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ON INTERVALLEY DIFFUSION OF HOT-ELECTRONS

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Abstract. - This paper presents an analysis of the applicability of the Shockley formula to the evaluation of the intervalley diffusion coefficient $D^1$ of electrons for a realistic case of many-valley semiconductor. In particular it is shown that the simplifying hypothesis of a constant time $\tau$ for carrier intervalley transfer leads to an overestimation of $D^1$. For a determination of $D^1$ from Monte Carlo simulation particular care must be put in the definition and the evaluation of the valley contributions to diffusion. Numerical results are presented for the case of Si at $T = 77$ K and $T = 200$ K, and compared with the results obtained by means of the Shockley formula.

1. Intervalley diffusion. - If we apply a static uniform electric field $\vec{E}$ to a many valley semiconductor, electrons in valleys differently oriented with respect to the field orientation have different drift velocities. This fact brings about an intervalley diffusion $D^1$, which must be added in the longitudinal diffusivity if the valley drift velocities have different components parallel to $\vec{E}$, and/or to the transverse diffusivity if valley drift velocities have different components perpendicular to $\vec{E}$. The physical reason of this phenomenon is shown in Fig. 1 for a two-valley semiconductor.

In the first case (Fig. 1-a) if electrons are in $x = 0$ at $t = 0$, at increasing time they will spend part of their time in one type of valley and part in the other type, so that they will drift part of their time with velocity $v_1$ and part with $v_2$. Thus an initial bunch will spread along the direction of the field even in absence of thermal diffusion.

In the second case, even though the average drift velocity is parallel to $\vec{E}$, in each valley electrons have drift velocities not parallel to $\vec{E}$, the components of $v_1$ and $v_2$ being equal in modulus, but with opposite orientations. This fact, together with the coupling of the two valleys, leads to the presence of a transverse intervalley diffusion.

For silicon, which is the material considered in this paper, these two cases occur when $\vec{E}$ is along a (100) direction or a (111) direction, respectively. If one considers other symmetry directions, such as a (110) direction, parallel and transverse intervalley diffusivities are present simultaneously.
2. **Shockley formula.** - For a model with two types of valleys the total diffusivity $D$ is given by the expression:

$$D = n_1 D_1 + n_2 D_2 + D^i$$

where $n_1$ and $n_2$ are the fractions of electrons in valleys of type 1 and 2 respectively, $D_1$ and $D_2$ are the single-valley contributions to the diffusion, and $D^i$ is the intervalley diffusion coefficient. In this case for the evaluation of the intervalley diffusion a general expression has been given by Shockley \(^1\):

$$D^i = n_1 n_2 (v_1 - v_2)^2 \tau_i$$

$$1/\tau = 1/\tau_i + 1/\tau_t$$

where $\tau_i$ is the inverse rate for electron transfer from a valley of type 1 to any valley of type 2, and similarly for $\tau_t$. Eq. (2) has been obtained for a simplified model in which the inter-valley-transfer times $\tau_i$ and $\tau_t$ are supposed to be constant in time. This hypothesis, however, is far from reality in actual semiconductors. In fact, when a carrier undergoes an inter-valley scattering it arrives in the final valley with an energy which is, in general, lower than the mean energy of the valley, because intervalley-phonon absorption is less frequent than emission, so that the carrier energy grows up during the first time spent in the new valley. Therefore, the intervalley scattering probability, which is strongly energy-dependent, also varies with time.

This phenomenon can be made particularly apparent for a semiconductor model in which the intervalley scattering occurs only if, and as soon as, the electrons reach a value of energy $\epsilon_5$, and intravalley scattering is absent. In this case Eq. (2) leads to an intervalley diffusion
sion different from zero, $\tau$, and $\tau_Z$ being equal to the times necessary for the carrier energy to reach the value $E$. The intervalley diffusion, however, is zero, because the electron dynamics is no more stochastic: if we consider, for example, a two-valley model with the electrons in $x = 0$ at $t = 0$ with $k = 0$, after any time $t$ all of them have spent the same time in each type of valley, and the indetermination on these times, which brings about intervalley diffusion, is lost. The simplifying hypothesis of a constant $\tau$ leads to an indetermination on the time of occurrence of an intervalley transition of the order of $\tau$, while for the stepwise probability function considered above the indetermination is zero. For a real physical case the scattering probability again increases rapidly at the energy range of the intervalley phonons, and the indetermination on $\tau$ is intermediate between the two cases. So we can conclude that Eq.(2) gives a general overestimate of $D_1$.

3. On the definition of single-valley diffusion. - The general considerations reported above suggest the convenience of an evaluation of $D_1$ independent of Eq.(2), which can be achieved by calculating $D_1$ as the difference between the total diffusivity $D$ and the single-valley contributions $D_v$. An appropriate definition of $D_v$ is however not trivial. One can think of defining $D_v$ in the same way as $D$ using the expression:

$$\lim_{t \to \infty} \frac{1}{2} \frac{d}{dt} \langle (x - \langle x \rangle)^2 \rangle$$

where now $x(t)$ is the space covered by the carrier when it is in the valley of interest, and $t$ is the time spent by the carrier in the same valley. This definition however is not correct, because if only the time spent by the carrier in a valley is taken into account, intervalley transitions break the correlation between "the past" and "the future" of the carrier: coming back in the valley, the carrier has lost memory of the values of its dynamical properties (namely velocity and energy fluctuations above their mean values) before it had been scattered away. In particular some contribution to the diffusivity, related to velocity fluctuations, is lost. If we remember that intervalley transitions bring about negative correlations of velocity fluctuations, we can expect that Eq.(3) overestimates $D$.

