

Rigorous Modeling of Mobilities and Relaxation Times Using Six Moments of the Distribution Function

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Abstract

Mobilities and relaxation times are the fundamental parameters of macroscopic transport models. They are determined by the scattering integral of Boltzmann's equation and thus depend on the shape of the distribution function. They are normally modeled in an empirical way because knowledge of the distribution function is difficult to obtain. Based on an analytic expression for the distribution function which exactly reproduces its first six moments we present models for these parameters which are highly accurate even for nanometer devices. We show that this accuracy cannot be obtained within the conventional heated and shifted Maxwellian approximation.

1 Introduction

Since the proposal of hydrodynamic models over forty years [1, 2] ago the modeling of the transport parameters like mobilities and relaxation times has been a hot topic of research. Since the fluxes are proportional to the mobilities these parameters are of fundamental importance. One of the most accurate physics-based models for the carrier mobility so far has been proposed by Hänsch [3] whereas the energy relaxation time is commonly assumed to be constant [4]. Although the energy relaxation time can be more accurately modeled as a function of the average carrier energy by fitting Monte Carlo data, this is not possible for the mobilities which are not single-valued functions of the average carrier energy [4]. Similar difficulties are observed for the energy flux mobility which is frequently modeled as equal to the carrier mobility [5].

Despite these difficulties hydrodynamic models suffer from additional limitations. Most of them are related to the fact that they do not provide enough information about the distribution function and a heated and drifted Maxwellian approximation is frequently assumed. It has been shown that this is not sufficient to model hot carrier processes like impact ionization [6, 7] and that much more accurate results can be obtained by including the next two equations of the moment hierarchy which results in a six moments transport model [8]. There, in addition to the carrier mobility μ_n , the energy flux mobility μ_S , and the energy relaxation time τ_E required also by hydrodynamic models, the kurtosis flux mobility μ_K , and the kurtosis relaxation time τ_β have to be modeled. The solution variables of the

six moments transport model are the moments of the distribution function, which are defined by the weight functions $\phi_i = \mathcal{E}^i$ for the even moments, giving the balance equations, and $\Phi_i^{\mathbf{u}} = \mathbf{u}\mathcal{E}^i$ for the flux equations.

2 Distribution Function Model

The distribution function is split into its symmetric and antisymmetric parts $f(\mathbf{k}) = f_S(\mathcal{E}) + f_A(\mathbf{k})$ where the symmetric part is assumed to depend only on the energy.

In the following we will use Kane's dispersion relation [9] with $\gamma(\mathcal{E}) = \mathcal{E}(1 + \alpha\mathcal{E}) = \mathcal{E}H_{\mathcal{E}}(\alpha\mathcal{E})$. The density of states evaluates to

$$g(\mathcal{E}) = g_0\sqrt{\mathcal{E}}\sqrt{1 + \alpha\mathcal{E}}(1 + 2\alpha\mathcal{E}) = g_0\sqrt{\mathcal{E}}H_g(\alpha\mathcal{E}) \quad (1)$$

and the group velocity to

$$\mathbf{u} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}(\mathbf{k}) = \frac{\hbar\mathbf{k}}{m^*}\frac{1}{1 + 2\alpha\mathcal{E}} = \frac{\hbar\mathbf{k}}{m^*}H_u(\alpha\mathcal{E}) \quad (2)$$

To obtain closed form expressions for the moments of the even part of the distribution function we use the approximation $H_g(\alpha\mathcal{E}) \approx 1 + \gamma_g(\alpha\mathcal{E})^{\lambda_g}$.

