increasing longer and the dominant frequencies in the noise become lower. In the evolution of the total energy three regions with different relaxation constants can be seen; these correspond to the loss of energy in each of the valleys.

The evolution of the TSD for the same field change in InP (Fig. 12) is similar, except that since the dispersion in velocity for 25 kV/cm is much larger than for 1 kV/cm, the TSD is greater than the stationary value for 1 kV/cm at all times. The effect of high frequencies is also stronger because the free flights are shorter.

If one wishes to observe the effect of the change in the electric field on the initial SSD with greater clarity, in the time of analysis, \( t = t_1 + t_2 \), can be considered a first part \( t_1 \) corresponding to the first field in the stationary situation, and a second part \( t_2 \) corresponding to the second field. The time \( t_1 \) is taken long enough to give a value of \( S_0(f) \) in Eq. (7) corresponding to the SSD of the first field, and short enough not to give too much weight in \( S_0(f) \) to the initial stationary situation.

Figure 13 shows the transient from 1 to 25 kV/cm in GaAs analyzed in this way, with \( t_1 = 12 \) ps (sufficient time for the curve corresponding to 12 ps to be the stationary one for 1 kV/cm) and different \( t_2 \) up to 30 ps. It is seen that the SSD for 1 kV/cm becomes modified by the effect of the mechanisms occurring in the transient. Interestingly, there is one frequency whose spectral density remains almost constant throughout the process.

The velocity of the change in the spectral density from one situation to another depends on two factors. The first is the time \( t_1 \) considered. The smaller this is, the less will be the weight of the effect of the first field in Eq. (7) and the spectral density will evolve more quickly toward the stationary situation corresponding to the second field. The second is the magnitude of the SSD of each of the fields,
which will lead them to exert a greater or smaller effect. Thus, in the case of InP in the same transition (Fig. 14) and with $\tau_1 = 12$ ps and different $\tau_2$ up to 16 ps, since the SSD is much higher for 25 kV/cm, much less time corresponding to $\tau_2$ is required than in GaAs to similarly approach the stationary situation, $\tau_1$ being the same for both. In this case there is also a frequency, lower than in GaAs, that has a constant value in the transient.

Figure 15 shows a change in GaAs from 25 to 3 kV/cm, with $\tau_1 = 8$ ps and different $\tau_2$ up to 12 ps. In this, one observes the progressive shift of the dominant frequencies in the spectral density from high to low values, because the free flights increase as the carriers lose energy and the frequencies characteristic of the dominant intervalley mechanisms are different. In this case there is no frequency with constant amplitude.

FIG. 13. Spectral density of velocity fluctuations in the direction of the electric field as a function of frequency in the transient from 1 to 25 kV/cm in GaAs for several times $\tau_2$ from the change in the field, considering $\tau_1 = 12$ ps of the initial stationary situation for 1 kV/cm.

FIG. 15. Spectral density of velocity fluctuations in the direction of the electric field as a function of frequency in the transient from 25 to 3 kV/cm in GaAs for several times $\tau_2$ from the change in the field, considering $\tau_1 = 8$ ps of the initial stationary situation for 25 kV/cm.

V. CONCLUSIONS

Using a multiparticle Monte Carlo method we have presented a theoretical analysis of the spectral density of velocity fluctuations under both stationary and transient conditions in the two III-V semiconductors most widely used today: GaAs and InP. The main novelty lies in the transient analysis, for which a new method is used, since for finite times the method traditionally employed, consisting in calculating spectral density as the Fourier transform of the autocorrelation function, is not valid. The new method consists in calculating the Fourier transform of the velocity fluctuations particle per particle up to finite times in the transient.

Together with the calculation of the spectral density, the evolution of different magnitudes in the transient were recorded; these permit one to gain further insight into the microscopic processes responsible for noise. Significant differences are observed between the behaviors of both materials, mainly owing to the different band structures, especially due to the high value of the $\Gamma$-$L$ gap in InP as compared with GaAs. However, it was observed that both materials show similar behaviors, but in different ranges of the field applied.

The presence of a high proportion of carriers in the $\Gamma$ valley was found as the main source of the velocity fluctuations. Here they evolve with a low effective mass and when they are subjected to high fields, very high velocity electrons appear, causing large deviations from the mean value. Another important source of noise is the intervalley mechanisms (isotropic) that delocalize the orientation of the velocity of the carriers and cause the appearance of maxima in the spectral density.

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