Spatial extent of the correlation between local diffusion noise sources in GaAs

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We present a microscopic analysis of the spatial correlation between local diffusion noise sources in homogeneous GaAs. The calculations are performed by using an ensemble Monte Carlo simulation. The spatial extent of the correlations is determined for different applied electric fields. It is confirmed that the space correlations do exist over short distances, ranging from 0.1 to 0.6 μm depending on the electric field. This correlation length is much longer in GaAs than in Si. It is shown that the diffusion coefficient can be decomposed into the contribution of cross-correlations between close cells inside a homogenous sample. Under far-from-equilibrium conditions, the forward correlations at low frequency are found to be spatially shorter than those with the backward positions due to the effect of the randomizing scattering mechanisms. © *1995 American Institute of Physics.*

I. INTRODUCTION

Traditional techniques dealing with the study of noise in electronic devices, such as the impedance-field method,[1,2] need, apart from the calculation of the impedance field, the knowledge of the local noise sources. These methods usually assume that there is no correlation between the diffusion noise sources at two different positions.[3] This assumption has been demonstrated to be false.[4,5] On the contrary, the spatial correlations are quite important over distances of the order of some mean free paths of the carrier in the semiconductor. The reason is that over lengths shorter than the distance traveled by a carrier between two scattering mechanisms, the fluctuation in its velocity is only slightly modified by the electric field (as compared with the randomizing effect of the collisions), and hence the velocity fluctuations remain strongly correlated. So, to account for all the noise contributions related to a given point, it is necessary to consider a volume around it. The works on this topic performed to date consist of a theoretical demonstration of the spatial correlation,[4] the derivation of an analytical expression for the spatial cross-correlation at thermal equilibrium,[6] and an approximate evaluation of the correlation length in a Si nonhomogeneous structure.[5,7] To our knowledge, the results given so far correspond to Si. In the case of GaAs, due to the nonrandomizing nature of the dominating scattering mechanisms at low fields, the space correlation is expected to remain for longer distances.

The purpose of this work is to demonstrate the existence of spatial correlation between local noise sources and compute the distance over which it extends in homogeneous GaAs under different applied electric fields. To this end, we shall use the Monte Carlo method,[8] which has the advantage over all other techniques of making no supposition about the behavior of the noise sources. Particularly, we shall study diffusion noise due to carrier velocity fluctuations.

This article is organized as follows. Section II presents the theoretical basis of the subject and their equivalence in a Monte Carlo simulation. In Sec. III the details of the Monte Carlo simulation used for the calculations and the physical model employed for GaAs are described. The results are reported and discussed in Sec. IV. Finally, in Sec. V the main conclusions are summarized.

II. THEORETICAL ANALYSIS

The local current density $\mathbf{j}(\mathbf{r},t)$ at point $\mathbf{r}$ and time t is given by the sum of a steady-state current $\mathbf{j}_0(\mathbf{r})$ and a fluctuation $\Delta\mathbf{j}(\mathbf{r},t)$:

$$\mathbf{j}(\mathbf{r},t)=\mathbf{j}_0(\mathbf{r})+\Delta\mathbf{j}(\mathbf{r},t). \tag{1}$$

The two-point cross-correlation function of the current density is defined as:

$$C_{J\alpha\beta}(\mathbf{r},\mathbf{r}',\theta)=\langle j_\alpha(\mathbf{r},t)\Delta j_\beta(\mathbf{r}',t+\theta)\rangle^t, \tag{2}$$

where α and β are any of the x, y, or z directions, and the angular brackets indicate time average.

The noise-source term associated to this correlation is the Fourier transform of the cross-correlation function, which for a frequency f is:

$$S_{J\alpha\beta}(\mathbf{r},\mathbf{r}',f)=4\int_0^\infty C_{J\alpha\beta}(\mathbf{r},\mathbf{r}',\theta)\cos 2\pi f\theta\, d\theta. \tag{3}$$

In the following we shall suppress the subscripts indicating direction, since in our case only correlations in the direction of the electric field will be calculated.

