Diagonal and Off-Diagonal Contributions to Autocorrelation of Velocity Fluctuations in Semiconductors

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A theoretical analysis of velocity fluctuations in semiconductors is presented, and results obtained from a Monte Carlo procedure are shown for Si. It has been found in particular that (i) off-diagonal contributions to the velocity autocorrelation function must be taken into account; (ii) the convective contribution is positive; and (iii) a long tail in the autocorrelation function, due to intervalley fluctuations, may be present.

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In recent times the analysis of velocity fluctuations of charge carriers in semiconductors in presence of high external electric fields has received renewed attention[1-11] both because of its relevance in microelectronics applications,[12] and because an analysis of noise at sufficiently high frequencies can yield significant information on the microscopic processes involved in transport physics. However, no rigorous account has yet been given of the different sources for such fluctuations. In the present paper a general analysis of carrier velocity fluctuations in semiconductors will be given.

Let us consider a homogeneous ensemble of electrons subject to a uniform static electric field $\vec{E}$ of arbitrary strength, and in steady-state conditions. Considering for simplicity only the field direction, we define v_d as the drift velocity, i.e., the mean velocity of all electrons, $v_v(t)$ as the valley drift velocity, i.e., the mean velocity of electrons in valley $V(t)$ in which an electron under consideration is at time t, and $v_\epsilon(t)$ as the mean velocity of electrons with energy between ϵ and $\epsilon + d\epsilon$ in valley $V(t)$, where $\epsilon(t)$ is the energy of the considered electron at time t. The fluctuation of the instantaneous velocity $v(t)$ of each electron over the drift value can then be written as a sum of a number of terms which account for the different physical sources of fluctuations:

$$\delta v(t) \equiv v(t) - v_d = \delta v_v(t) + \delta v_\epsilon(t) + \delta v_k(t), \qquad (1)$$

where $\delta v_v(t) = v_v(t) - v_d$ is the fluctuation associated with the drift velocity of the valley in which an electron lies at time t with respect to the total drift velocity, $\delta v_\epsilon(t) = v_\epsilon(t) - v_v(t)$ is the velocity fluctuation associated with the fluctuation of electron energy at time t, with respect to the valley drift velocity, and $\delta v_k(t) = v(t) - v_\epsilon(t)$ is the velocity fluctuation associated with the fluctuation of the electron momentum $k(t)$, with respect to the average velocity of all electrons with the same energy $\epsilon(t)$.

The autocorrelation function of velocity fluctuations,

$$C(\tau) \equiv \langle \delta v(t)\, \delta v(t+\tau) \rangle, \qquad (2)$$

becomes, by use of the expression in Eq. (1),

$$C(\tau) = \sum_{i,j=1}^{3} \langle \delta v_i(t)\, \delta v_j(t+\tau) \rangle = \sum_{i,j=1}^{3} C_{ij}(\tau), \qquad (3)$$

where $i, j = v, \epsilon, k$. The three diagonal terms $(i=j)$ in the above equation are at the origin of intervalley,[13] convective,[14] and thermal[14] noise, respectively.

Equation (3) shows that off-diagonal terms $(i \neq j)$ may also contribute to the total autocorrelation function and, therefore, to diffusion and noise. It has sometimes been implicitly assumed in the literature that the total noise due to velocity fluctuations is given by the sum of the three diagonal contributions. This restrictive assumption is correct only when the relaxation times of the various fluctuating terms have well differentiated values,[14] so that in calculating the off-diagonal terms one of the two fluctuating terms can be assumed as constant, while the other averages to zero.

As is well known, diffusion and noise are strictly connected with the autocorrelation function of velocity fluctuations through the equation

$$D(\omega) = \int_0^{+\infty} C(\tau) e^{i\omega\tau}\, d\tau = \tfrac{1}{2} S_v(\omega). \qquad (4)$$

As a result of the linearity of the above expression, we can associate specific terms in the autocorrelation function with corresponding terms in the diffusion constant and noise, thus making explicit their physical origins.

