Monte Carlo analysis of the transient spectral density of velocity fluctuations in semiconductors

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A multiparticular Monte Carlo method has been developed to calculate the spectral density of velocity fluctuations in transient conditions, when the electric field applied to a semiconductor changes. This method has been employed in the study of an instantaneous change in the electric field from 1 to 25 kV/cm in N-type GaAs. The results obtained are interpreted in terms of the phenomena occurring during the transient. The evolution of the transient spectral density for long times was found to converge at the steady state one of the final field.

One of the sources of noise in a semiconductor device is that inherent to the bulk material of which the device has been constructed. The Monte Carlo method is a powerful tool for the analysis of such problems. Using this method, different studies have been performed with the aim of analyzing the velocity fluctuations under steady-state conditions, and calculating their spectral density for different semiconductor materials[1–5] and in some devices.[6] Exhaustive research works on current spectral density have also been performed.[7–9] The frequency analysis can be done simply, applying the Wiener–Kintchine theorem,[10] by calculating the spectral density as the Fourier transform of the autocorrelation function.

However, in view of the high-working frequencies currently reached by such devices, and especially when these work under switching conditions, the semiconductor is not very often in a steady-state situation. There are also different factors that cause the appearance of noise in the output signal when a transient occurs. In particular, the study of the contribution of the noise inherent to the material in the transients has received little attention, and even less, its frequency analysis. Until the present, Monte Carlo simulations have been performed to analyze the evolution in the transient of velocity, energy, diffusion coefficient, and valley population;[11–13] and analyses have even been made of velocity fluctuations through transient autocorrelation functions,[5] but the spectral density in the transient has not been calculated. The main problem involved in calculating the spectral density resides in the fact that since the study of velocity fluctuations is performed over finite times during the transient, the Wiener–Kintchine theorem[10] cannot be applied, and the spectral density cannot be obtained as the Fourier transform of the autocorrelation function.

In the present letter, we describe a method for obtaining the spectral density of velocity fluctuations of electrons for different times in the transient. This is done starting from the values of velocity obtained from a Monte Carlo simulation.

Let us consider an ensemble of electrons undergoing, at $t=0$, a change in the value of the electric field to which they are subject. Let τ be the time up to which we wish to study the velocity fluctuations in the transient. Then, the function to be analyzed will be given by

$$\delta v_\tau(t)=\begin{cases}0 & \text{for } t<0,\\ \delta v(t) & \text{for } 0\leqslant t\leqslant\tau,\\ 0 & \text{for } t>\tau,\end{cases} \tag{1}$$

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

The Fourier transform of $\delta v_\tau(t)$, $\delta V_\tau(\omega)$, is

$$\delta V_\tau(\omega)=\int_{-\infty}^{\infty}\delta v_\tau(t)e^{j\omega t}\,dt=\int_0^\tau \delta v(t)e^{j\omega t}\,dt. \tag{2}$$

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

$$\overline{\delta v_\tau^2}=\frac{1}{\tau}\left\langle\int_0^\tau \delta v^2(t)dt\right\rangle. \tag{3}$$

By the Parseval theorem,[14] and because $\delta v(t)$ is real, it follows that

$$\overline{\delta v_\tau^2}=\frac{1}{\tau}\left\langle\frac{1}{2\pi}\int_{-\infty}^{\infty}\left|\delta V_\tau(\omega)\right|^2 d\omega\right\rangle$$
$$=\int_{-\infty}^{\infty}\frac{1}{2\pi\tau}\langle|\delta V_\tau(\omega)|^2\rangle d\omega. \tag{4}$$

Now we define the transient spectral density up to a time τ, $S_\tau(f)$, with $f=\omega/2\pi$, by

$$\overline{\delta v_\tau^2}=\int_{-\infty}^{\infty}S_\tau(f)df, \tag{5}$$

and we obtain

$$S_\tau(f)=\frac{1}{\tau}\langle|\delta V_\tau(\omega)|^2\rangle=\frac{1}{\tau}\left\langle\left|\int_0^\tau \delta v(t)e^{j\omega t}dt\right|^2\right\rangle. \tag{6}$$

$S_\tau(f)$ provides information about the mean power dissipated between 0 and τ in the transient by velocity fluctuations of frequencies ranging between f and $f+df$.

Using this technique, we analyze a transient in N-type homogeneous GaAs ($N_D=10^{15}\ \mathrm{cm}^{-3}$) at 300 K, in which the electric field rises from 1 to 25 kV/cm. An ensemble Monte Carlo with 100 000 particles has been used to perform the simulation. We consider the conduction band

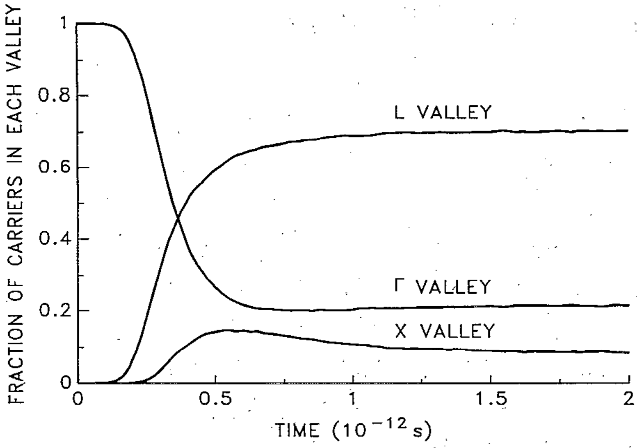

FIG. 1. Fraction of electrons in each valley as a function of the time elapsed from the change in the electric field from 1 to 25 kV/cm.

