

Auto-Correlation of Velocity-Fluctuations and Frequency-Dependent Diffusion Constant for Hot Electrons

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Abstract. A method has been developed for determining the auto-correlation functions of the fluctuations in the transverse and the parallel components of hot carrier-velocity in a semiconductor by Monte Carlo simulation. The functions for electrons in InSb are determined by this method for applied electric fields of 50 V/cm, 75 V/cm, and 100 V/cm. With increasing value of the time interval the transverse auto-correlation function falls nearly exponentially to zero, but the parallel function falls sharply to a negative peak, then rises to positive values and finally becomes zero. The interval beyond which the auto-correlation function is zero and the correlation time are also evaluated. The correlation time is found to be approximately 1.6 times the relaxation time calculated from the chord mobility. The effect of the flight sampling time on the value of variance of the displacement, is investigated in terms of the low frequency diffusion constants, determined from the variation of the correlation functions. It is found that the diffusion constants become independent of the sampling time if it is of the order of one hundred times the relaxation time. The frequency-dependent diffusion constants are calculated from the correlation functions. The transverse diffusion constant falls monotonically with frequency for all the field strengths studied. The parallel diffusion constant has similar variation for the lower fields (50 V/cm and 75 V/cm) but it has a peak at about 44 GHz for the field of 100 V/cm.

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Solid-state microwave devices used in oscillators and amplifiers generally operate under hot-electron conditions, and the hot-electron thermal noise is a significant component of the total noise of these devices. The noise under hot-electron conditions have been studied experimentally by several workers [1–8]. Theory of hot-electron noise has been discussed by Price [9]. It is also known that the diffusion constant is directly related to the noise spectrum and the noise behaviour may be studied from the diffusion constant [10]. Hill et al. [11] studied the frequency dependence of the diffusion constant in InP from the spectral density of the velocity fluctuations obtained by the Monte Carlo method and reported some interesting results.

The spectral density of velocity fluctuations is, however, directly related to its auto-correlation function [12]. Hence one may study the frequency dependence of the noise power or of the diffusion constant also from the correlation function. It is further expected that the study of the auto-correlation function will provide a better insight into the physical origin of the frequency dependence. The importance of choosing a proper sampling time for the Monte Carlo calculation of various transport parameters would also be evident from this study.

We have developed a Monte Carlo program for obtaining the auto-correlation function of velocity fluctuations under hot-electron conditions. The method

and the results obtained by applying the same to InSb are presented in this paper.

1. Theoretical Background

The relation between the spectral density of the fluctuations in velocity, its auto-correlation function and the diffusion constant are well discussed in the literature [10, 12, 13]. However, as these relations are used in our calculations we quote, in this section, the relevant formulas.

The spectral density $S_{\Delta v_\alpha}(\omega)$ and the auto-correlation function $C_\alpha(s)$ of the fluctuations $\Delta v_\alpha(t)$ of the velocity $v_\alpha(t)$ of an electron in the direction α are related according to the Wiener-Khintchine theorem [12]

$$S_{\Delta v_\alpha}(\omega) = 4 \int_0^\infty C_\alpha(s) \cos \omega s ds, \quad (1)$$

where

$$C_\alpha(s) = \langle \Delta v_\alpha(t) \cdot \Delta v_\alpha(t+s) \rangle, \quad (2)$$

and

$$\Delta v_\alpha(t) = v_\alpha(t) - \langle v_\alpha(t) \rangle. \quad (3)$$

In (2) and (3) the angular brackets represent average values. The velocity function $v_\alpha(t)$ may be taken to be ergodic so that the time and the ensemble-averages are identical.

It follows from (1) that the spectral density of the noise current in the direction α in a semiconductor block of length L , area of cross-section A and electron density N is [10]

$$S_{\Delta I}(\omega) = \frac{4e^2 AN}{L} \int_0^\infty C_\alpha(s) \cos \omega s ds. \quad (4)$$

The diffusion constant $D_\alpha(\omega)$ at an angular frequency ω in the direction α is also related to $C_\alpha(s)$ as [13]

$$D_\alpha(\omega) = \int_0^\infty C_\alpha(s) \cos \omega s ds. \quad (5)$$

Thus

$$S_{\Delta I}(\omega) = \frac{4e^2 AN}{L} D_\alpha(\omega). \quad (6)$$

The spectral density of the noise current is thus proportional to $D_\alpha(\omega)$ which can be obtained from the auto-correlation function $C_\alpha(s)$ of the velocity fluctuations $\Delta v_\alpha(t)$ by using (5). Further the noise characteristics of a semiconductor device can be ascertained by studying $D_\alpha(\omega)$.

