JOURNAL DE PHYSIQUE
Colloque C7, supplément au n°10, Tome 42, octobre 1981 *page* C7-123

FREQUENCY AND WAVEVECTOR DEPENDENT DIFFUSION COEFFICIENT OF ELECTRONS FROM MONTE CARLO CALCULATIONS

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Résumé.- Quand un gradient de concentration $\partial n/\partial x$ de particules est présent dans un système physique et ses variations temporelles et/ou spatiales sont très rapides, une généralisation de la loi de Fick conduit à la définition d'un coefficient de diffusion $D(q,\omega)$, qu'on doit écrire en fonction du vecteur d'onde q et de la pulsation ω de la composante de Fourier de $\partial n/\partial x$. L'expression générale pour $D(q,\omega)$ est obtenue, et la méthode de Monte Carlo est appliquée à son calcul. Les valeurs numériques des résultats sont données dans le cas du Si.

Abstract.- If in a physical system a particle-concentration gradient $\partial n/\partial x$ is present which varies rapidly in time and/or in space, a generalization of Fick's law leads to a definition of a diffusion constant $D(q,\omega)$ which is a function of the wavevector q and of the frequency ω of the Fourier component of $\partial n/\partial x$. A general expression of $D(q,\omega)$ is obtained, and a Monte Carlo procedure is presented which leads to its evaluation. Numerical results are presented for the case of Si.

1. Introduction. - In the last years a considerable amount of work has been devoted to the study of hot-carrier diffusion properties at small distances and/or short times, that is , in conditions such that Fick's law does not hold. This problem may become very important in connection with the modelling of small semiconductor devices or when alternating fields are applied, with frequency comparable with the inverse of some electronic relaxation time and/or wavevector comparable with the inverse of the electronic mean free path.

The aim of this paper is to present, for such types of problems, an extension of the theory which leads to Fick equation by making use of the Fourier analysis, which allows us to define a frequency and wavevector dependent diffusion coefficient $D(q,\omega)$. For q and ω different from zero it describes the diffusion properties of the system in steady-state conditions when a particle gradient $\partial n(q,\omega)/\partial x$ is present. Furthermore, it will be shown that $D(q,\omega)$ reduces to the known static value when both q and ω tend to zero.

2. Theory. - Let us consider a system of particles subject to an external uniform static electric field E. A particle source of sinusoidal type:

$$S(x,t) = C\left\{1+\cos(qx-\omega t)\right\} \tag{1}$$

is then introduced, where x is the direction of the drift produced by $\vec{E}$, together with a trapping mechanism with a constant rate γ . The source amplitude C and γ are connected through the condition of particle conservation over a wavelength λ :

$$\int_\lambda C\{1+\cos(qx-\omega t)\}\,dx = \int_\lambda \gamma n(x,t)\,dx \,. \tag{2}$$

The particles are thus trapped and redistributed in space. If we make use of the more convenient complex formalism, the Fick' s law for such a system would be written in the one-dimensional case as:

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} - v_d\frac{\partial n}{\partial x} + C\left\{1+e^{i(qx-\omega t)}\right\} - \gamma n \,, \tag{3}$$

where D is the diffusion constant and v_d is the steady-state drift velocity.

The general solution of Eq.(3) is:

$$n(x,t) = n_0 + n_1\, e^{i(qx-\omega t+\varphi)} \,, \tag{4}$$

where n_0 is a constant average term, n_1 and φ are the amplitude and the phase-shift of the harmonic disturbance, respectively. By substituting Eq.(4) into Eq.(2), we obtain:

$$C = n_0\gamma \,,$$

and Eq.(3) becomes:

$$-i\omega + q^2 D + iqv_d + \gamma = \frac{n_0}{n_1}\gamma\, e^{-i\varphi} \,. \tag{5}$$

As far as we deal with problems linear in n, this equation can be used also at frequencies and wavevectors so high that Fick' s law does not hold /1,2/ ; in this case D, however, must be taken as a function of q and ω. Thus from Eq.(5) we obtain an expression for D(q, ω, γ) in terms of the relative amplitude n_1/n_0 and of the phase-shift φ of the disturbance:

$$D = \frac{1}{q^2}\left\{\frac{n_0}{n_1}\gamma e^{-i\varphi} + i(\omega - qv_d) - \gamma\right\} \,. \tag{6}$$