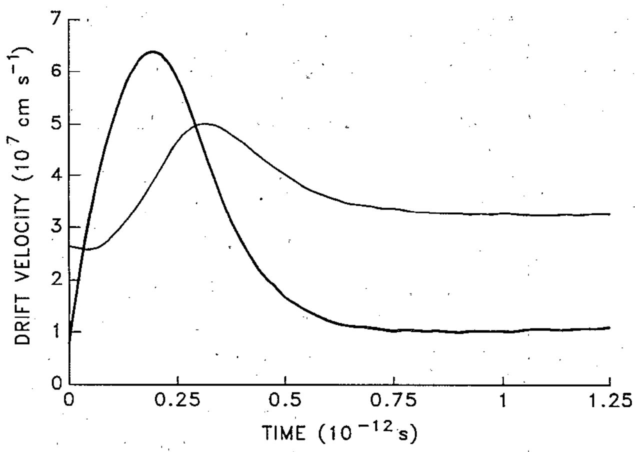

FIG. 2. (━) Average drift velocity in the electric field direction, and (—) its standard deviation as a function of the time elapsed from the change in the electric field from 1 to 25 kV/cm.

formed of three nonparabolic spherical valleys. The scattering mechanisms taken into account are: ionized impurities, acoustic, piezoelectric, polar optical, nonpolar optical, and intervalley (equivalent and nonequivalent) mechanisms. The physical parameters of the GaAs used in the simulation are the same as those used for the valleys of the first conduction band in previous works,[15] and already used by other authors.[16,17]

Initially, the 100 000 carriers are placed in the Γ valley with the thermic energy, and they move under the action of an electric field of 1 kV/cm for sufficient time (6 ps) for the steady state to be reached. When this time has elapsed, an instantaneous change occurs in the field to a value of 25 kV/cm, the moment at which the time origin is taken up again, thereafter recording the velocity of each of the particles every 1.25×10^{-14} s. At the same time, the evolution of different magnitudes (valley population, mean energy, and mean velocity) is registered during the transient. These magnitudes are useful for the microscopic interpretation of the results obtained for $S_T(f)$. Following this, the calculations indicated in Eq. (6) are performed. Seventy hours of CPU time were spent on an IBM RISC 6000/320 system to obtain the results that are shown below.

Figure 1 shows the evolution in the transient of the population in each valley. Initially (steady-state situation for 1 kV/cm), all the carriers are in the Γ valley. When the electric field rises to 25 kV/cm, the electrons evolve in that valley (mainly interacting with ionized impurities and polar optical phonons), where they gain energy and velocity very fast owing to the low effective mass and the high value of the electric field, until they acquire sufficient energy for the intervalley scattering mechanisms to transport them to the higher L and X valleys. At that moment (0.18 ps) the mean drift velocity reaches a maximum (Fig. 2), thereafter decreasing with the rise in the effective mass of the carriers in the L and X valleys. As from 0.75 ps, a steady-state situation is reached in the velocity, but not in the population of the valleys, which does not become stabilized until 1.5 ps.

The analysis of the dispersion of the carrier velocities over the mean value is of great interest for later interpreting the transient spectral density. At the beginning of the transient, while the carriers remain in the Γ valley, their velocities evolve uniformly towards high values, with which the standard deviation (Fig. 2) takes a low value, in fact lower than the steady state one for 1 kV/cm. For longer times, intervalley scattering mechanisms begin to appear, which delocalize the carrier velocity and cause this to evolve under the effect of very different effective masses (that of the Γ valley and that of the L valley), this in turn causing an increase in dispersion, as observed in Fig. 2 for times between 0.15 and 0.35 ps. Finally, when the population of the valleys begins to become stabilized, the deviation decreases, until after 0.75 ps it remains constant (steady-state value).

Figure 3 shows the transient spectral density of the noise up to different times. Up to 0.15 ps, all the carriers evolve uniformly in the Γ valley, barely undergoing any isotropic mechanisms, and with quite long free flights,

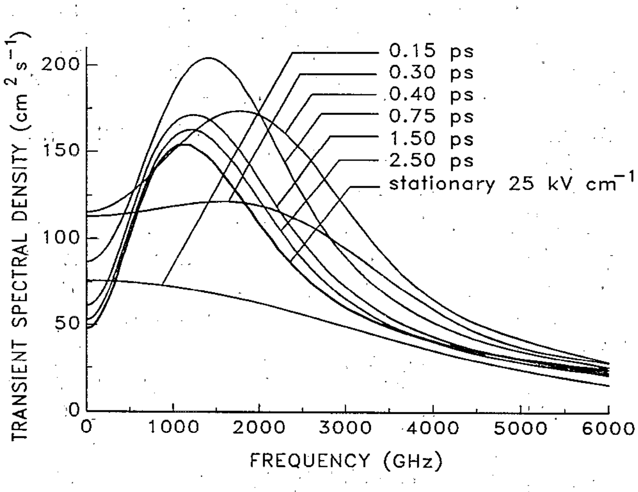

FIG. 3. Transient spectral density of electron velocity fluctuations vs frequency at several times in the transient from 1 to 25 kV/cm, and stationary spectral density for 25 kV/cm.

