High-field transport properties of bulk Si: A test for the Fokker-Planck approach

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High-field transport parameters are calculated using an analytical Fokker-Planck approach (FPA), where transport is modeled as a drift-diffusion process in energy space. We have applied the theory to the case of Si, taking into account the six intervalley phonons, aiming to test the FPA. The obtained results show a quite reasonable agreement with experimental data and Monte Carlo simulations confirming in this case that the FPA works very well for high enough electric fields.

PACS numbers: 72.10.Di; 72.20.Ht.

More than three decades ago the Fokker-Planck approach (FPA) was proposed as an alternative for the Boltzmann transport equation (BTE) in the calculation of semiconductor transport properties. Recently the theory has been revisited in a series of works where a relatively detailed analysis of both mathematical and physical aspects of this formalism was developed. In these papers the same model system was considered in calculations using the FPA and the BTE by means of the Monte Carlo method. The results of both approaches showed good agreement in the high electric-field regime for the mentioned model system. In spite of this, there remains a certain degree of doubt about how the FPA could handle a more realistic model of a concrete semiconductor with several possible scattering mechanisms and complicated band structure. The FPA considers transport, in the opposite regime of the ballistic one, as a certain diffusive-drifting “motion” of the carriers in the energy space and it is valid when \( \tau(\vec{p}) < t < \tau_E \), where \( \tau(\vec{p}) \) is the momentum relaxation time and \( \tau_E \) is the energy relaxation time. The method is semiclassical by its own nature and applicable when the energy exchange between the carriers and the surrounding medium can be assumed quasicontinuous which excludes highly inelastic scattering processes. It is valid when the average carrier energy is much larger than the exchanged energy as in the case of high-field transport. The FPA has the advantage of being analytical, and, whenever it can be applied, saves computational time and allows a more transparent physical interpretation.

In this report, we present results within the FPA for bulk Si and compare them with experimental data and previous Monte Carlo simulations (using the BTE). We show that the FPA leads to good results as compared with those data whatever several scattering mechanisms (six intervalley phonons between the Si \( \Delta \) valleys in the conduction band) are taken into account. The intravalley acoustic phonons were ignored, and thus our results are reliable just for high enough temperatures.

The evolution of the energy distribution function (DF) \( f(E,t) \) is governed by the Fokker-Planck equations

\[
\frac{\partial}{\partial t} f(E,t) + \frac{1}{N(E) \partial E} J(E,t) = 0, \tag{1}
\]

where

\[
J(E,t) = W(E)N(E)f(E,t) - \frac{\partial}{\partial E} [D(E)N(E)f(E,t)], \tag{2}
\]

such that \( f(E,t)N(E) \) gives the number of carriers at time \( t \) with energies in the interval \( (E, E + dE) \), while the function \( N(E) \) represents the density of states (DOS). In Eq. (2) \( W(E) \) represents a certain “drift velocity” in energy space and in fact gives the rate of energy balance of the carrier, \( D(E) \) is a kind of diffusion coefficient and \( J(E,t) \) represents thus the carrier current density in energy space. Under steady state conditions, the Eq. (2) transforms into

\[
\frac{\partial}{\partial E} [D(E)N(E)f(E)] = W(E)N(E)f(E). \tag{3}
\]

The carriers interact with the phonons and the applied dc electric field \( \vec{F} \). We assume a phonon reservoir in thermal equilibrium at the temperature \( T \) and that the continuous exchange of phonons between the carriers and the bath does not affect the thermal equilibrium of the latter. Hence, the coefficients \( W(E) \) and \( D(E) \) are split as follows

\[
D(E) = D_F(E) + D_{ph}(E), \quad W(E) = W_F(E) + W_{ph}(E). \tag{4}
\]
The label "F" ("ph") denotes the electric field (phonon) contribution to these coefficients, whose explicit forms will be given below. Equation (3) has the simple solution

\[ f(E) = \exp \left\{ \int \frac{W_{ph}(E)}{D_F(E)} dE \right\} \]

(5)

where \( D_{ph}(E) \) was neglected. This approximation is very well fulfilled in all the cases of interest for us.

We consider transport of electrons in the Si conduction band (CB) in a high dc electric field regime \( (F > 10 \text{ kV/cm}) \). We take into account the six ellipsoidal energy valleys of Si at the \( \Delta \) points of the Brillouin zone (along the \( <100> \) direction). To be specific, let us take \( \vec{F} = (0, 0, F) \), where the \( z \) axis is taken along one high symmetry direction, and denote by \( "F" \) ("tr") the valleys with principal axis parallel (perpendicular) to \( \vec{F} \).