Let i be the ith carrier inside a sample. The local current density fluctuation in the field direction at a time t is given by

$$\Delta j(\mathbf{r},t)=q\sum_i [v_i(t)-v_0(\mathbf{r})]\delta[\mathbf{r}-\mathbf{r}_i(t)]$$

$$=q\sum_i \Delta v_i(\mathbf{r},t)\,\delta[\mathbf{r}-\mathbf{r}_i(t)], \tag{4}$$

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where q is the absolute value of the electron charge, $v_i(t)$ the instantaneous velocity of the ith carrier in the field direction, $v_0(\mathbf{r})$ the average longitudinal velocity at point $\mathbf{r}$, and $\mathbf{r}_i(t)$ the instantaneous position of the ith carrier. The summation extends over all the carriers inside the sample.

By carrying (4) into (2), we have

$$C_J(\mathbf{r},\mathbf{r}',\theta)=q^2\sum_{i,j}\langle\Delta v_i(\mathbf{r},t)\delta[\mathbf{r}-\mathbf{r}_i(t)] \times\Delta v_j(\mathbf{r}',t+\theta)\delta[\mathbf{r}'-\mathbf{r}_j(t+\theta)]\rangle^t. \quad (5)$$

In the Monte Carlo simulation the sample is divided into cells. For each of them we store, at every time interval dt, the mean velocity of the carriers that are inside them at that moment. Considering the whole simulation time, we have the average velocity in each cell n, $v_0(n)$, and the cross correlations are calculated from the fluctuations of the carrier mean velocity at each time interval. It must be clarified that, in this way, the cross-correlations are not calculated between points, but between meshes. So, in the following we shall denote them as $C_J(n,m,\theta)$, where n and m indicate the meshes they are referred to. Thus, to obtain analytically $C_J(n,m,\theta)$, Eq. (5) must be integrated on $\mathbf{r}$ over the volume V_n corresponding to the cell n, and on $\mathbf{r}'$ over the volume V_m of the cell m. In this way we arrive at

$$C_J(n,m,\theta)=\int_{V_n}\int_{V_m} d^3\,r d^3\,r' C_J(\mathbf{r},\mathbf{r}',\theta) =q^2\sum_{i,j}\langle\Delta v_i(n,t)\Delta v_j(m,t+\theta)\rangle^t, \quad (6)$$

where $\Delta v_i(n,t)=v_i(t)-v_0(n)$. Now the summation over i extends to the carriers that are in the cell n at the instant t, and the summation over j to those in the cell m at the instant $t+\theta$. The correlation is expected to persist over distances that carriers may travel without undergoing any randomizing scattering mechanism.

We define $\Delta\bar{v}_n$ as the fluctuation of the mean velocity of the carriers present inside the cell n

$$\Delta\bar{v}_n(t)=\sum_i \Delta v_i(n,t)/N_n(t), \quad (7)$$

where $N_n(t)$ is the number of carriers in the cell n at time t. We are interested in studying only diffusion noise. Therefore, we shall focus in the contribution to the current fluctuations coming from the velocity fluctuations, without considering that of the carrier number and its cross-correlation with the velocity.[9] Consequently, for diffusion noise we have:

$$C_J(n,m,\theta)=q^2N_nN_m\langle\Delta\bar{v}_n(t)\Delta\bar{v}_m(t+\theta)\rangle^t =q^2N_nN_mC_v(n,m,\theta), \quad (8)$$

where N_n is the average number of carriers in the cell n during the simulation, and $C_v(n,m,\theta)$ is the cross-correlation function of mean velocity fluctuations corresponding to the cells n and m, which is the magnitude to be calculated in the simulation.

In this way, from (3) we can express the noise-source term associated with the meshes n and m as

$$S_J(n,m,f)=4q^2N_nN_m\int_0^\infty C_v(n,m,\theta)\cos 2\pi f\theta\, d\theta. \quad (9)$$