2.1 Symmetric Part

The symmetric part is modeled according to our previous works [10] as consisting of a hot (f_h) and a cold distribution (f_c).

$$f_S(\mathcal{E}) = A\left\{\exp\left[-\left(\frac{\mathcal{E}}{a}\right)^b\right] + c\exp\left[-\frac{\mathcal{E}}{a_c}\right]\right\} \quad (3)$$

$$= A\left\{f_h(\mathcal{E}) + cf_c(\mathcal{E})\right\} \quad (4)$$

The five parameters A , a , b , c , and a_c , are calculated in such a way that f_S exactly reproduces the first three even moments provided by the six moments model. In addition, the conditions $a_c = k_B T_L$ and $\langle \mathcal{E}^2 \rangle_c = h(\langle \mathcal{E} \rangle_c)$ are assumed, where $h(\langle \mathcal{E} \rangle)$ is the relationship between $\langle \mathcal{E}^2 \rangle$ and $\langle \mathcal{E} \rangle$ in bulk and $\langle \cdot \rangle_c$ is the moment of f_c only. Note that the cold population only exists inside the drain regions and that inside channel regions c vanishes [10].

We define the even moments of the distribution function using the weight functions $\phi_i = \mathcal{E}^i$ as $\langle \phi_i \rangle = \frac{1}{n}\int \phi_i f_S(\mathcal{E}) d^3\mathbf{k}$. Introducing the auxiliary functions

$$I(x, z) = \frac{a^{x+\frac{3}{2}}}{b}\Gamma\left(\frac{x+\frac{3}{2}}{b}\right) + za_c^{x+\frac{3}{2}}\Gamma\left(x+\frac{3}{2}\right) \quad (5)$$

$$m_y(x) = I(x, c) + \gamma_y\alpha^{\lambda_y}I(x + \lambda_y, c) \quad (6)$$

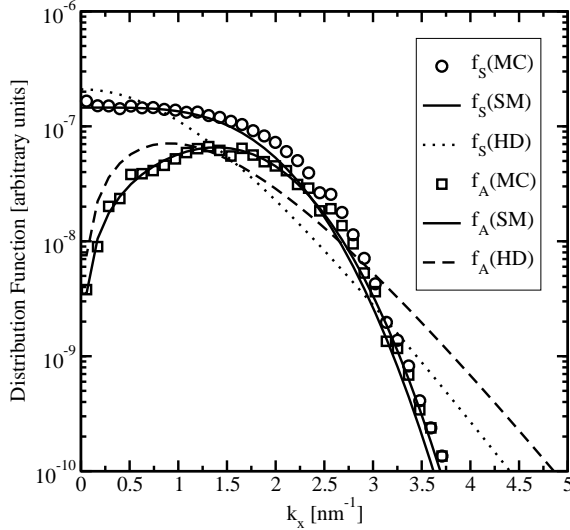


Figure 1: Cuts through the symmetric and antisymmetric parts of the distribution function at the end of the channel region.

and $C_m = Ag_0$ we obtain

$$n = C_m m_g(0) \quad \text{and} \quad \langle \phi_i \rangle = \frac{m_g(i)}{m_g(0)} \quad (7)$$

with $m_y(x)$ being the generalized moment of f_S using the parameters γ_y and λ_y .

2.2 Antisymmetric Part

The antisymmetric part is obtained by shifting the symmetric part and applying the diffusion approximation

$$f_A(\mathbf{k}) = \sum_{j=0}^2 \mathcal{E}^j \mathbf{B}_j \cdot \mathbf{k} f_{\mathcal{E}}(\mathcal{E}) \quad (8)$$

with $f_{\mathcal{E}}(\mathcal{E}) = f_h(\mathcal{E}) + c_A f_c(\mathcal{E})$. Note that a different prefactor appears in front of f_c because the cold electron gas has a different average energy and velocity. This prefactor is empirically modeled as $c_A/c = a_c/a$ in this work.