Using Chambers method we can obtain an integral expression for n(x,t):

$$n(x,t) = n_0\int_{-\infty}^{t} dt'\gamma \int_{-\infty}^{+\infty} dx' \left\{1+e^{i(qx'-\omega t')}\right\} P(x',t',x,t)\, e^{-\gamma(t-t')} \,, \tag{7}$$

where P(x',t',x,t) is the probability that, without trapping, a particle in x' at t' will be in x at t. The integral of the first term in the brackets in Eq.(7) is equal to n_0, since going from the time $-\infty$ to t all the particles have been trapped and redistributed by the source. P(x',t',x,t) is a function of x', t', x, and t only through the differences ξ = x–x' and ϑ = t – t', so that Eqs.(7) and (4) yield:

$$n(x,t) - n_0 = n_0\, e^{i(qx-\omega t)} \int_0^{\infty}\frac{d\vartheta}{\tau_d}\int_{-\infty}^{\infty} d\xi\, e^{-i(q\xi-\omega\vartheta)-\vartheta/\tau_d}\, P(\xi,\vartheta) \,, \tag{8}$$

where $\tau_d = \gamma^{-1}$. From Eqs.(4) and (8), we then have:

$$R \equiv \frac{n_1}{n_0} e^{i\varphi} = \int_0^{\infty} \frac{d\vartheta}{\tau_d} \int_{-\infty}^{\infty} d\xi \, e^{-i(q\xi - \omega\vartheta) - \vartheta/\tau_d} P(\xi, \vartheta) \quad , \tag{9}$$

and Eq.(6) yields finally:

$$D(q, \omega, \tau_d) = \frac{1}{q^2 \tau_d R} \left\{ 1 - R + i\tau_d R \left(\omega - q v_d \right) \right\} \tag{10}$$

Eqs.(10) and (9) provide an expression for $D(q, \omega, \tau_d)$ valid for any frequency, wavevector, and particle lifetime τ_d. When τ_d is much larger than both ω^{-1} and any microscopic time, $D(q, \omega) \equiv D(q, \omega, \infty)$ is obtained for steady-state conditions. $P(\xi, \vartheta)$ must be derived from the knowledge of the particle dynamics; a Monte Carlo method for the determination of R will be shown later. For finite τ_d a transient diffusivity is obtained, whose value depends upon the dynamical initial conditions when particles are created.

3. <u>Comparison with previous definitions for D(q) and D(ω).</u> - The problem of defining a q-dependent diffusion coefficient $D(q) \equiv D(q,0)$ and an ω-dependent diffusion coefficient $D(\omega) = D(0, \omega)$ has been analysed in several papers /1,3-6/ . For what concerns the limit $\omega \to 0$ Eq.(10) gives:

$$D(q, 0, \tau_d) = \frac{1}{q^2 \tau_d R} \left\{ 1 - R - i\tau_d R q v_d \right\} \quad , \tag{11}$$

where R becomes:

$$\int_0^{\infty} \frac{d\vartheta}{\tau_d} \int_{-\infty}^{\infty} d\xi \, e^{-iq\xi - \vartheta/\tau_d} P(\xi, \vartheta) . \tag{12}$$

This result is in agreement with that of /1/ .

As regards the expression of $D(\omega)$, let us consider the limit of our results as q approaches zero. R can be expanded in series of q:

$$R = R_0 + R_1 q + R_2 q^2 + \dots \tag{13}$$

Expressions for R_0, R_1, and R_2 can be obtained from the expansion of Eq.(9), after some non totally trivial calculations:

$$R_0 = \int_0^{\infty} e^{-(1 - i\omega\tau_d)\vartheta/\tau_d} \frac{d\vartheta}{\tau_d} = \frac{1}{1 - i\omega\tau_d} \tag{13.1}$$

$$R_1 = -i \int_0^{\infty} e^{-(1 - i\omega\tau_d)\vartheta/\tau_d} \langle \xi \rangle_\vartheta \frac{d\vartheta}{\tau_d} = -i \frac{v_d \tau_d}{(1 - i\omega\tau_d)^2} \tag{13.2}$$

$$R_2 = -\frac{1}{2}\int_0^\infty e^{-(1-i\omega\tau_d)\vartheta/\tau_d} \langle \xi^2 \rangle_\vartheta \frac{d\vartheta}{\tau_d}$$

$$= -\frac{v_d^2 \tau_d^2}{(1-i\omega\tau_d)^3} - \frac{\tau_d}{(1-i\omega\tau_d)^2}\int_0^\infty C(\vartheta)\, e^{i\omega\vartheta} e^{-\vartheta/\tau_d}\, d\vartheta \tag{13.3}$$

where $C(\vartheta)$ is the autocorrelation function of velocity fluctuations:

$$C(\theta) = \langle \delta v(\theta)\, \delta v(0) \rangle$$

$\langle\ \rangle$ being the ensemble average.