Within the impedance-field method it is usually considered that the local source of diffusion noise is[2,3]

$$S_J(\mathbf{r},\mathbf{r}',f)=4q^2n(\mathbf{r})D(\mathbf{r},f)\delta(\mathbf{r}-\mathbf{r}'), \quad (10)$$

where $D(\mathbf{r},f)$ is the frequency-dependent longitudinal diffusion coefficient corresponding to the local electric field and $n(\mathbf{r})$ the carrier density, both referred to the point $\mathbf{r}$. Equation (10) assumes that there is no spatial correlation between the noise sources, so that all the noise contribution associated with the position $\mathbf{r}$ is localized at $\mathbf{r}$, and is characterized by the diffusion coefficient. In the case of a whole cell, and following the same scheme already employed to pass from (5) to (6), Eq. (10) becomes

$$S_J(n,f)=4q^2N_nD_n(f) \quad (11)$$

with $D_n(f)$ the longitudinal diffusion coefficient corresponding to the electric field present at the cell n. Equation (11) indicates again that all the noise contributions associated with the cell n are localized inside it and characterized by the diffusion coefficient.

From (9) we can define

$$D_{nm}(f)=N_m\int_0^\infty C_v(n,m,\theta)\cos 2\pi f\theta\, d\theta \quad (12)$$

as the contribution to the diffusion coefficient in the cell n from the correlation with the cell m, so that

$$S_J(n,m,f)=4q^2N_nD_{nm}(f). \quad (13)$$

Forward and backward correlations are studied according to the conditions $n<m$ and $n>m$, respectively. To take into account all the noise sources associated with the cell n, it is necessary to add up the correlations with close cells

$$S_J(n,f)=\sum_m S_J(n,m,f)=4q^2N_n\sum_m D_{nm}(f). \quad (14)$$

By comparing (11) with (14), Eq. (11) holds only if

$$D_n(f)=\sum_m D_{nm}(f), \quad (15)$$

where the summation extends over the cells within a distance long enough for the space correlation to disappear. Of course, the difference between (11) and (14) is that while in the former all the noise source is spatially localized in one cell, in the latter it is distributed into those over which the correlation persists. As we shall see, there are situations in which (15) is not true.

III. MONTE CARLO SIMULATION

The theory previously reported in Sec. II has been applied to the case of homogeneous samples of n-type GaAs at 300 K. The calculations are performed by using an ensemble Monte Carlo simulation, three dimensional in momentum space and one dimensional in real space. The samples are divided into equal cells of 100 Å. The number of simulated

particles range between 15 000 and 21 000 depending on the length of the structures, so that at least 100 carriers were initially placed at each mesh. This number of carriers in each cell is large enough for its relative fluctuation during the simulation to be lower than 10%. In order to assure the homogeneity of the semiconductor, periodic boundary conditions are considered at the ends of the samples.[9] The length of the simulated structures is always longer than the double of the distance over which the spatial correlations persist. In other cases, and due to the boundary conditions, artificial correlations could be introduced, since the influence of both directions would overlap. In any case, it has been concluded that the results are the same when the length of the samples is increased twice. During the simulation the electric field is kept constant (Poisson's equation is not solved) in order to avoid coupling between the fluctuations of carrier velocity and electric field.[5,9] The carrier kinetics inside the samples are simulated during 1 ns (divided into time steps of 10 fs) in order to achieve an adequate resolution of the cross-correlation functions.

The model for the GaAs conduction band consists of three nonparabolic spherical valleys (Γ, L and X). The scattering mechanisms taken into account are the following: ionized impurities, polar optical, both assumed as anisotropic; nonpolar optical, acoustic, and intervalley (equivalent and nonequivalent), all of which are considered isotropic. The GaAs physical parameters employed in the simulation are the same as those used for the valleys of the first conduction band in previous works,[10] except for the acoustic deformation potential, whose value is 5 eV in the three valleys. At low fields the dominating scatterings are the interaction with ionized impurities and the polar optical. Due to the anisotropic nature of both mechanisms, a longer correlation length than in Si is expected.