As ω approaches zero, $D_\alpha(\omega)$ equals the low frequency diffusion constant D_α which is given by

$$D_\alpha = \int_0^\infty C_\alpha(s) ds. \quad (7)$$

D_α is also related to the variance $\langle (\Delta \alpha)_T^2 \rangle$ of the displacement of the electron in the direction α in the interval T provided T is chosen much larger than the correlation time \mathcal{T}_c . This relation is obtained as follows

$$\langle (\Delta \alpha)_T^2 \rangle = \int_0^T dt \int_{-t}^{T-t} C_\alpha(s) ds. \quad (8)$$

If $T \gg \mathcal{T}_0$, where \mathcal{T}_0 is the value of s beyond which $C_\alpha(s)$ is zero, then

$$\begin{aligned} \int_{-t}^{T-t} C_\alpha(s) ds &= \int_{-\infty}^{\infty} C_\alpha(s) ds \\ &= 2 \int_0^\infty C_\alpha(s) ds \\ &= 2D_\alpha \end{aligned} \quad (9)$$

and

$$\langle (\Delta \alpha)_T^2 \rangle = 2TD_\alpha. \quad (10)$$

Equation (8) shows that D_α calculated by using (10) depends on T unless $T \gg \mathcal{T}_0$.

2. The Method

A Monte Carlo program [14–16] was set up to study the trajectory of a single electron in the semiconductor in the presence of an electric field F in the Z direction. The trajectory is followed for 1000 real collisions and the following quantities are stored in the computer: (i) the instant at which each collision takes place, (ii) the components of the velocity $v_x, v_y,$ and v_z immediately after each collision, and (iii) the average acceleration due to the electric field during the interval between two successive collisions (inter-collision period).

The effective mass of the electron, however, is dependent on its energy due to the non-parabolic energy-band structure. As the electron accelerates under the influence of the field, its energy changes and so does its effective mass. Thus the acceleration does not remain constant during the inter-collision period. To simplify calculations we have computed the average acceleration during the period on the basis of an average mass given by

$$m_{av}^* = \frac{m^*}{1 + \alpha(E_1 + E_2)}, \quad (11)$$

where E_1, E_2 are the energies of the electron at the beginning and at the end of the period. The components of the initial velocity $v_x, v_y,$ and v_z have also been evaluated from the initial values of the wave vector using this average effective mass. The error introduced by this procedure has been found to be less

than 1% in the case of InSb for the fields considered by us.

The average values $\langle \Delta v_\alpha(t), \Delta v_\alpha(t+n \cdot \Delta t) \rangle$ for $\alpha = x, y, z$ and $0 \leq n \leq 100$ are analytically computed from the stored data by the steps explained below. Let T_i be the instant at which the i th collision takes place. From the series of instants T_i another series $T'_i = T_i + s$, where $s = n \cdot \Delta t$, is obtained. Against a common coordinate axis of time these two series appear, as shown in Fig. 1.

If T'_0 is taken as the origin of the time axis the points on the lower straight line represent t , while those on the upper line give $(t+s)$. The interval $(0$ to $T)$ over which the average is taken, can be divided into smaller intervals like $(T'_0$ to $T_2)$, $(T_2$ to $T'_1)$, $(T'_1$ to $T_3)$, $(T_3$ to $T'_2)$, ... Over each of these periods both $v_\alpha(t)$ and $v_\alpha(t+s)$ are given by simple expressions and $\int v_\alpha(t) \cdot v_\alpha(t+s) dt$ can be obtained analytically. Thus during the period $(T'_0$ to $T_2)$

$$v_z(t) = v_{z1} + a_1 t \quad (12)$$

and

$$v_z(t+s) = v_{z2} + a_2(T'_0 - T_1) + a_2 t, \quad (13)$$

where v_{zi} and a_i , respectively, are the component of the initial velocity and the average acceleration during the inter-collision period immediately preceding the i th collision.