To determine the coefficients \mathbf{B}_i we calculate the moments of the antisymmetric part of the distribution function

$$\begin{aligned} \langle \Phi_i^u \rangle &= \frac{\hbar}{m^* n} \sum_{j=0}^2 \mathbf{B}_j \int \mathcal{E}^{i+j} (\mathbf{k} \otimes \mathbf{k}) H_u(\alpha \mathcal{E}) f_{\mathcal{E}}(\mathcal{E}) d^3 \mathbf{k} \\ &= C_M \sum_{j=0}^2 \mathbf{B}_j \int \mathcal{E}^{i+j+3/2} H_M(\alpha \mathcal{E}) f_{\mathcal{E}}(\mathcal{E}) d\mathcal{E} \end{aligned}$$

Here we introduced $C_M = 2g_0/(3\hbar n)$ and $H_M(\alpha \mathcal{E}) = H_u(\alpha \mathcal{E}) H_g(\alpha \mathcal{E}) H_{\mathcal{E}}(\alpha \mathcal{E}) = (1 + \alpha \mathcal{E})^{3/2}$ which will be approximated as $1 + \gamma_M(\alpha \mathcal{E})^{\lambda_M}$ to obtain closed form solutions. Introducing the auxiliary functions

$$M_y(x) = I(x, c_A) + \gamma_y \alpha^{\lambda_y} I(x + \lambda_y, c_A) \quad (9)$$

and requiring that f_A reproduces the moments $\langle \Phi_i^u \rangle$ we obtain a linear equation system

$$\langle \Phi_i^u \rangle = C_M \sum_{j=0}^2 \mathbf{B}_j M_M(i+j+1) = \sum_{j=0}^2 \mathbf{B}_j C_{ij} \quad (10)$$

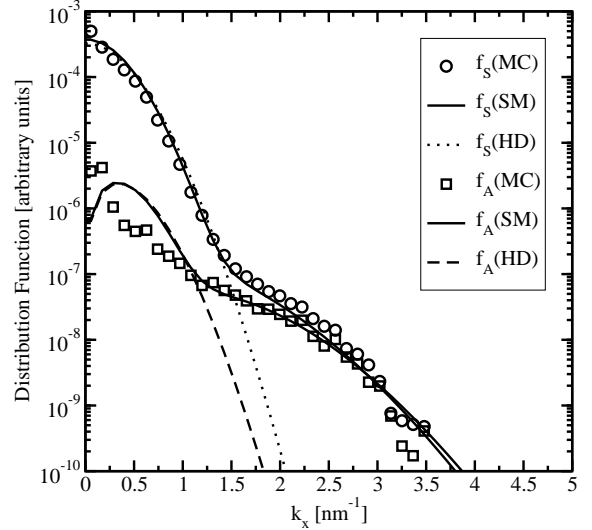


Figure 2: Cuts through the symmetric and antisymmetric parts of the distribution function inside the drain region.

where the C_{ij} have the property $C_{ij} = C_{kl}$ for $i+j = k+l$. Solving for \mathbf{B}_i gives $\mathbf{B}_i = \sum_{j=0}^2 D_{ij} \langle \Phi_i^u \rangle$ where the D_{ij} are the components of the inverted tensor \hat{C}^{-1} which have the property $D_{ij} = D_{ji}$. The antisymmetric part of the distribution function can now be written as

$$f_A(\mathbf{k}) = f_{\mathcal{E}}(\mathcal{E}) \sum_{i=0}^2 d_i(\mathcal{E}) \langle \Phi_i^u \rangle \cdot \mathbf{k} \quad (11)$$

$$d_i(\mathcal{E}) = \sum_{j=0}^2 D_{ji} \mathcal{E}^j \quad (12)$$

A comparison of the analytic model with Monte Carlo data is given in Fig. 1 for the end of the channel region and in Fig. 2 for the beginning of the drain region of an n^+-n-n^+ structure with $L_c = 100$ nm. A hydrodynamic version of this model is obtained by assuming a heated Maxwellian distribution for the even part and considering only \mathbf{B}_0 and \mathbf{B}_1 in (8). The results are also shown in Figs. 1 and 2 which are much less accurate than the six moments version.