IV. RESULTS

Before reporting the results of the spatial correlation analysis, we consider it interesting to show the values obtained for the longitudinal diffusion coefficient as a function of the electric field in GaAs with the present model (Fig. 1). These values were calculated by using the two conventional techniques[8] (from the autocorrelation function of velocity fluctuations of a single carrier, and from the second central moment of an ensemble of carriers), which were found to give practically the same results. Two different doping levels were analyzed: 5×10^{15} cm^{-3} and 10^{17} cm^{-3}. The main differences between them appear at low fields, where the effect of the interaction with ionized impurities is more important, reducing considerably the values of the diffusion coefficient for 10^{17} cm^{-3}. Also plotted in Fig. 1 (squares) are the results obtained for the low-frequency value of the diffusion coefficient through Eq. (15), by adding the contributions from the cross-correlation with the cells over which the spatial correlation extends. As can be observed, these values are in good agreement with those obtained by the other techniques within the statistical error of the Monte Carlo method. The uncertainty in these calculations has been estimated to be within a $\pm15\%$ due to the long time tail of the cross-correlation functions (which do not vanish completely, but oscillate around zero) when integrated to calculate the Fourier transforms. To increase the accuracy, a higher number of carriers and a longer simulation time are needed: requirements which are not always affordable from the point of view of computation time.

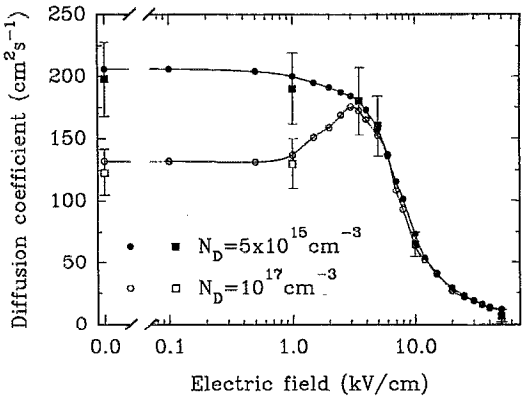

FIG. 1. Low-frequency value of the longitudinal diffusion coefficient as a function of the electric field in GaAs for two impurity concentrations: 5×10^{15} and 10^{17} cm^{-3}. The squares correspond to the values obtained by adding the contributions from the cross-correlations.

Figure 2 shows the cross-correlation functions of carrier velocity fluctuations between cells placed at different distances, $C_v(n,m,t)$, for an electric field of 10 kV/cm and a doping of 5×10^{15} cm^{-3}. It can be observed how the correlation decreases as the distance grows. The peak of the cross-correlation functions takes place for the average time spent by the carriers to cover the distance between cells without undergoing any randomizing interaction, thus appearing for shorter times in the forward correlations than in the backward ones. Moreover, the forward correlations exhibit a higher peak, which, however, drops faster. Hence, their contributions to the diffusion coefficient (at low frequency) are smaller than those of the opposite direction. The longer time tail of the backward cross-correlation functions is associated

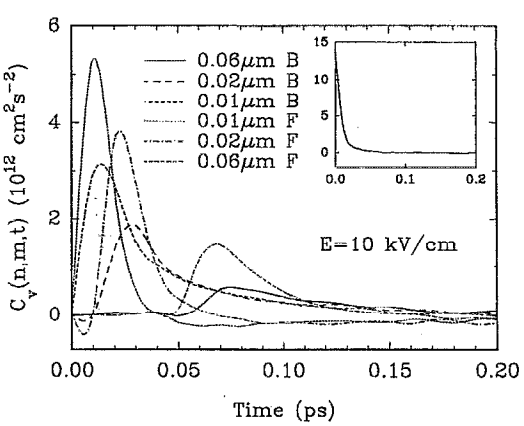

FIG. 2. Autocorrelation (inset) and cross-correlation functions of velocity fluctuations between cells at distances of 0.01, 0.02 and 0.06 μm in both directions: forwards (F) and backwards (B). The electric field is 10 kV/cm.

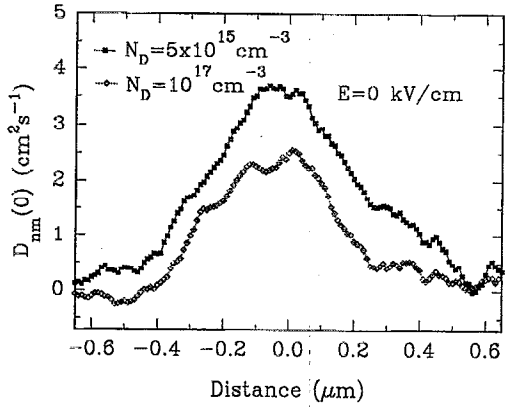

FIG. 3. Contribution to the low-frequency diffusion coefficient in a cell located at 0.0 μm from the correlation with cells at different distances for two impurity densities, 5×10^{15} and 10^{17} cm^{-3}, at thermal equilibrium.