The explicit expressions for \( D_F(E) \) and \( W_{ph}(E) \) are

\[ D_F(E) = \left\{ \tau(\vec{p}) |q\vec{F} \cdot \nabla \epsilon(\vec{p})|^2 \right\} \]

(6)

\[ W_{ph}(E) = \hbar \omega_1 \left[ \frac{1}{\tau_{abs}(\vec{p})} - 1 / \tau_{em}(\vec{p}) \right] \]

(7)

where the brackets represent an average over the constant energy surface \( \epsilon(\vec{p}) = \text{const} \), \( \tau(\vec{p}) \) is the total relaxation time due to the electron-phonon scattering, and \( "abs" \) ("em") denotes phonon absorption (emission) by the electron due to the several scattering mechanisms.

A straightforward evaluation of Eq. (6) leads to

\[ D_F(E) = \frac{2e^2F^2}{3m_j} \tau(\epsilon) \gamma(\epsilon) / (\gamma'(\epsilon))^2 \]

\[ j = l, \text{tr}, \]

(8)

where \( \gamma'(\epsilon) \) denotes the derivative of the function \( \gamma(\epsilon) = \epsilon(1 + \alpha \epsilon) \) responsible by the non-parabolicity of the band structure with \( \epsilon = \epsilon(\vec{p}) \) being the energy dispersion for a given valley. For \( \tau(\epsilon) \) we shall consider the six intervalley phonons responsible for transitions between the equivalent \( \Delta \)-valleys of Si. Then the total relaxation time reads as

\[ \frac{1}{\tau(\epsilon)} = \sum_{i=1}^{6} C_{oi} \left\{ n_i(T) \sqrt{\gamma(\epsilon + \hbar \omega_i)} [1 + 2\alpha(\epsilon + \hbar \omega_i)] \right\} \]

\[ + (n_i(T) + 1) \sqrt{\gamma(\epsilon - \hbar \omega_i)} [1 + 2\alpha(\epsilon - \hbar \omega_i)] \Theta(\epsilon - \hbar \omega_i) \]

(9)

where \( \Theta(\epsilon) \) is the step function, \( n_i(T) \) is the phonon distribution function, and

\[ C_{oi} = (m_{tr}m_l^{1/2}D_{oi}^2) / (\sqrt{2\pi \rho \hbar^3 \omega_i}) \]

with \( m_{tr} \) \( (m_l) \) being the transverse (longitudinal) effective mass, \( \rho \) the semiconductor density, \( \omega_i \) and \( D_{oi} \) the frequency and deformation-potential constant respectively for intervalley phonons of type \( i \). In Eq. (9), the first and second terms correspond to \( 1 / \tau_{abs}(\epsilon) \) and \( 1 / \tau_{em}(\epsilon) \) respectively. The phonon contribution can be written as

\[ W_{ph}(E) = \sum_{i=1}^{6} W_{ph}(E) \]

(10)

where \( W_{ph}(E) \) is given by Eq. (9) for each \( i \). Intravalley optical phonons do not contribute to transition rates, because the corresponding transitions are forbidden by the selection rules and we assume that, for high \( T \) and \( E \), the contribution of intravalley acoustic phonons should be neglected.

Once, we have evaluated \( W_{ph}(E) \) and \( D_F(E) \), we have to calculate the integral in Eq. (9) to obtain the two DF, \( f_l(E) \) and \( f_{tr}(E) \), corresponding to the \( l-tr \) valleys respectively. Of course, the FPA is of practical use only in the case where such integration can be analytically performed which is not the case for expressions of \( D_F \) and \( 1 / \tau(E) \) given by Eqs. (8) and (9). So, we consider a single effective intervalley phonon with energy \( \hbar \omega_0 = 0.0343 \, \text{eV} \), obtained from an average of different phonon frequencies given in Table VI of [9], and with constant \( D_0 \) obtained by the superposition of the different deformation-potential constants, but also including the number of final equivalent valleys for each kind of transition. With this approximation we obtain the following result

\[ \sum_{i=1}^{6} \frac{W_{ph}(E)}{D_F(E)} = \frac{3m_j\hbar\omega_0}{2e^2F^2} \sum C_{oi}C_{ot} \Phi(E, T), \quad j = l, tr, \]

(11)
with

$$\Phi(E, T) = n^2(T)(E + 1)(1 + E_0(E + 1))(1 + 2E_0(E + 1))^2$$

$$- (n(T) + 1)^2(E - 1)(1 + E_0(E - 1))(1 + 2E_0(E - 1))^2\Theta(E - 1),$$

(12)

where hereafter $E$ is in units of $\hbar\omega_0$ and $E_0 = \hbar\omega_0\tau$. Considering the contributions from different valleys and using Eq.(8), again applying the parameters from Table VI Ref. [9], we are led to:

$$f(E) = \exp \left[ \beta_j \int \Phi(x, T)dx \right],$$

(13)

with $\beta_j = (3m_jm_o^3D^2_o)/4\pi^2\rho^2e^2F^2\hbar^4$ and $D_o$ is the effective deformation-potential constant defined through $D^2_o = \sum D^2_jD^2_{ok}$. We have estimated $D_o = 12.09 \times 10^8$ eV/cm and in all the above expressions the overlapping integral (see Ref. [9]) was taken equal to unity. However, for numerical computations it should be useful consider it as a fitting parameter.