We have obtained the autocorrelation function $C(\tau)$, as given in Eq. (3), from a Monte Carlo procedure; then the noise spectral density was calculated by means of a numerical evaluation of Eq. (4). In the following, results for Si as a typical example will be analyzed. The model used in calculations is that reported in Ref. 15.

Figure 1 shows the autocorrelation function of velocity fluctuations for electrons in Si at 77 K with an electric field $E = 10$ kV/cm applied along $\langle 111\rangle$ and $\langle 100\rangle$ directions. After an initial sharp decay, a negative part of $C(\tau)$ is present in both cases. When $\vec{E}$ is along a $\langle 111\rangle$ direction, the negative part goes directly to zero, while in the other case a positive slowly decaying contribution is present, which also reduces the negative part of $C(\tau)$.

In order to understand the physical origin of these curves, it is useful to analyze the different contributions $C_{ij}(\tau)$. Figure 2(a) reports the diagonal terms of $C(\tau)$ when $\vec{E}$ is along a $\langle 100\rangle$ direction. The intervalley contribution $C_{vv}(\tau)$ is seen to be responsible for the long tail of the total autocorrelation function; in fact the intervalley transition time is the longest of the characteristic times of the transport process under these conditions of field and temperature.

The convective contribution $C_{\epsilon\epsilon}(\tau)$ has a regular behavior with a small negative part, while the thermal contribution $C_{kk}(\tau)$ has a large negative part to which most of the negative part of the total $C(\tau)$ can be ascribed. Furthermore the off-diagonal term $C_{\epsilon k}(\tau)$, shown in Fig. 2(b), also contributes appreciably to the negative part of $C(\tau)$, partially compensated by the positive $C_{k\epsilon}(\tau)$ (other off-diagonal terms are negligible in this case).

The particular form of these contributions is related to the energy dependence of the scattering mechanisms. In fact, if at a given time t a positive fluctuation of the electron momentum occurs, then at a later time, because of the larger absorbed power, a positive fluctuation of energy is likely to occur, which, in turn, leads to an increase of the scattering efficiency, so that a scattering will occur with larger probability. Since each scattering mechanism is momentum randomizing, at longer times negative fluctuations of momentum will follow. Furthermore the Monte Carlo analysis has proved that in our case v_ϵ is an increasing function of ϵ, as shown in

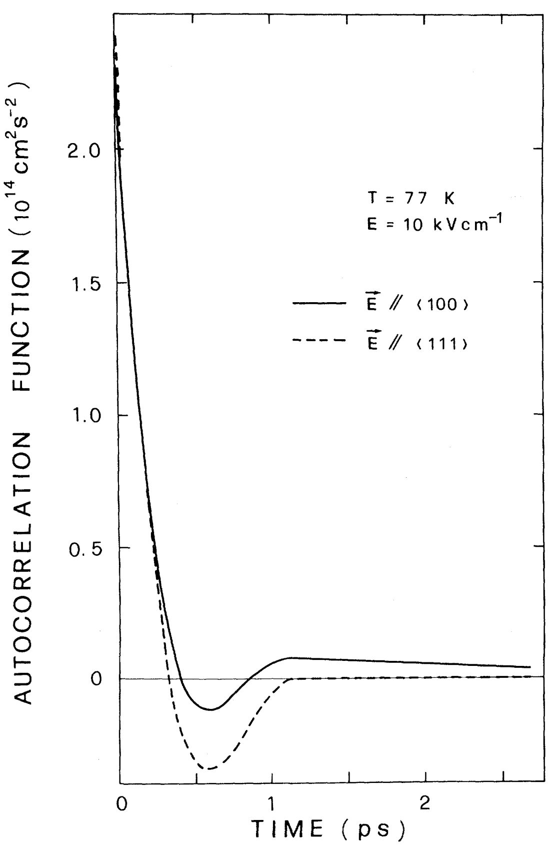

FIG. 1. Autocorrelation function of velocity fluctuations for electrons in Si at the indicated temperature and fields.