Putting $T_2 - T'_0 = \Delta T$, and $T'_0 - T_1 = \Delta T'$

$$\begin{aligned} \int_{T'_0}^{T_2} v_z(t) \cdot v_z(t+s) dt &= v_{z1}(v_{z2} + a_2 \Delta T') \cdot \Delta T \\ &+ [a_1(v_{z2} + a_2 \Delta T') \\ &+ a_2 v_{z1}] \cdot \frac{(\Delta T)^2}{2} \\ &+ a_1 a_2 \frac{(\Delta T)^3}{3}. \end{aligned} \quad (14)$$

For $\alpha = x, y$ the terms containing a_i 's do not appear in (12)–(14) and subscripts z are replaced by x or y . Over the period $(0$ to $T)$

$$\begin{aligned} \langle v_\alpha(t) \cdot v_\alpha(t+s) \rangle &= \frac{1}{T} \left[\int_{T'_0}^{T_2} v_\alpha(t) \cdot v_\alpha(t+s) dt \right. \\ &\left. + \int_{T_2}^{T'_1} v_\alpha(t) \cdot v_\alpha(t+s) dt + \dots \right]. \end{aligned} \quad (15)$$

The auto-correlation functions are given by

$$\langle \Delta v_\alpha(t) \cdot \Delta v_\alpha(t+A) \rangle = \langle v_\alpha(t) \cdot v_\alpha(t+s) \rangle - \langle v_\alpha(t) \rangle^2. \quad (16)$$

For $\alpha = x, y$

$$\langle v_\alpha(t) \rangle = 0 \quad (17a)$$

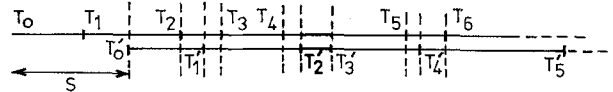


Fig. 1. Instants of collisions for the velocity functions $v_\alpha(t)$ and $v_\alpha(t+s)$

and for $\alpha = z$

$$\langle v_\alpha(t) \rangle = v_d, \quad (17b)$$

where v_d = the drift velocity.

For the period $(0$ to $T)$

$$v_d = \frac{1}{T} \left[\int_{T'_0}^{T_2} v_z(t) dt + \int_{T_2}^{T'_1} v_z(t) dt + \dots \right]. \quad (18)$$

The drift velocity is also calculated from the displacement of the electron in the z direction which in the i th inter-collision period is

$$(\Delta z)_i = \frac{(\Delta E)_i}{F}, \quad (19)$$

where $(\Delta E)_i$ is the change in the energy of the electron during the period and F the intensity of the applied electric field.

Thus

$$v_d = \frac{1}{T} \sum_i (\Delta z)_i. \quad (20)$$

Comparison of the values of v_d obtained by (18) and (20) provides a check on the correctness of the computation.

It may be noted that for determining the correlation functions over the period 0 to T , the values of $v_{\alpha i}$ and a_i for the period 0 to $(T+s)$ for the highest value of s required, must be available. For this reason the averages for the period covering the first 500 collisions are computed from the stored data for 1000 collisions.

T_i , $v_{\alpha i}$, and a_i for $1001 \leq i \leq 1500$ are then computed and the averages for the period covering the first 1000 collisions are obtained by combining the previous results with the data stored for $500 \leq i \leq 1500$.

The process is continued till the average values converge to give the auto-correlation functions $C_i(s)$ and $C_p(s)$. The frequency-dependent diffusion constant $D_i(\omega)$ and $D_p(\omega)$ are obtained from these functions using (5).