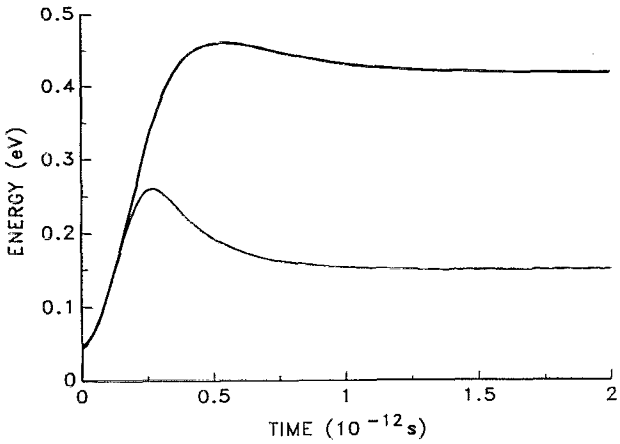

FIG. 4. (━) Average total energy, and (—) average kinetic energy as a function of the time elapsed from the change in the electric field from 1 to 25 kV/cm.

since their kinetic energy is low (Fig. 4). This is why the spectral density takes low values and decreases continuously with the increase in frequency. As longer times are reached (0.3 ps), the carriers begin to acquire greater energy and the appearance of intervalley mechanisms (Γ–L and Γ–X) causes a delocalization of the velocities, thus implying an increase in the noise spectrum, especially for high frequencies (1500–2500 GHz), as corresponds to the increase in mean kinetic energy (Fig. 4). Between 0.4 and 0.75 ps, the greatest number of intervalley mechanisms occurs, which means that at this range the highest values of spectral density are reached and, in turn, the mean kinetic energy of the carriers decreases, such that the free flights are longer and the dominant frequencies of the noise begin to decrease. As from 0.75 ps, the population of the different valleys begins to stabilize; the number of isotropic mechanisms decreases, noise decreasing with this and the frequencies at which the maximum appears becoming lower. Finally, for longer times (2.5 ps, when the steady state has already been reached) the effects of the transient up to that time have very little effect, such that the spectral density approaches that corresponding to the steady-state situation for a field of 25 kV/cm (obtained as the Fourier transform of the autocorrelation function[5]). As expected, the evolution of the transient spectral density converges toward that corresponding to the steady-state situation for a field of 25 kV/cm as τ increases.

We are currently analyzing several transients both in GaAs and in InP. The first results obtained show very interesting differences in transient frequency behavior between both materials. These results will be published elsewhere.

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[1] G. Hill, P. N. Robson, and W. Fawcett, J. Appl. Phys. **50**, 356 (1979).
[2] R. Fauquembergue, J. Zimmermann, A. Kaszynski, and E. Constant, J. Appl. Phys. **51**, 1065 (1980).
[3] D. K. Ferry and J. R. Barker, J. Appl. Phys. **52**, 818 (1981).
[4] R. Brunetti and C. Jacoboni, Phys. Rev. Lett. **50**, 1164 (1983).
[5] R. Brunetti and C. Jacoboni, Phys. Rev. B **29**, 5739 (1984).
[6] J. Zimmermann and E. Constant, Solid-State Electron. **23**, 915 (1980).
[7] T. Kuhn, L. Reggiani, L. Varani, and V. Mitin, Phys. Rev. B **42**, 5702 (1990).
[8] T. Kuhn, L. Reggiani, and L. Varani, Phys. Rev. B **42**, 11 133 (1990).
[9] T. Kuhn, L. Reggiani, and L. Varani, J. Appl. Phys. **69**, 7097 (1991).
[10] D. A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976), pp. 553–559.
[11] J. G. Ruch, IEEE Trans. Electron Devices **ED-19**, 652 (1972).
[12] M. Abe, S. Yanagisawa, O. Wada, and H. Takanashi, Appl. Phys. Lett. **25**, 674 (1974).
[13] T. J. Maloney and J. Frey, J. Appl. Phys. **48**, 781 (1977).
[14] P. M. Morse and F. Herman, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 1, pp. 456–458.
[15] T. González, J. E. Velázquez, P. M. Gutiérrez, and D. Pardo, Semicond. Sci. Technol. **6**, 862 (1991).
[16] M. A. Littlejohn, J. R. Hauser, and T. H. Glisson, J. Appl. Phys. **48**, 4587 (1977).
[17] K. Brennan and K. Hess, Solid-State Electron. **27**, 347 (1984).