3 Scattering Models

By introducing a relaxation time $\tau_{\phi}(\mathcal{E})$ related to the weight function ϕ the scattering integral can be rearranged formally as [11]

$$\begin{aligned} \int \phi(\mathbf{k}) Q[f(\mathbf{k})] d^3 \mathbf{k} &= - \left\langle \frac{\phi(\mathbf{k})}{\tau_{\phi}(\mathcal{E})} \right\rangle \\ \frac{1}{\tau_{\phi}(\mathcal{E})} &= \int \left[1 - \frac{\phi(\mathbf{k}')}{\phi(\mathbf{k})} \right] S(\mathbf{k}, \mathbf{k}') d^3 \mathbf{k}' \end{aligned}$$

In the following we will evaluate the scattering integral considering acoustic deformation potential scattering (ADP), intravalley scattering (IVS), and impurity scattering (IMP) [12]. For IMP the Brooks-Herring model is used for simplicity, although more accurate models can be treated in the same manner.

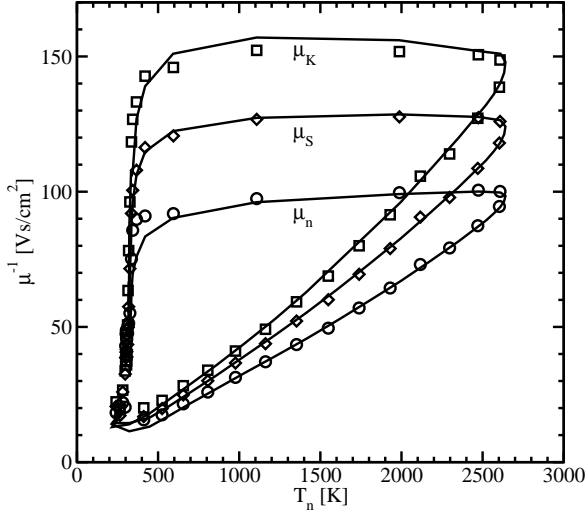


Figure 3: Mobilities required for the six moments model. The symbols are the Monte Carlo results whereas the solid lines are obtained by the analytic distribution function model.

3.1 Mobilities

We now define the scalar mobilities via

$$-\left\langle \frac{\Phi_i^{\mathbf{P}}}{\tau_p(\mathcal{E})} \right\rangle = q \frac{\langle \Phi_i^{\mathbf{u}} \rangle}{\mu \langle \Phi_i^{\mathbf{u}} \rangle} \quad (13)$$

Note that we *do not* employ the relaxation time approximation as we evaluate the scattering integral directly, using the microscopic relaxation times of the odd moments $\Phi_i^{\mathbf{P}} = \hbar \mathbf{k} \mathcal{E}^i$. For all scattering processes considered here the microscopic relaxation times related to $\tau_{\Phi_i^{\mathbf{P}}}(\mathcal{E})$ are equal the momentum relaxation time $\tau_p(\mathcal{E})$. This gives

$$\begin{aligned} -\left\langle \frac{\Phi_i^{\mathbf{P}}}{\tau_p(\mathcal{E})} \right\rangle &= C_Q \sum_{j=0}^2 \mathbf{B}_j \int \mathcal{E}^{i+j+3/2} H_Q(\alpha \mathcal{E}) \frac{f_{\mathcal{E}}(\mathcal{E})}{\tau_p(\mathcal{E})} d\mathcal{E} \\ &= \sum_{j=0}^2 Z_{ij} \langle \Phi_j^{\mathbf{u}} \rangle \end{aligned}$$

with the definitions $C_Q = m^* C_M$, $H_Q(\alpha \mathcal{E}) = (1 + \alpha \mathcal{E})^{3/2} (1 + 2\alpha \mathcal{E})$, and

$$Z_{ij} = C_Q \sum_{l=0}^2 D_{lj} Q_{il} \quad (14)$$

$$Q_{ij} = \int \mathcal{E}^{i+j+3/2} H_Q(\alpha \mathcal{E}) \frac{f_{\mathcal{E}}(\mathcal{E})}{\tau_p(\mathcal{E})} d\mathcal{E} \quad (15)$$

