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THE METHOD OF MOMENTS FOR THE ANALYSIS OF TRANSIENT HOT-CARRIER PHENOMENA

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Résumé.— La méthode des moments est proposée pour analyser le comportement de la vitesse de dérive et du coefficient de diffusion en régime non stationnaire. Les résultats obtenus avec la méthode de Monte Carlo dans Si, Ge, CdTe sont interprétés par référence aux collisions des porteurs avec le réseau et à la structure des bandes d'énergie de conduction.

Abstract.— The method of moments is here suggested to analyse the transient behaviour of drift velocity and diffusion coefficient. Monte Carlo results obtained for Si, Ge and CdTe are reported and interpreted with reference to scattering mechanisms and peculiarities of the band structure of these semiconductors.

1. Introduction.— The microscopic definition of the transport coefficients related to the phenomenological current equation, in one dimension for simplicity,

\[ j(x,t) = e \left[ n(x,t) v_d(E) - D_{\parallel}(E) \frac{\partial}{\partial x} n(x,t) \right] \]  

\( j \) being the current density, \( n \) the carrier concentration, \( v_d \) the drift velocity, \( D_{\parallel} \) the longitudinal diffusion coefficient, \( E \) the electric field and \( e \) the unit charge, is still a debated problem in the study of high-field transport phenomena /1-3/. Gantsevich et al. /4/ demonstrated that Eq.(1) can be derived from the linearized Boltzmann equation under the assumption that: i) the concentration gradient is small and, ii) the time is long enough for the momentum distribution function to be the stationary one. Owing to these limitations, any analysis of transient phenomena will require an "a priori" operative definition of the transport coefficients.

The aim of this paper is to present the method of moments as a suitable technique to overcome the limitations cited above, and to illustrate some applications to cases of general interest.

2. Theory.— Under transient conditions and high fields a one-dimensional current equation of the following form is assumed /5,6/ :

\[ j = e \left[ a n + b \frac{\partial n}{\partial x} + c \frac{\partial n}{\partial t} \right] \]  

where the coefficients \( a \), \( b \) and \( c \) can depend upon time and bias field. Eq.(2) differs from Eq.(1) for the presence of a time-derivative term. The justification and the physical meaning of the different coefficients of Eq.(2) can be directly obtained by using the continuity equation and the moments of the spatial distribution /6/, thus obtaining:

\[ a = \frac{d}{dt} \langle x \rangle \]
Table 1 - Physical parameters used in calculations.

<table>
<thead>
<tr>
<th>Type of Intervalley scattering</th>
<th>Phonon mode</th>
<th>Eq. temp. (K)</th>
<th>Coup. const. (10^-8 eV/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F₁</td>
<td>(TA)</td>
<td>220</td>
<td>0.3</td>
</tr>
<tr>
<td>F₂</td>
<td>(LA)</td>
<td>550</td>
<td>2.0</td>
</tr>
<tr>
<td>F₃</td>
<td>(TO)</td>
<td>685</td>
<td>2.0</td>
</tr>
<tr>
<td>G₁</td>
<td>(TA)</td>
<td>140</td>
<td>0.5</td>
</tr>
<tr>
<td>G₂</td>
<td>(LA)</td>
<td>215</td>
<td>0.8</td>
</tr>
<tr>
<td>G₃</td>
<td>(LO)</td>
<td>720</td>
<td>11.0</td>
</tr>
</tbody>
</table>

Ge-holes

Band parameter | A | 13.18 |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>B</td>
<td>8.48</td>
</tr>
<tr>
<td>n</td>
<td>C</td>
<td>13.14</td>
</tr>
</tbody>
</table>
Spin-orbit energy | Δ | 0.295 eV |
Crystal density | ρ | 5.32 gr/cm³ |
Sound velocity | vₐ | 3.93 x 10⁵ cm/sec |
Acoustic deformation potential | E₁ | 4.6 eV |
Optical deformation potential | δₚ | 40.3 eV |
Optical phonon temperature | Θₒ | 430 K |

CdTe-electrons

T' - effective mass | mₚ | 0.0963 |
L - effective mass | mᵢ | 0.5 |
Crystal density | ρ | 6.06 gr/cm³ |
Optical phonon temperature | Θₒ | 248 K |
Intervalley phonon temperature | Θᵢ | 220 K |
Static dielectric constant | ε₀ | 10.6 |
High-frequency dielectric constant | εₐ | 7.13 |
T' - L intervalley deformation potential | (δK)ₐL | 1.5 eV |
L - T intervalley deformation potential | (δK)ₐL | 10.9 eV/cm |

\[-b + ac = \frac{1}{2} \frac{d}{dt} \langle (x - \langle x \rangle)^2 \rangle\]  

(4)

\[6c (-b + ac) = \frac{d}{dt} \langle (x - \langle x \rangle)^2 \rangle\]  

(5)

where brackets indicate ensemble average.