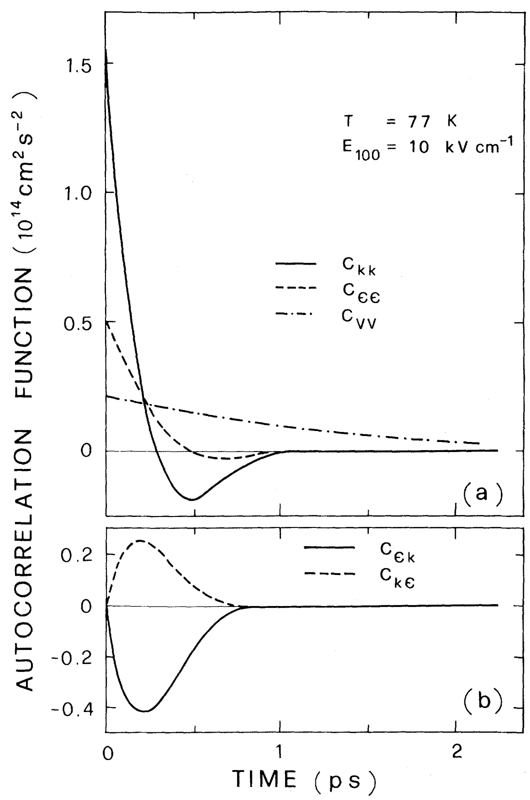

FIG. 2. (a) Diagonal and (b) off-diagonal terms of the autocorrelation function of velocity fluctuations for electrons in Si at the indicated temperature and field.

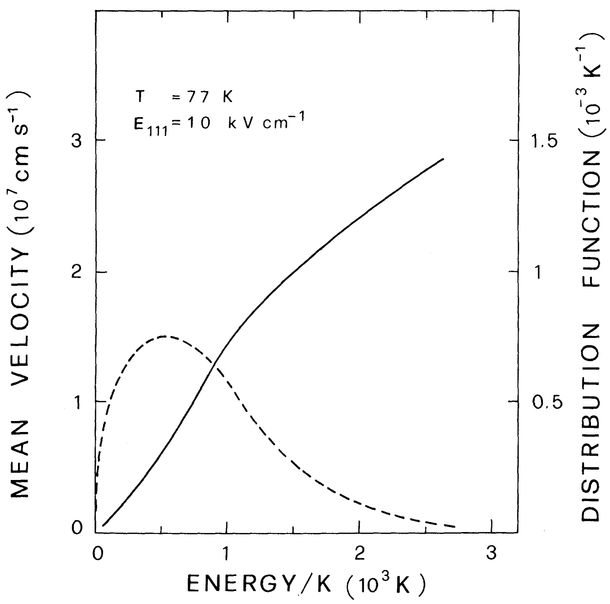

FIG. 3. Mean velocity (continuous line and left scale), and distribution function (dashed line and right scale), as functions of energy for electrons in Si at the indicated temperature and field (in kilovolts per centimeter).

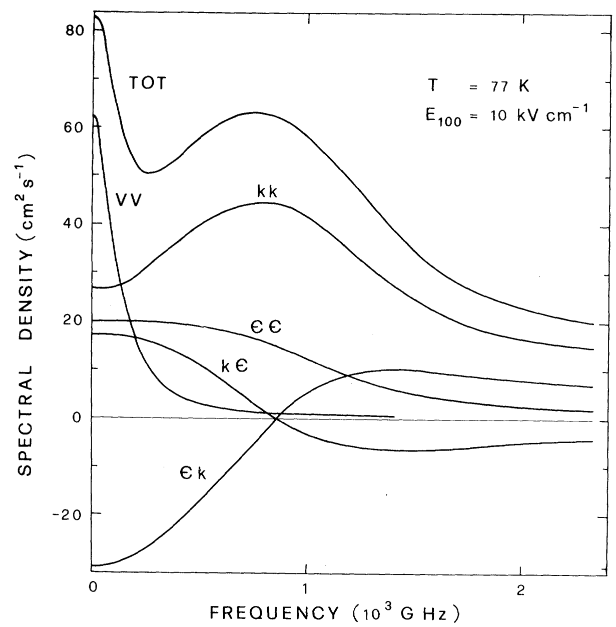

FIG. 4. Spectral density of velocity fluctuations and its components for electrons in Si at the indicated temperature and field.