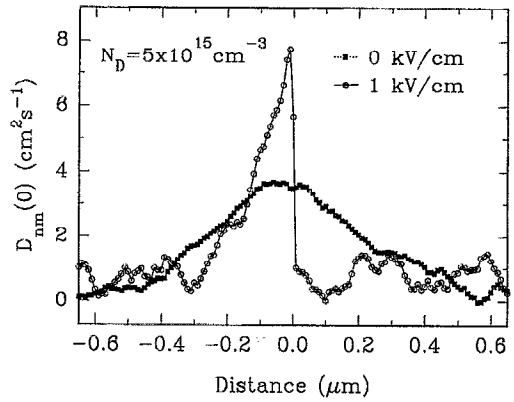

FIG. 4. Contribution to the low-frequency diffusion coefficient in a cell located at 0.0 μm from the correlation with cells at different distances for electric fields of 0 and 1 kV/cm (in negative direction.

with the carriers traveling against the electric field, which reduces their velocity, and consequently the time they spend to cover the distance between two cells is longer.

Figure 3 reports the values of $D_{nm}(0)$ at thermal equilibrium for two different impurity concentrations. In spite of the "noise" present in the results (whose origin has been already commented), it can be observed that the correlation persists for a distance around 0.6 μm. So, it is confirmed that the space correlation in GaAs is longer than in Si, where it extends over a length around 0.1 μm.[5,6] This is due to the predominance of the anisotropic mechanisms and to the higher velocity of the carriers in GaAs.

It is detected that when the doping increases, the correlation length is slightly shortened, and that the decrease of the diffusion coefficient (Fig. 1) comes mainly from the reduction of the correlation between close cells originated by the impurity scattering. This type of scattering modifies the direction of the carrier wave vector and may produce significant changes in the velocity of the electrons for high dopings. Consequently, the correlation is reduced for 10^{17} cm^{-3}, and is lost for shorter lengths. When the applied electric field is greater than the threshold for negative differential-mobility, the intervalley scattering mechanisms are dominant and the influence of the impurities is much smaller. This causes both the diffusion coefficient and the correlation functions to become independent of the doping (Fig. 1).

The values of $D_{nm}(0)$ as a function of the distance for different applied fields (in negative direction) are shown in Figs. 4 and 5. First of all it is noticed that the space correlations are not symmetric. To understand this effect it is necessary to take into account that the electrons moving towards the right (forward) are accelerated by the electric field. This makes their energy increase and accordingly the probability of isotropic scatterings to happen (mostly intervalley). When a mechanism of this type occurs, the velocity is randomized and the correlation tends to lose. The intervalley transfers can also lead to negative values of the cross-correlation function for long times because of the change in the sign of the velocity fluctuation.[11,12] This fact contributes to reduce $D_{nm}(0)$, which may even take negative values. As the electric field is increased, the appearance of isotropic scatterings is more probable, and that is why the forward correlation length is drastically reduced (around 0.1 μm) with respect to the case of equilibrium. The carriers moving to the left suffer the opposite effect: they are slowed down by the field, their energy is lowered, and the most probable mechanisms are anisotropic. So, the correlation persists over longer distances (around 0.2 μm).

Figure 6 shows the results for D_{nm} at two different frequencies, 0 and 600 GHz, for a field of 10 kV/cm. The high frequency behavior of the noise sources is found to be very different from that at low frequency. The forward correlation takes higher values and extends over a longer length. This effect is related to the intervalley mechanisms between the Γ and the upper valleys. These transfers usually take place when the carriers gain enough energy after traveling some distance in the field direction. Although this kind of scattering is isotropic, the correlation is not completely lost when it occurs. On the contrary, it frequently leads to a change in the sign of the carrier velocity fluctuation due to the different effective mass of the valleys involved (positive fluctuation in