The method of calculation described above has the advantage of reducing the computation time compared to that required in the method using Simpson's rule for obtaining the integral $\int v_\alpha(t) \cdot v_\alpha(t+s) dt$. The approximation regarding the effective mass given by (11) enables us to carry out these integrations analytically. On the other hand, in the method using Simpson's rule for integration it is necessary to calculate the components of the velocity at the beginning

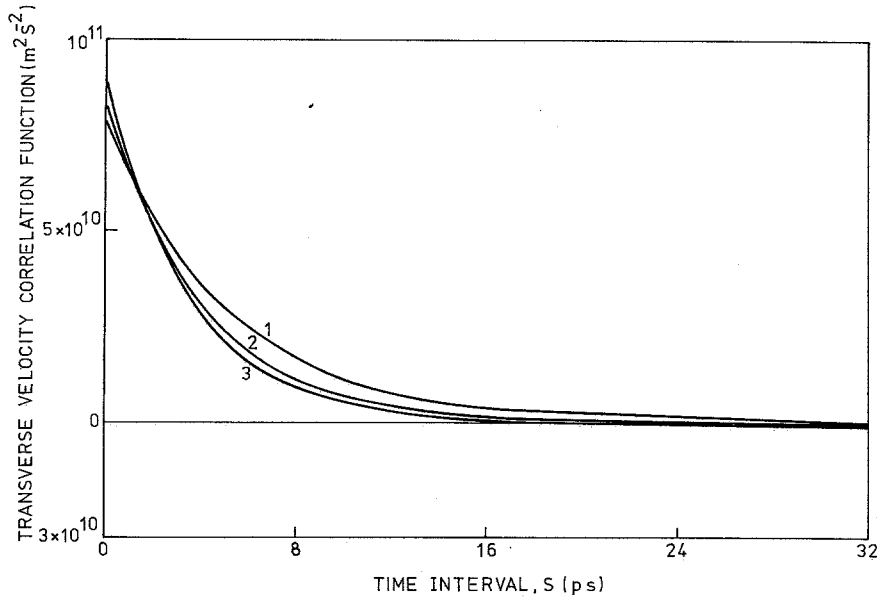


Fig. 2. Autocorrelation function of fluctuations in electron velocity in *n*-InSb transverse to the applied electric field (1 50 V/cm, 2 75 V/cm, 3 100 V/cm)

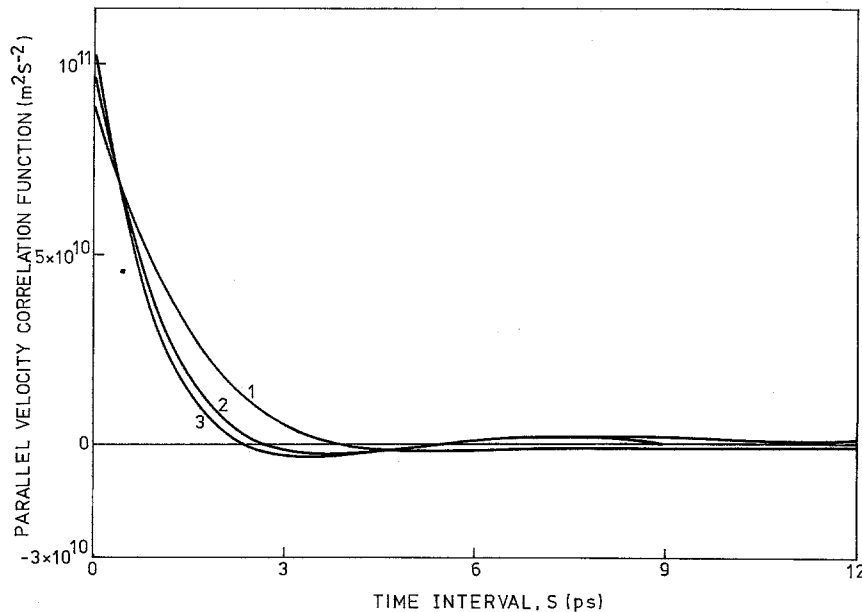


Fig. 3. Autocorrelation function of fluctuations in electron velocity in *n*-InSb parallel to the applied electric field (1 50 V/cm, 2 75 V/cm, 3 100 V/cm)

of intervals δt which are required to be taken so small that there are about ten such intervals in the average inter-collision period. This calculation at so many instants of time makes the over-all computation time much longer than that for the proposed method.

3. Results

The above method has been used to calculate the autocorrelation function and the frequency-dependent diffusion-constant of electrons in *n*-InSb as an example for studying their nature. A non-parabolic energy-band structure has been assumed and scattering by ionized impurity atoms, polar optic and acoustic pho-

nons has been considered. The following values of the parameters for the material *n*-InSb have been used [17]

$E_g = 0.225$ eV, $m^*/m_e = 0.014$, $K_s = 16.00$, $K_\infty = 18.70$,
 $\rho = 5.79 \times 10^3$ kg/m³, velocity of sound: 3.7×10^3 m/s,
 polar optic phonon energy: 0.025 eV,
 concentration of ionized impurity atoms:
 1.6×10^{20} m⁻³.