Under stationary conditions (i.e. in the limit t → ∞), α reduces to the drift velocity; c = 0, as expected because the solution of Eq. (1) is symmetric; -b coincides with the longitudinal diffusion coefficient defined by Fick's law.

Under transient conditions, α is by definition the time-dependent drift velocity and a value of c different from zero, as indicated by Nag /5/, weights the contribution of the drift velocity to the time-derivative of the mean square displacement.

Owing to its stationary limiting value, the term

\[(-b + ac) = \frac{1}{2} \frac{d}{dt} \langle (x - \langle x \rangle)^2 \rangle\]

seems to be a plausible definition for a generalized diffusion coefficient allowed to depend on time in accord with Ref. (3). Consequently, Eq. (2) should be quite appropriate to study transient phenomena from ballistic up to stationary regimes in terms of the time dependence of the coefficients a, b and c or of the first three moments as defined by Eqs. (3-5).

3. Results and discussion. - The dependence with time of the different moments is calculated making use of an ensemble Monte Carlo technique. The initial conditions of motion are taken with all carriers starting from the same point (x = 0) and, energy distributed according to an equilibrium maxwellian distribution for Ge and CdTe, at fixed energy equal to (3/2) KT with K orthogonal to E for the case of Si. To exemplify the method, in Fig. 1 the first three moments of the distribution are reported for the case of electrons in CdTe. The time simulation has been taken long enough to match the stationary conditions. For the initial conditions here chosen the first moment and the second central moment exhibit in the transient region (up to about 10 psec) a time dependence which leads to overshoot of the drift velocity and, more generally, to a non-Langevin behaviour of the longitudinal diffusion coefficient. Furthermore, the third central moment evidences a significant time dependence which, in terms of Eq. (2), is interpreted as a relevant contribution of drift to spreading through a non-zero value of c.

* This assumption has been made for simplicity reasons
At times longer than 10 psec a linear least-square interpolation of the results well reproduces the stationary values with \( v_d = 1.4 \times 10^7 \) cm/sec and \( D_Q = 85 \) cm\(^2\)/sec (see the lines in Fig. 1). The same fitting procedure still yields a small negative slope of the third central moment which leads to \( c = -1.9 \times 10^{-6} \) cm. However, this non-zero value of \( c \) should not be significant because of the large uncertainty (25% which increases with time) associated with the calculation of the third central moment.

Of course, quantitative results reflect the microscopic properties of the material under investigation such as its polar or covalent nature and its band structure. To present a systematic analysis, in the following the results for the case of electrons in Si, holes in Ge and electrons in CdTe will be briefly surveyed. The uncertainty of the results is estimated to be within 5% for the drift velocity and 10% for the diffusion coefficient. The microscopic models used for these semiconductors have been found to interpret satisfactorily drift, diffusion and, for the case of Si and Ge, noise measurements in a wide range of electric field strengths and temperatures /7,8,9/, and are reported in Table 1.

**Si-electrons.** - Fig. 2 reports the results obtained at 300 K for field strengths of 20 and 100 kV/cm along a \( \langle 100 \rangle \) direction. At both fields drift and diffusion exhibit overshoot effects with peaks which are more pronounced at the highest field strength. Since the higher the acceleration the faster the dissipation starts, the peaks occur at shorter times by increasing the field strength. It is quite natural to correlate the overshoot of the diffusion coefficient to the overshoot of the drift velocity. On this correlation it has to be noted that the peak of the diffusion occurs somewhat delayed in time with respect to that of the drift velocity, furthermore, within the uncertainty of the calculations, transverse diffusion has not evidenced overshoot effects. The values of the transport coefficients in the transient are found to be practically independent from the orientation of the field, a result which is consequence of the initial equal population for different valleys here assumed. Finally, the times involved in the transient here studied are below about 0.5 psec which in turn means that detectable effects will require structure of the order of 500 \( \AA \).

