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NOISE AND DIFFUSION IN p-TYPE SILICON

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RESUME: La théorie des fluctuations de la fonction d'occupation d'états, développée très récemment, et la notion de temps de relaxation différentiel, permettent de donner ici l'expression du coefficient de diffusion transversal, qui est calculé numériquement dans si-p en fonction du champ électrique à 300 K entre 0 et 50 kV/cm.

ABSTRACT: The theory of the fluctuations of the state occupancy function, recently developed, together with the differential relaxation time, allow getting the transverse diffusion coefficient, which is computed in p-type Silicon, as a function of the electric field, at 300 K, from 0 to 50 kV/cm.

1. INTRODUCTION:

Except Monte Carlo simulations, which are much time consuming and thus very expensive, all the device modeling methods use transport equations, which require the knowledge of the diffusion coefficient $D(E)$ as a function of the electric field E . $D(E)$ is difficult to obtain. One way to get it is to study the diffusion noise, experimentally or theoretically. The purpose of this paper is to propose a new theoretical method for determining the diffusion coefficients, based on the differential relaxation time and on the fluctuation of the state occupancy function.

2. STATE OCCUPANCY FUNCTION:

In a previous paper [1], we settled a theory, derived from a series of nice papers from Gansevitch, Gurevitch and Katilius, they gathered in a review article [2]. In that paper, we studied the fluctuations of the State Occupancy Function $f(\mathbf{k},t)$ of hot carriers (labelled SOF in the following for convenience). $f(\mathbf{k},t)$ is a random function which takes the value 1 when the state $\mathbf{k}$ is occupied by a carrier, and the value 0 when the state $\mathbf{k}$ is empty. The SOF depends on the external electric field E , but for convenience we shall omit E , wherever it is possible. $f(\mathbf{k},t)$ fluctuates, due to the random motion of the carriers, which undergo scattering events. If $N(t)$ is the total number of carriers inside the sample at time t , one has :

$$N(t) = \sum_{\mathbf{k}} f(\mathbf{k},t) \quad (1)$$

The ensemble average $\langle f(\mathbf{k},t) \rangle$ of $f(\mathbf{k},t)$ is then the distribution function at time t , governed by the Boltzmann equation (labelled BE in the following). As $t \rightarrow \infty$, $\langle f(\mathbf{k},t) \rangle \rightarrow f_s(\mathbf{k},E)$, solution of the steady state BE in the uniform electric field E .

3. THE DIFFERENTIAL RELAXATION TIME:

Since we intend to study small fluctuations around the steady state, we are interested in small deviations of the distribution function $\langle f(\mathbf{k},t) \rangle$ around its steady state value $f_s(\mathbf{k},E)$. This can be done

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using the differential relaxation time concept, introduced some years ago [3], defined as follows: When a small perturbation δE is applied, the new steady state distribution is $f_s(\mathbf{k}, E + \delta E)$. When the perturbation δE is removed, $\langle f(\mathbf{k}, t) \rangle$ evolves from $f_s(\mathbf{k}, E + \delta E)$ to $f_s(\mathbf{k}, E)$. The differential relaxation time $\tau(\mathbf{k}, E)$ is then defined as:

$$\lim_{|\delta E| \rightarrow \infty} \left(\frac{\partial \langle f(\mathbf{k}, t) \rangle}{\partial t} \right)_{t=0} = - \lim_{|\delta E| \rightarrow \infty} \left(\frac{f_s(\mathbf{k}, E + \delta E) - f_s(\mathbf{k}, E)}{\tau(\mathbf{k}, E)} \right) \quad (2)$$

Indeed, as shown in [3], $\tau(\mathbf{k}, E)$ can be expressed, using the steady state BE for $f_s(\mathbf{k}, E + \delta E)$ and $f_s(\mathbf{k}, E)$, and the transient BE for $\langle f(\mathbf{k}, t) \rangle$. One then finds that $\tau(\mathbf{k}, E)$ depends on the direction of the perturbation δE with respect to the electric field E :

$$\tau(\mathbf{k}, E) = - \frac{\hbar}{q} \frac{\delta E \cdot \nabla_E f_s(\mathbf{k}, E)}{\delta E \cdot \nabla_E f_s(\mathbf{k}, E)} \quad (3)$$