The acoustic deformation potential has been taken as 20 eV [18]. The values of s have been chosen at intervals of 0.6 picosecond so that the correlation functions are evaluated at a reasonably large number (40–50) of points on the s -axis within the limits of

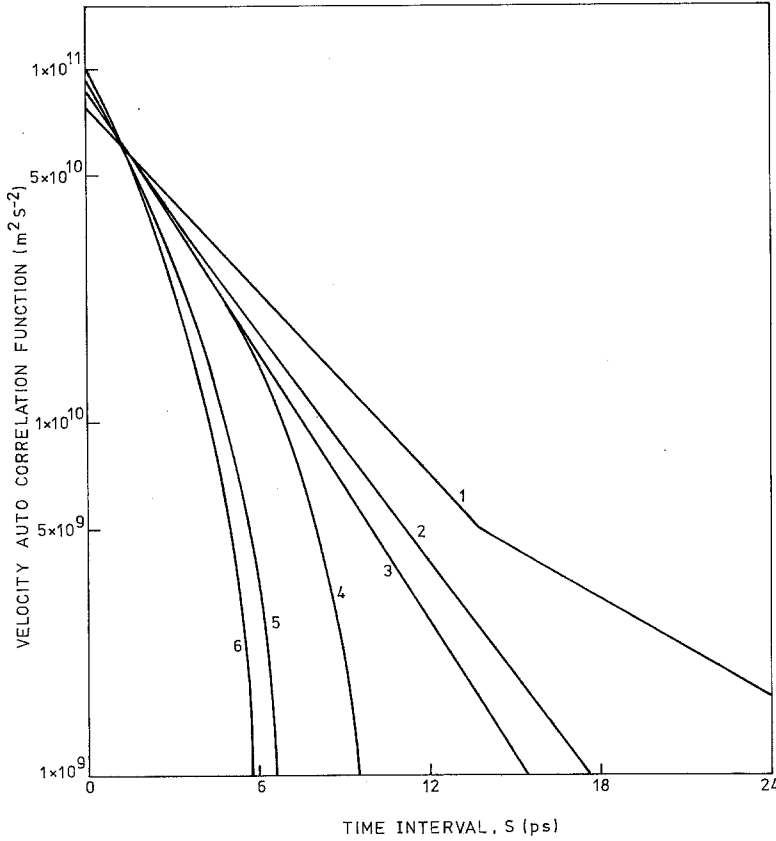


Fig. 4. Autocorrelation function of fluctuations in electron velocity in *n*-InSb in logarithmic scale. For the transverse component of velocity (1 50 V/cm, 2 75 V/cm, 3 100 V/cm and for the parallel component of velocity (4 50 V/cm, 5 75 V/cm, 6 100 V/cm)

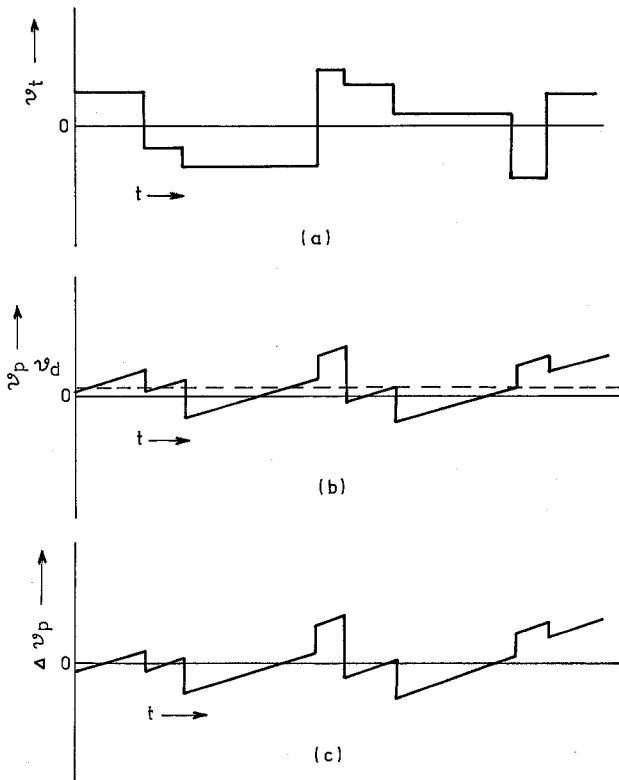


Fig. 5a-c. Typical plot of electron-velocity against time: (a) transverse component, (b) parallel component, (c) fluctuations in the parallel component