These considerations have been checked in the case of Si with $E$ parallel to a $(111)$ direction: in this case all valleys are equivalent with respect to the field direction and, for symmetry, $D_v = D$. Fig. 2 shows that $D_v$ calculated with Eq.(3) is, instead, greater than $D$. Results also show that when the number $N$ of valleys considered in the evaluation of Eq.(3) increases $D_v$ tends to $D$ as expected, when all the six valleys are considered, the correlation between the various fragments of the particle history is correctly taken into account and $D_v$ beco
As further support to this physical interpretation, the autocorrelation function of the velocity fluctuations:

\[
\mathcal{C}(\theta) = \left\langle \delta v(t) \delta v(t+\theta) \right\rangle
\]

where \( \theta \) indicates time average and \( \langle \rangle \) ensemble average, has been calculated for both the case in which all the particle history is considered and the case in which only the single-valley history is studied. Results, reported in Fig. 3, show that the negative part of \( \mathcal{C}(\theta) \), which is connected to the existence of negative correlations due to intervalley transitions, is reduced, as expected from the considerations reported above.

When \( \mathbf{E} \) is along a \( (100) \) direction we have hot and cold valleys, and consequently, an intervalley term is added to the longitudinal diffusivity. For this reason care must be put in order to obtain an estimate of the \( D_{1c} \)'s, without having interference with intervalley diffusion. Eq. (3) can be used for a single cold or hot valley, thus obtaining \( D_{1c} \) and \( D_{1h} \), respectively; furthermore Eq. (3) can be used with the collection of all equivalent cold or hot valleys, thus obtaining \( D_{2c} \) and \( D_{2h} \), respectively. If we assume that each \( f \) or \( g \) scattering event plays the same role in the determination of \( D_{1c} \), then \( D_{2c} \) which collects information only from the cold valleys, corrects \( D_{1c} \) for all \( g \) scatterings and no \( f \) scattering, while \( D_{2h} \), which collects information only from hot valleys, corrects \( D_{1h} \) for all \( g \) and half \( f \) scatterings.

Thus an estimate of \( D_{vc} \) and \( D_{vh} \) can be obtained as follows:

\[
D_{vc} = D_{1c} + (D_{2c} - D_{1c}) \frac{N_f + N_g}{N_f + N_g/2}
\]

\[
D_{vh} = D_{1h} + (D_{2h} - D_{1h}) \frac{N_f + N_g}{N_f + N_g/2}
\]

where \( N_f \) and \( N_g \) are the number of \( f \) and \( g \) scattering events, as obtained from the Monte Carlo simulation, respectively. The above procedure has been checked in the case of \( \mathbf{E} \) along a \( (111) \) direction: \( D_{1c} \), evaluated from Eq. (5), where \( D_2 \) and \( D_4 \) have been obtained collecting results on two valleys and four valleys respectively, is equal to the total diffusion coefficient \( D \), as expected.

4. Numerical results. - Once the valley diffusion constants have been obtained by means of Eq (5) with the procedure described in the previous section, the intervalley diffusivity \( D^1 \) can be obtained by difference, from Eq. (1).

Numerical results have been obtained from a Monte Carlo silicon model whose characteristics are described in detail in /4/. Fig. 4 shows the results for \( D^1 \) compared with the predictions of Eq. (2) for which \( \mathcal{C} \) has been obtained from the simulation /4/. For comparison, the total longitudinal diffusivity \( D \) has been reported.

At 200 K the difference between \( D^1 \), as evaluated from Eq. (1), and from Eq. (2) is small, comparable to the statistic uncertainty of the results. At 77 K, on the contrary, the difference is quite large, and decreases as the field strength increases. This behaviour can be under...
stood by considering that at higher electron energies the time dependence of $\zeta$, caused by the energy-loss due to intervalley emission, is reduced.

In order to check the physical interpretation of the above results, a simple model has been analysed in which acoustic intravalley scattering is strongly depressed and a very strong intervalley scattering is present, with equivalent temperature $T_e = 500$ K. The lattice temperature has been kept low, in order to eliminate phonon absorption. In this way we approach the limiting situation discussed in section 2.

Fig. 5 shows the autocorrelation function of velocity fluctuations obtained for a field of 500 V/cm along a $\langle 111 \rangle$ direction, whose long oscillatory character indicates a strong streaming behaviour, which, in turn, corresponds to a strong time dependence of $\zeta$. For $E$ parallel to a $\langle 100 \rangle$ direction the Shockley formula yields, with this model, an intervalley diffusivity which is even greater than the total $D$ (Fig. 6). The correct evaluation of $D^l$ from Eq.(1)
on the contrary, gives values well below $D$, as expected.

We have seen that in Eq. (2) $\tau$ plays the role of the uncertainty in the time of occurrence of intervalley transitions; by consideration of the connection between noise and diffusion and of the Wiener–Khinchine theorem, it seems reasonable that a better approximation would be obtained by using $\tau$ in Eq. (2) as the autocorrelation time of the fluctuations of the number of carriers in hot and cold valleys, defined as the integral of their autocorrelation function $C_n(\theta)$ divided by its value at $\theta = 0$.

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References.