When δE is perpendicular to E , one gets $\tau_{\perp}(\mathbf{k}, E)$. In polar coordinates with the polar axis along E , $\mathbf{k} = (k, \theta)$ with $k = |\mathbf{k}|$ and $\theta = (E, \mathbf{k})$. $\tau_{\perp}(\mathbf{k}, E)$ is then easily expressed as [3]:

$$\tau_{\perp}(\mathbf{k}, E) = \frac{\hbar k}{qE} \frac{\partial f_s(\mathbf{k}, E) / \partial \theta}{(\partial f_s(\mathbf{k}, E) / \partial \theta) \cos \theta + k (\partial f_s(\mathbf{k}, E) / \partial k) \sin \theta} \quad (4)$$

Within the above hypothesis, the evolution of the distribution function $\langle f(\mathbf{k}, t) \rangle$, around its steady state value $f_s(\mathbf{k}, E)$, is governed by the equation:

$$\frac{\partial \langle f(\mathbf{k}, t) \rangle}{\partial t} = - \frac{\langle f(\mathbf{k}, t) \rangle - f_s(\mathbf{k}, E)}{\tau(\mathbf{k}, E)} \quad (5)$$

As an example, figure 1 shows the variations of $\tau_{\perp}(\mathbf{k}, E)$ versus $k = |\mathbf{k}|$, along three directions with respect to the electric field E ($\theta = 0$, $\theta = \pi/2$, and $\theta = \pi$), in undoped p-type Silicon at 300 K, $E = 2$ kV/cm (fig. 1a) and $E = 20$ kV/cm (fig. 1b). $f_s(\mathbf{k}, E)$ was computed numerically, using a matrix method, so as $\tau_{\perp}(\mathbf{k}, E)$ through eq. (4). We used a one spherical non parabolic band model. As can be seen fig. 1, $\tau_{\perp}(\mathbf{k}, E)$ is in the range 0.01 to 0.2 ps at 20 kV/cm, and increases as the field strength decreases.

4. FLUCTUATION OF THE STATE OCCUPANCY FUNCTION:

In order to study the fluctuations of the SOF, we apply the general theory developed in [1], to the particular case studied here, where the BE is replaced by eq. (5). According to [1], one sets: $\langle f(\mathbf{k}, t) \rangle = f_s(\mathbf{k}, E) + \delta f(\mathbf{k}) \exp(i\omega t)$. This expression, carried into eq. (5), gives for the first order terms, $\delta f(\mathbf{k})$ as a solution of:

$$\left[i\omega + \frac{1}{\tau(\mathbf{k}, E)} \right] \delta f(\mathbf{k}) = 0 \quad (6)$$

The Langevin theory then relies the fluctuation $\hat{f}(\mathbf{k}, \omega)$ to the white noise source term $\xi(\mathbf{k})$ by:

$$\left[i\omega + \frac{1}{\tau(\mathbf{k}, E)} \right] \hat{f}(\mathbf{k}, \omega) = \xi(\mathbf{k}) \quad (7)$$

This gives, for the spectral density $S_f(\mathbf{k}, \mathbf{k}', \omega)$ of the fluctuations of the SOF:

$$S_f(\mathbf{k}, \mathbf{k}', \omega) = \frac{\tau^2(\mathbf{k}, E)}{1 + \omega^2 \tau^2(\mathbf{k}, E)} S_g(\mathbf{k}) \delta_{\mathbf{k}\mathbf{k}'} \quad (8)$$

where $\delta_{\mathbf{k}\mathbf{k}'} = 1$ if $\mathbf{k} = \mathbf{k}'$, and $\delta_{\mathbf{k}\mathbf{k}'} = 0$ if $\mathbf{k} \neq \mathbf{k}'$. $S_g(\mathbf{k})$ can be evaluated using the variance $\langle \Delta f^2(\mathbf{k}, t) \rangle$ which writes [1]:

$$\langle \Delta f^2(\mathbf{k}, t) \rangle = f_s(\mathbf{k}, E) [1 - f_s(\mathbf{k}, E)] = \int_0^\infty S_f(\mathbf{k}, \mathbf{k}, \omega) d\omega \quad (9)$$