integration for determining $D_t(\omega)$ and $D_p(\omega)$ by Simpson's rule. Averages have been taken in each case over 50,000 real collisions which gave satisfactory convergence. Computations have been made for three values of the applied electric field, namely, 50, 75, and 100 V/cm.

We discuss below the characteristics of the auto-correlation functions and the frequency-dependence of the diffusion constant as obtained from these studies.

3.1. Auto-Correlation Functions

Figures 2 and 3 show the variation of the auto-correlation functions $C_t(s)$ and $C_p(s)$, respectively, with the time interval s . Figure 4 depicts the same variation with $C_t(s)$ and $C_p(s)$ plotted on a logarithmic scale. As expected both correlation functions fall with increasing s but while $C_t(s)$ fall nearly exponentially, as indicated by its linear variation in the logarithmic plot, the rate of fall of $\log C_p(s)$ increases with s . Figure 3 shows that $C_p(s)$ falls sharply, attains negative values after passing through zero, reaches a negative maximum, becomes positive again and finally becomes zero.

The nature of variation of the correlation functions can be explained by considering the way in which the respective component of velocity changes with time. In

Table 1. Computed values of correlation time, relaxation time and diffusion constant for n -InSb

Field [V/cm]	\mathcal{T}_0		\mathcal{T}_c	\mathcal{T}_μ	D_t [$\text{m}^2 \text{s}^{-1}$]		D_p [$\text{m}^2 \text{s}^{-1}$]	
	1st zero s_1 for Z_t [ps]	3rd zero s_3 for C_p [ps]			from		from	
			[ps]	[ps]	$C_t(s)$	$\langle(\Delta\alpha)^2\rangle$	$C_p(s)$	$\langle(\Delta\alpha)^2\rangle$
50	31.8	33.6	5.04	3.10	0.406	0.362	0.272	0.270
75	27.0	29.4	4.20	2.59	0.325	0.310	0.215	0.210
100	21.0	26.4	3.60	2.24	0.307	0.275	0.202	0.179

\mathcal{T}_0 : The interval beyond which the auto-correlation functions become zero

\mathcal{T}_c : Correlation time

\mathcal{T}_μ : Relaxation time

D_p : Diffusion constant in the direction parallel to the applied electric field

D_t : Diffusion constant in the direction transverse to the applied electric field

Fig. 5a and b the transverse and the parallel components of the electron-velocity are plotted against time. Figure 5c shows the fluctuations in the parallel velocity $\Delta v_p(t)$ against the same time axis. The transverse component of the velocity may be assumed to be approximately constant during the inter-collision periods. The auto-correlation function for such velocity is known [19] under certain simplifying conditions, namely, (i) the probability that the electron does not suffer a collision for a time t_c after last collision is proportional to $\exp(-t_c/\mathcal{T}_c)$, and (ii) the velocity after the collision has a Gaussian distribution. In this case the autocorrelation function is proportional to $\exp(-s/\mathcal{T}_c)$. The observed exponential fall of $C_t(s)$ confirms that these conditions are reasonably satisfied in the case of the transverse component of the velocity.

The abrupt changes in the parallel velocity being caused by the same randomizing collisions (Fig. 5b), the conditions (i) and (ii) mentioned above are equally applicable to this case as well. So the interval \mathcal{T}_0 beyond which the correlation function becomes zero is likely to be nearly the same in both cases. The monotonic increase in the parallel velocity during each inter-collision period due to the applied electric field leads to a finite value of its average which is called the drift velocity v_d .