The integral involved in Eq.(13) can be analytically performed in a straightforward way and the general structure of the DF has the form:

$$f(E) = E^A(1 + E_0E)^B \exp(C \cdot P(E)),$$

(14)

where $A$, $B$ and $C$ are parameters dependent on $T$ and $F$ and $P(E)$ is a polynomial. This structure is far from a Maxwellian one. The DF describes the stationary non-equilibrium configuration where an electron temperature $T_e$ cannot be defined. From Eq.(14), we can immediately obtain the average electron energy, estimated as $E_{av}(T, F) = (E_{av}^l + 2E_{av}^{tr})/3$ with

$$E_{av}^j = \left[ \int Ef_j(E)N(E)dE \right] / \int f(E)_jN(E)dE \quad j = l, tr.$$

(15)

In Fig. 1, the electric-field dependence of $E_{av}$ is depicted for different temperatures. As expected, we found a weak temperature dependence. We can see that the average electron energy increases for larger electric fields. Moreover, the condition $E_{av}^l >> \hbar\omega_0$ is fairly well accomplished, ensuring that the FPA is within its range of validity for the given temperatures. Our results cannot be expected to be correct for low temperatures (or too low carrier energies) because we neglect intravalley acoustic phonons.

The drift velocity $v_d = (v_{dl} + 2v_{dtr})/3$ can be also evaluated from (12)

$$v_{dl} = \frac{2eF}{3m_j} \int \frac{\gamma(E)\tau(E)}{(\gamma'(E))^2} \left[ - \frac{df_j(E)}{dE} \right] N(E)dE / \int f(E)_jN(E)dE.$$

(16)

In Fig. 2, we show $v_d$ as a function of $F$ for two different temperatures. We see that the general behavior of the curve is qualitatively correct if compared with experimental results and Monte Carlo simulations. For a more quantitative comparison, we present in Fig. 3 our results together with the experimental data and those from Monte Carlo simulations [11,12]. As it can be seen, we obtained a good agreement with both results for $T = 300$ K in the high electric-field regime. However, in the opposite limit, the results from FPA do not reproduce those from experiments and Monte Carlo calculations, as should be expected. For comparison with experimental data we have taken $\beta_j$ as a fitting parameter, an issue which can be reasonably understood considering the overlapping integral for the electron-phonon scattering probabilities. Another point to be stressed is that reliable results were obtained just for high temperatures. However this is not a limitation of the FPA itself but of our present calculations since we have ignored intravalley acoustic phonons.

In conclusion, we have shown that transport problems can be tackled by the mathematically simple FPA even in the case of a concrete semiconductor. We can also emphasize that the possibility for achieving correct results from the FPA depends on the chance of performing good enough approximations for the relaxation processes, allowing the analytical evaluation of the integral in Eq.(8) and still retaining the essential physical picture. The results, being acceptable just for the higher electric fields, in fact are very close to those of Monte-Carlo simulations. Additional calculations for $T = 430$ K also revealed good agreement with those of [10]. The saturation effect, however, is not predicted by FPA. For higher electric field intensities a slow but ever decreasing behaviour is achieved.

We acknowledge financial support from the Fundação de Amparo à Pesquisa de São Paulo. F. C. is grateful to Departamento de Física, Universidade Federal de São Carlos, for hospitality.
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FIG. 1. Average electron energy (in units of $\hbar\omega_0$) as a function of the electric field for three different temperatures. It is clearly seen that the average energy is actually much larger than the phonon energy.

FIG. 2. Drift velocity for three different temperatures as a function of the electric field. The general trend of the curves corresponds with what is seen in experiments and Monte Carlo simulations.

FIG. 3. Drift velocity as a function of electric field for 300 K for Si. Our results (solid curve) are compared with Monte Carlo simulations (dotted curve) and experimental data.
BULK Si

T=300 K
T=10 K
T=200 K

AVERAGE ENERGY $/\hbar\omega$
ELECTRIC FIELD [kV/cm]
BULK Si  T=300  K

DRIFT VELOCITY [$10^6$ cm/s]

ELECTRIC FIELD [kV/cm]

- **EXPERIMENT**
- **FOKKER PLANCK**
- **MONTE CARLO**