Carrying eq.(8) in eq.(9) readily gives $S_g(\mathbf{k})$, so that finally, with $F_s(\mathbf{k}, E) = f_s(\mathbf{k}, E)[1 - f_s(\mathbf{k}, E)]$:

$$S_f(\mathbf{k}, \mathbf{k}', \omega) = \frac{4\tau(\mathbf{k}, E)}{1 + \omega^2 \tau^2(\mathbf{k}, E)} F_s(\mathbf{k}, E) \delta_{\mathbf{k}\mathbf{k}'} \quad (10)$$

5. DIFFUSION COEFFICIENT:

The spectral density $S_{j\alpha\beta}(\omega)$ of the fluctuations of the current density writes [2][1]:

$$S_{j\alpha\beta}(\omega) = \frac{q^2}{\Omega^2} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} v_{\alpha}(\mathbf{k}) v_{\beta}(\mathbf{k}') S_f(\mathbf{k}, \mathbf{k}', \omega) \quad (11)$$

where Ω is the volume of the sample, and α and β mean directions with respect to the electric field. The local noise source term $K_{\alpha\beta}(\omega)$ is:

$$K_{\alpha\beta}(\omega) = \Omega S_{j\alpha\beta}(\omega) = 4 q^2 n D_{\alpha\beta}(\omega) \quad (12)$$

which gives, using eqs.(11) and (10), replacing summations over $\mathbf{k}$ by integrations over $\{\mathbf{k}\}$ space, and taking into account the density of states $1/8\pi^3$:

$$D_{\alpha\beta}(\omega) = \frac{\int \frac{\tau(\mathbf{k}, E) v_{\alpha}(\mathbf{k}) v_{\beta}(\mathbf{k})}{1 + \omega^2 \tau^2(\mathbf{k}, E)} F_s(\mathbf{k}, E) d^3\mathbf{k}}{\int f_s(\mathbf{k}, E) d^3\mathbf{k}} \quad (13)$$

Using this method, we computed the transverse diffusion coefficient $D_{\perp}(E)$ in p-type Silicon, with doping impurity concentrations $N_A = 0$ and $N_A = 10^{17} \text{ cm}^{-3}$, at $t = 300 \text{ K}$, as a function of the electric field intensity E . Then, in eq.(13), $v_{\alpha}(\mathbf{k}) = v_{\beta}(\mathbf{k}) = v \sin \theta \cos \phi$, $\tau(\mathbf{k}, E) = \tau_{\perp}(\mathbf{k}, E)$ and $F_s(\mathbf{k}, E) \approx f_s(\mathbf{k}, E)$ since in our case the semiconductor is non degenerate. $D_{\perp}(E)$ was also computed using a Monte Carlo simulation. The results are shown figure 2: taking into account the statistical dispersion of the Monte Carlo simulation, the results are in excellent agreement.

The result presented here is the first theoretical determination of the hot carrier diffusion coefficient using the distribution function, with non randomizing scattering mechanisms. Depending on the electric field strength, it is 10 to 50 CPU time less consuming than the Monte Carlo simulation.

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Figure 1: $\tau_{\perp}(\mathbf{k}, E)$ for holes in undoped Silicon, as a function of $k=|\mathbf{k}|$, at 300 K, along three directions $\theta=0$ ($\bullet$), $\theta=\pi/2$ ($\triangle$), and $\theta=\pi$ ($\blacksquare$), with respect to the electric field E . (a) $E=2$ kV/cm, (b) $E=20$ kV/cm.

Figure 2: Transverse diffusion coefficient $D_{\perp}(E)$ of holes, as a function of the electric field intensity E , in pure ($N_A=0$) and doped ($N_A=10^{17}\text{cm}^{-3}$) p-type Si at 300 K.
 Monte Carlo simulation: $N_A=0$ (—) and $N_A=10^{17}\text{cm}^{-3}$ (----)
 Computed using eq.(13): $N_A=0$ ($\blacksquare$) and $N_A=10^{17}\text{cm}^{-3}$ ($\bullet$)