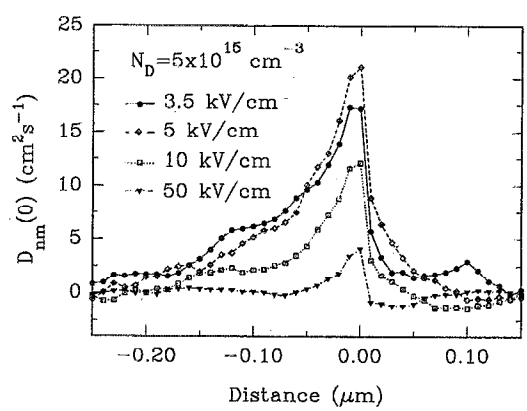

FIG. 5. Contribution to the low-frequency diffusion coefficient in a cell located at 0.0 μm from the correlation with cells at different distances for electric fields of 3.5, 5, 10, and 50 kV/cm (in negative direction).

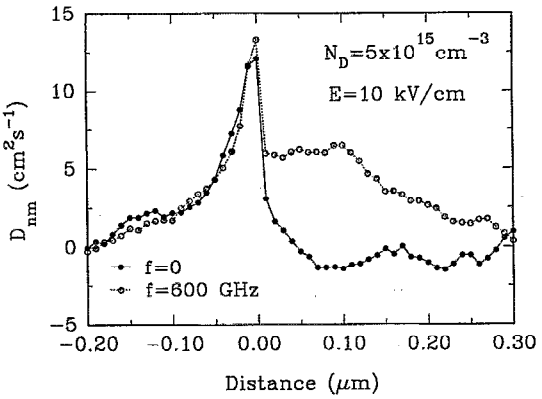

FIG. 6. Contribution to the diffusion coefficient in a cell located at 0.0 μm from the correlation with cells at different distances from an electric field of 10 kV/cm (in negative direction) at two frequenices: 0 and 600 GHz.

the Γ valley and later, in time and space, negative in the L or X valley),[11,12] thus introducing a negative correlation between cells. This phenomenon appears mainly in the forward direction, and that is why the high-frequency value of D_{nm} is higher and extends over a longer distance in such a direction. The negative part in the cross-correlation functions provokes the appearance of a well known peak at high frequency in $D_n(f)$.[11,12]

In view of the previous results, we can finally remark that only in the case of long devices (as compared with the correlation length) the utilization of the diffusion coefficient to characterize the local noise sources is meaningful, since in such a case the error introduced when all the spatial correlations are associated with just one point (through the diffusion coefficient) is negligible. However, when dealing with submicron and/or strongly nonhomogeneous devices this is not true, because it is likely that not all the cross-correlations were present, or were different from those of the uniform case due to changes in the material or in the electric field. In these cases the diffusion coefficient is meaningless and the spatial correlations must be taken into account.

The next step in this work is the analysis of the contributions to the spatial correlation between local current noise sources coming from carrier number fluctuations and from their cross correlation with velocity fluctuations, which can also be very significant. Moreover, the importance of the spatial correlations in submicron nonhomogeneous structures (like n^+nn^+ diodes) can be readily studied with the present technique. These will be the subjects of forthcoming papers.

V. CONCLUSIONS

In this paper we have presented a theoretical analysis of the spatial correlation between local diffusion noise sources in GaAs. The theory underlying the subject has been extended for the case of regions of a given length (cells) instead of points. By using an ensemble Monte Carlo simulation of carrier transport in GaAs homogenous samples, the following has been found:

(i) The diffusion coefficient can be decomposed into the contributions of the cross-correlation between the local velocity fluctuations at close cells.

(ii) The space correlations do exist in GaAs over distances ranging between 0.1 and 0.6 μm depending on the applied electric field. The correlation length near equilibrium is longer than in Si due to the predominance of the nonrandomizing scatterings.

(iii) Under far from equilibrium conditions, the forward correlations at low frequency are found to be shorter than those with the backward cells due to the increasing effect of the isotropic scatterings.

(iv) For fields higher than the threshold, the intervalley scattering mechanisms between the Γ and the upper valleys leads to the appearance of a negative part in the cross-correlation functions, which makes the high-frequency correlation increase and extend longer forwards.

(v) The usual expression for the local diffusion noise source [Eq. (10)] is appropriate for the case of long devices where the field and the carrier distribution are homogenous over distances much longer than the correlation length. However, for short and/or strongly nonhomogeneous devices, it is not correct, and the spatial correlations must be taken into account.

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