The nonlinear variation of $\log C_p(s)$ against s (Fig. 4) may be explained by referring to Fig. 5c. It is seen that for a number of inter-collision periods $\Delta v_p(t)$ starts with a negative value but ends up with a positive one. These intervals make a negative contribution to $C_p(s)$. The interval s over which such negative contribution is made can at most be $T_{ci}/2$, where T_{ci} is the inter-collision period under consideration. These negative values are added to the positive exponentially falling values arising in the manner similar to the transverse case. In both cases the positive values fall to zero in a

period approximately five times the correlation time \mathcal{T}_c . The negative contributions, however, persist at most for one half of the longest inter-collision period. Thus compared to the positive values the negative values fall to zero for smaller values of s . So the superposition of the negative values makes $C_p(s)$ fall more sharply than $C_t(s)$ and become negative. Thereafter the positive values predominate to make $C_p(s)$ positive again and finally zero. This explanation is confirmed by the fact that the third zero s_3 of $C_p(s)$ and the first zero s_1 of $C_t(s)$ occur for nearly the same values of s as shown in Table 1. These values of s give \mathcal{T}_0 the interval beyond which the correlation function may be taken as zero and these have been taken as the upper limit of integration in calculating $D_t(\omega)$ and $D_p(\omega)$ from the respective correlation function.

It may be noted from the above discussion that the correlation time \mathcal{T}_c can be obtained from the slope of the logarithmic plots of $C_t(s)$ against s as these are nearly linear. Values of \mathcal{T}_c as obtained from these slopes for different field strength are given in Table 1 along with the relaxation time \mathcal{T}_μ calculated from the chord mobility given by Deb Roy and Nag [17]. It is found that \mathcal{T}_c is approximately 1.6 times \mathcal{T}_μ .

We give in Table 1 the values of \mathcal{T}_0 , the interval beyond which the autocorrelation functions $C_t(s)$, $C_p(s)$ are zero. These are found to lie in the range 20–30 ps. We note that while calculating D_t and D_p for electrons in n -InSb using (10) in our earlier work [17] we could get satisfactory convergence in their values for the time of flight $T \gtrsim 250$ ps. It may therefore be concluded that the sampling time T for determining the diffusion constants D_t and D_p from the variance of the displacements is required to be about 10 times \mathcal{T}_0 or 60 times the correlation time \mathcal{T}_c or 100 times the relaxation time \mathcal{T}_μ since $\mathcal{T}_0 \approx 6\mathcal{T}_c$ and $\mathcal{T}_c \approx 1.6\mathcal{T}_\mu$.

It is also clear that if T is chosen to be smaller, the values of D_t and D_p obtained will be different from the

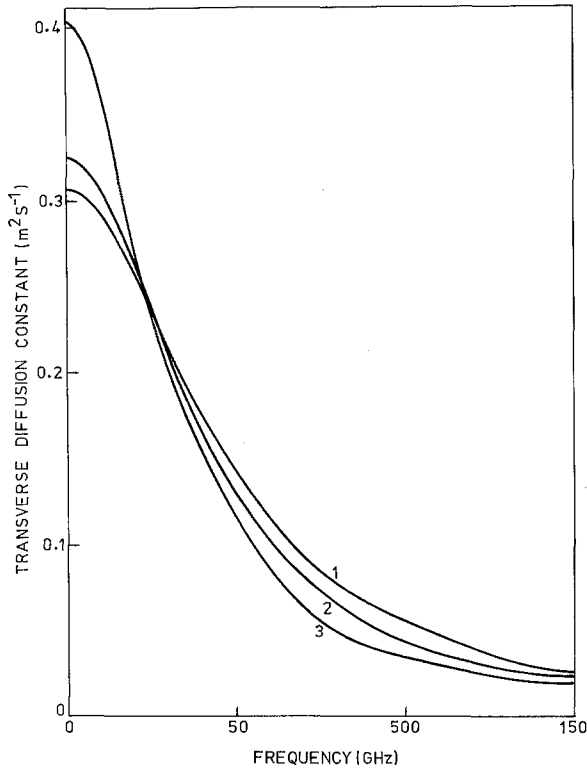


Fig. 6. Diffusion constant transverse to the applied electric field for electrons in n -InSb for different frequencies (1 50 V/cm, 2 75 V/cm, 3 100 V/cm)

low frequency values of the diffusion constants and the calculated values may be smaller or larger depending on the nature of variation of the correlation functions $C_t(s)$ and $C_p(s)$ with s . Since $C_t(s)$ does not have negative values D_t will increase monotonically with T towards its convergent value. But as $C_p(s)$ has negative values for some values of s , D_p will first increase with T , reach a maximum, then decrease and finally increase to reach a constant value. The variation of D_p with T , as reported by Hill et al. [11], may be explained by the observed nature of variation of the correlation function.