**Ge-holes.** - Fig. 3 reports the results obtained at 77 K for a field strength of 10 kV/cm oriented along \( \langle 100 \rangle \) and \( \langle 111 \rangle \) directions. The main features of the time dependence of drift and diffusion resemble the Si case. Here, as a consequence of the warped structure of the heavy-hole band, a strong anisotropy of the transport coefficients with values larger in \( \langle 100 \rangle \) than in \( \langle 111 \rangle \) direction is evidenced. In particular, overshoot of both drift and diffusion, as a result of a smaller effective mass, is better evidenced along a \( \langle 100 \rangle \) direction while along a \( \langle 111 \rangle \) direction it is smoothed remarkably for the drift velocity and suppressed for the diffusion.

**CdTe-electrons.** - Fig. 4 reports the results obtained at 300 K for field strengths of 10.5 and 40.5 kV/cm, the former being below and the latter above the value of threshold for negative
differential resistivity ($\Delta 15$ kV/cm). Below threshold the drift velocity exhibits a small overshoot, on the contrary a large overshoot is found for the longitudinal diffusion coefficient. In fact, at fields just below threshold, electrons have energy high enough to undertake those flights which, in absence of intervalley scattering, would produce polar runaway. These "superflights" are at the origin of a strong initial elongation in the forward direction of the spatial distribution function $/10/$. This effect persists in time, so that values of the order of 10 psec are needed before stationary conditions are achieved.

Above threshold, in analogy with the results found for GaAs and InP $/11/$, a large overshoot of the drift velocity is found. At this field the overshoot of the longitudinal diffusivity exhibits a negative peak before reaching its stationary value for times of about 1 psec. This peculiar behaviour of $D_L$ may be explained in terms of the dominant intervalley scattering between the satellites and central valley which privileges final states in the central valley with large $K$-wavevector antiparallel to $E$ $/12$, $13/$. These states are privileged in the sense that a carrier has the possibility to perform a long flight before suffering another intervalley scattering; under ideal conditions this long flight occurs periodically in real space and carries the electron to its initial position within a cycle. Consequently, when this process dominates, the ensemble of carriers, which are assumed to start at the same point, will spread initially according to its maxwellian momentum distribution to come closer at the end of the cycle. This "pulsed" character of the motion of the electron ensemble is damped fastly by the presence of shorter flights and other scattering mechanisms but, within the transient it is strong enough to produce the negative values of the longitudinal diffusion coefficient as reported in Fig. 4(b). The long times involved in the transient at fields near threshold and the high value of the drift velocity overshoot at fields well above threshold mean that detectable effects are possible in structure within $0.1 - 1 \mu m$. 

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**Fig. 2** - Drift velocity (a) and longitudinal diffusion coefficient (b) as a function of time for the case of electrons in Si at $T = 300$ K. Dashed and continuous curves refer to electric field strengths of 20 and 100 kV/cm, respectively.

**Fig. 3** - Drift velocity (a) and longitudinal diffusion coefficient (b) as a function of time for the case of holes in Ge at $T = 77$ K and $E = 10$ kV/cm. Continuous and dashed curves refer to field oriented along $(100)$ and $(111)$ directions, respectively.
4. Conclusions. - The study of the transient behaviour of drift and diffusion at high fields is carried out in terms of the time analysis of the first moment and the second and third central moments of the spatial distribution. In this way a generalized longitudinal diffusion coefficient at short times is defined through Eq. (4). For the initial conditions here assumed, the drift velocity and the longitudinal diffusion coefficient are found to exhibit overshoot effects. By increasing the electric field strength overshoot is favoured and its peak shifts at shorter times. The warped shape of the valence band is found to be at the origin of strong anisotropy effects in both drift and diffusion, higher values of these quantities being associated with the direction for which the effective mass of carriers is smaller. In CdTe, for a field strength just below threshold, when polar optical scattering is dominant over other scattering mechanisms overshoot effect of longitudinal diffusivity is quite larger and persists up to times of the order of 10 psec. For field strengths above threshold, the drift velocity is found to exhibit the highest peak of its overshoot for fields above threshold.

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**References.**

/3/ D.K. Ferry and J.R. Barker, J. Appl. Phys. 52, 818 (1981) and references therein
22, 103 (1973)