Fig. 3, so that a positive energy fluctuation will correspond to a positive velocity fluctuation δv_ϵ.

By collecting the above considerations, it can be understood why $C_{k\epsilon}$ is positive, $C_{\epsilon k}$ is negative, and C_{kk} is positive at smaller τ and negative at larger τ with a minimum which is reached at times greater than the extrema of $C_{k\epsilon}$ and $C_{\epsilon k}$. In this case, therefore, the fact that the scattering probability is an increasing function of energy yields a negative contribution to diffusivity[8,16] through a negative part in C_{kk} and in $C_{\epsilon k}$, and not through a negative convective contribution $C_{\epsilon\epsilon}$.

In a transverse direction, velocity fluctuations are only due to thermal fluctuations ($v_d = v_v = v_\epsilon = 0$); their autocorrelation is always positive, since no energy transfer is associated with velocity fluctuations. For this reason $D_\perp > D_\parallel$. When the electric field is applied along a $\langle 111\rangle$ direction, all the above considerations are still valid with the exception of the intervalley contribution which, in this case, is absent in the longitudinal direction, but present in a transverse direction.[15]

Recent energy-velocity cross correlations $\langle \delta\epsilon(t)\delta v(t+\tau)\rangle$ and $\langle \delta v(t)\delta\epsilon(t+\tau)\rangle$ have been presented for the case of Si with $\vec{E} \parallel \langle 111\rangle$[17]; their behaviors are similar to those of $C_{k\epsilon}$ and $C_{\epsilon k}$ shown in Fig. 2(b). This is so because, as we already noticed, a positive energy fluctuation is, in general, associated with a positive fluctuation of δv_ϵ and the major contribution to $\delta v(t)$ comes from $\delta v_k(t)$. However, in Ref. 17 no analysis of the different contributions to δv like that in Eq. (1) was introduced.

Figure 4 shows the noise spectral density $S_v(\omega)$ for the case of $\vec{E} \parallel \langle 100\rangle$ discussed above. Again, the peculiar shape of the total $S_v(\omega)$ can be understood from the analysis of its partial contributions, also shown in Fig. 4.

The white-noise value of the total spectrum, corresponding to a diffusion coefficient of 41 cm^2 sec^{-1}, is strongly influenced by the large intervalley contribution ($D_{int} = 31$ cm^2 sec^{-1}). This term shows the most rapid decrease at increasing frequencies as a result of the largest relaxation time of the intervalley velocity fluctuations. The thermal contribution to the white-noise level is relatively small ($D_{kk} = 14$ cm^2 sec^{-1}) as an effect of the cancellation of the negative and positive parts of C_{kk}, and a bump is present, due to the strong oscillation of C_{kk}. The convective contribution, with a white-noise level corresponding to $D_{\epsilon\epsilon} = 10$ cm^2 sec^{-1}, is present with a monotonically decreasing behavior, and is always positive. The off-diagonal terms $S_{k\epsilon}$ and $S_{\epsilon k}$ have similar shapes of opposite signs; their cumulative contribution, which is relatively small, is negative at low frequencies, corresponding to a negative contribution to diffusivity, and becomes positive at high frequencies.

Calculations have also been performed for GaAs at room temperature and $E = 10$ kV/cm. The results, which will be published elsewhere, are consistent with the above physical interpretation applied to the transfer-electron model of GaAs.

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