Substitution of Eqs.(13) into Eq.(10) yields, for vanishing small q:

$$D(0,\omega,\tau_d) = \int_0^\infty C(\vartheta)\, e^{i\omega\vartheta}\, e^{-\vartheta/\tau_d}\, d\vartheta \tag{14}$$

For $\tau_d \to \infty$:

$$D(\omega) = \int_0^\infty C(\vartheta)\, e^{i\omega\vartheta} d\vartheta \tag{15}$$

In agreement with the results of Price /3/ and Schlup /4/, we have thus found that for a time dependent density gradient the diffusion constant, defined by Eq.(5), can be obtained as the Fourier transform of the autocorrelation function of velocity fluctuations. Eq.(14) contains also the expression for a transient $D(\omega, \tau_d)$ observed at small times τ_d, with the initial conditions for the particle velocities given by the steady-state distribution. In particular, for vanishing small ω we obtain for the transient diffusivity:

$$D(\tau_d) = \int_0^\infty C(\vartheta)\, e^{-\vartheta/\tau_d}\, d\vartheta \tag{16}$$

4. Monte Carlo procedure for the calculation of $D(q,\omega,\tau_d)$. – In order to obtain $D(q,\omega,\tau_d)$ from a Monte Carlo simulation, it is sufficient to include among the scattering mechanisms a trapping mechanism with a constant inverse rate τ_d /1/ . After a trapping process, the particle starts again with the velocity it had when decayed; velocities are thus distributed according to the stationary-state distribution. If the particle is trapped after it has covered a distance ξ in a time ϑ, the quantity $\exp[-i(q\xi - \omega\vartheta)$ is recorded. Then $R(q,\omega,\tau_d)$ is obtained as the mean value of these quantities.

5. Numerical applications to silicon . - Numerical calculations have been performed for the case of silicon, using the Monte Carlo model described in /7/ . Figs.1 to 4 show some of the results obtained with the procedure discussed above.

Figs.1 and 2 show $D(q,\omega)$ for large τ_d at different values of q, as a function of ω. It must be noted that the frequency $\omega' = \omega - qv_d$ experienced by the electrons is Doppler shifted with respect to the frequency ω indicated in the figure. The zero-q curves have been obtained as Fourier transforms of the autocorrelation function, as in Eq.(15).

Fig. 1 refers to a low field value at T= 77 K. As q increases, $D(q,\omega)$ decreases because when ql (l being the electron mean free path) becomes larger than unity, electrons contributing to the current at any point x are coming with free fligths from regions far from x. Therefore an average over several wavelengths of carrier concentration lowers the diffusion current. This nonlocal behaviour of D(q) has been discussed in /1/ . Similar considerations hold when $\omega\tau$ (τ being the electron mean momentum relaxation time) is larger than unity;

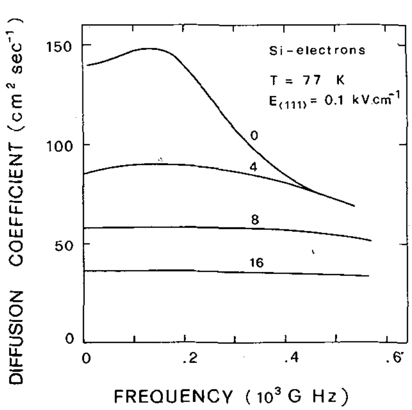

Fig.1 - Low-field diffusion coefficient as a function of frequency ω at the different values of q indicated by the numbers on the curves, in units of $10^4 cm^{-1}$.