3.2. Frequency Dependence of Diffusion Constant

Figures 6 and 7 show the variation of the transverse and the longitudinal diffusion constant $D_t(\omega)$ and $D_p(\omega)$ with frequency for three different values of the applied electric field (50, 75, and 100 V/cm). It is observed that for all the values of the applied field $D_t(\omega)$ falls monotonically with frequency. $D_p(\omega)$ varies similarly for the lower fields (50 and 75 V/cm) but for 100 V/cm it has a peak at a frequency of about 44 GHz. The peak in the curve for $D_p(\omega)$ was observed for InP by Hill et al. [11]. The appearance of the peak is caused by the negative values of $C_p(s)$. For the lower

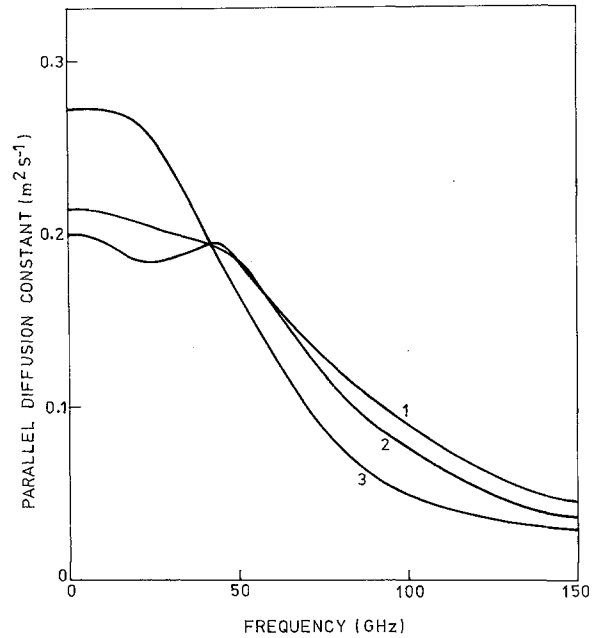


Fig. 7. Diffusion constant parallel to the applied electric field for electrons in n -InSb for different frequencies (1 50 V/cm, 2 75 V/cm, 3 100 V/cm)

fields (50 and 75 V/cm) the effect of the negative values of $C_p(s)$ is relatively small and so the peaks are absent.

As the frequency approaches zero, $D_t(\omega)$ and $D_p(\omega)$ reduce to the low frequency diffusion constants D_t and D_p . Figures 6 and 7 show that both D_t and D_p decrease as the field strength is increased and that for each field strength D_t is greater than D_p . These characteristics follow directly from the nature of variation of $C_t(s)$ and $C_p(s)$ with s .

In Table 1 the values of D_t and D_p given in Figs. 6 and 7 are compared with their values calculated from the variance of the displacement of the electron under similar conditions [17]. They agree within 10%. This discrepancy may be attributed to the different values of the acoustic deformation potential (30 eV) taken in this reference.

4. Conclusion

The results of our Monte Carlo calculations show how the autocorrelation functions of the fluctuations in transverse and parallel velocity of electrons in n -InSb, $C_t(s)$ and $C_p(s)$, vary with the interval s and how the diffusion constants $D_t(\omega)$ and $D_p(\omega)$ depend on the

frequency. The nature of variation of $C_t(s)$ and $C_p(s)$ has been explained on the basis of the nature of velocity fluctuations in the respective direction. The variation of $D_t(\omega)$ and $D_p(\omega)$ has been found to follow directly from the nature of variation of the respective correlation function with s . An estimation of the smallest sampling time T for determination of the low frequency diffusion constants D_t and D_p from the variance of the displacements of the electrons has been made. It has been found that for satisfactory results T should be at least 10 times \mathcal{T}_0 , the interval beyond which the correlation function is zero, or 100 times \mathcal{T}_ν , the relaxation time calculated from chord mobility.

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