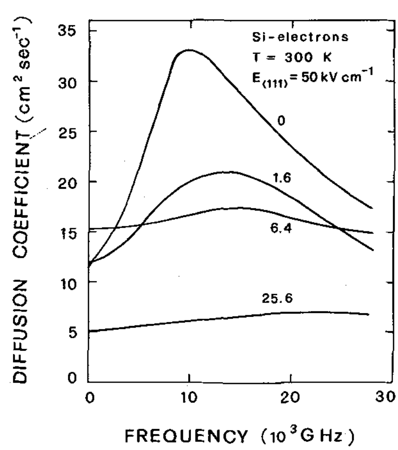

Fig.2 - High-field diffusion coefficient as a function of frequency ω at the different values of q indicated by the numbers on the curves, in units of 10^5 cm^{-1} .

at very large frequencies $D(q,\omega)$ decreases because electrons contribute to the diffusion current averaging over several periods of concentration in the past. The low-q curves show a maximum at intermediate frequencies related to the presence of active and passive regions of energy for intervalley scattering, as discussed in /5,6,8/ , which in turn can be seen in a negative part of the autocorrelation function $C(\vartheta)$. In /5/, however, this phenomenon is seen in GaAs but not in silicon. From the results presented there, this fact seems to be associated to the lack of a negative part of $C(\vartheta)$, a result which is in disagreement with the findings of the present authors. This feature is still more evident in the case of high fields, as shown in Fig. 2 .

The crossing of two curves in Fig. 2 at high frequencies can be due to their different Doppler shifts, however in the region of high frequencies the statistical uncertainties of the results become quite large. The crossing at low frequencies is due to the dependence of D upon q discussed below.

Figs. 3 and 4 show the results obtained for $D(q,\omega)$ as a function of q at low frequencies. The two figures refer to cases of low and high fields, respectively. As a general trend, D decreases at increasing q for the reason discussed above; however, at high fields, a maximum is present at intermediate values of q. The physical interpretation of this maximum is the same seen above for $D(0,\omega)$ as a function of ω . In fact the values of q at which $D(q,\omega)$ is

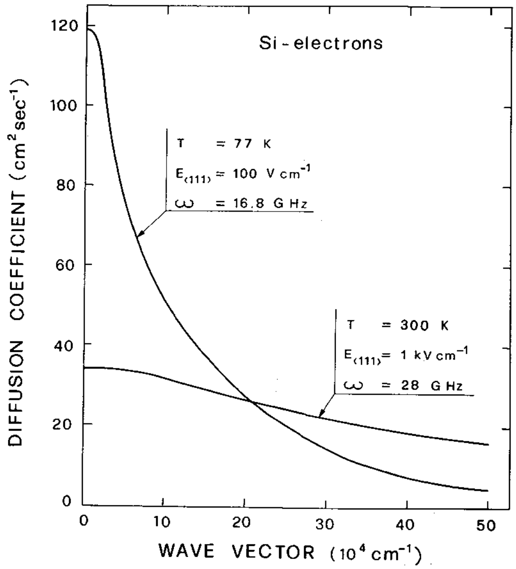

Fig.3 - Low-field and low-frequency diffusion coefficient as a function of wavevector at the indicated temperatures.

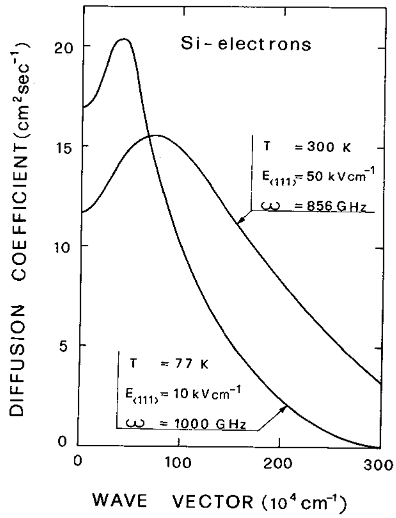

Fig.4 - High-field, low-frequency diffusion coefficient as a function of wavevector at the indicated temperatures.

maximum are corresponding to Doppler shifted frequencies at which $D(0,\omega)$ is maximum.

In conclusion, for situations in which the diffusion is to be analysed at short times or small distances because the gradient varies rapidly in time or in space, Fourier analysis can be performed, and $D(q,\omega)$ is a useful tool.

If, however, a transient phenomenon is to be studied, due to fast and short transits of carriers across small devices, then the initial conditions of the particle motion at the injection positions play a fundamental role in the determination of the features of the transient phenomenon, and particular attention must be payed in taking care of such initial conditions.

Acknowledgements . - We wish to thank for support the Centro di Calcolo Elettronico of the Modena University, where the computations have been performed.

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