3.2 Relaxation Times

The relaxation times for the balance equations are determined by the even moments ϕ_i as

$$-\left\langle \frac{\phi_i}{\tau_{\phi_i}(\mathcal{E})} \right\rangle = \frac{1}{m_g(0)} \int \phi_i \mathcal{E}^{1/2} H_g(\alpha \mathcal{E}) \frac{f_{\mathcal{E}}(\mathcal{E})}{\tau_{\phi_i}(\mathcal{E})} d\mathcal{E}$$

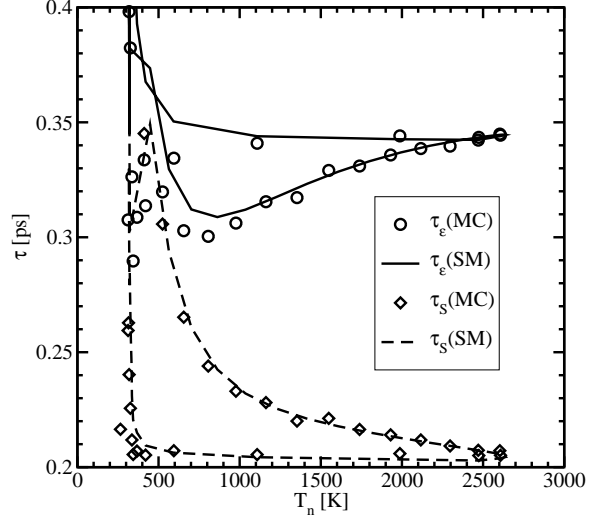


Figure 4: Relaxation times required for the six moments model. The symbols are the Monte Carlo results whereas the solid lines are obtained by the analytic model.

Since ADP and IMP are assumed to be elastic, they do not contribute to these relaxation rates. The relaxation times for the even moments determine the average relaxation times used in the macroscopic transport equations

$$\tau_{\langle \phi_i \rangle} = \frac{\langle \phi_i \rangle - \langle \phi_i \rangle_{\text{eq}}}{q_i} \quad \text{and} \quad \langle \phi_i \rangle_{\text{eq}} = \left. \frac{m_g(i)}{m_g(0)} \right|_{\text{eq}}$$

where under equilibrium $a = k_B T_L$, $b = 1$, and $c = 0$.

3.3 Scattering Rates

Since the scattering models we use are well known [12], they are only briefly sketched here:

$$\text{ADP} : \quad \frac{1}{\tau_p(\mathcal{E})} = K_{\text{adp}} g(\mathcal{E}) \quad (16)$$

$$\text{IVS} : \quad \frac{1}{\tau_p^{\pm}(\mathcal{E})} = K_{\text{ivs}}^{\pm} \sigma(\mathcal{E} \pm \mathcal{E}_0) g(\mathcal{E} \pm \mathcal{E}_0) \quad (17)$$

$$\text{IMP} : \quad \frac{1}{\tau_p(\mathcal{E})} = K_{\text{imp}} T(t) H_{\text{imp}}(\alpha \mathcal{E}) \mathcal{E}^{-3/2} \quad (18)$$

with the auxiliary definitions for IMP

$$T(t) = \left[\ln(1+t) - \frac{t}{1+t} \right]$$

$$t = \frac{4}{\mathcal{E}_\beta} \mathcal{E} (1 + \alpha \mathcal{E})$$

$$H_{\text{imp}}(\alpha \mathcal{E}) = \frac{1 + 2\alpha \mathcal{E}}{(1 + \alpha \mathcal{E})^{3/2}}$$

4 Results

In our Monte Carlo code we use the same scattering rates as given above and a single equivalent isotropic nonparabolic band. Although this band structure is unreliable above 0.5 eV, it allows us to write relatively simple closed form expressions when the integrals occurring in the evaluation of the scattering integral are

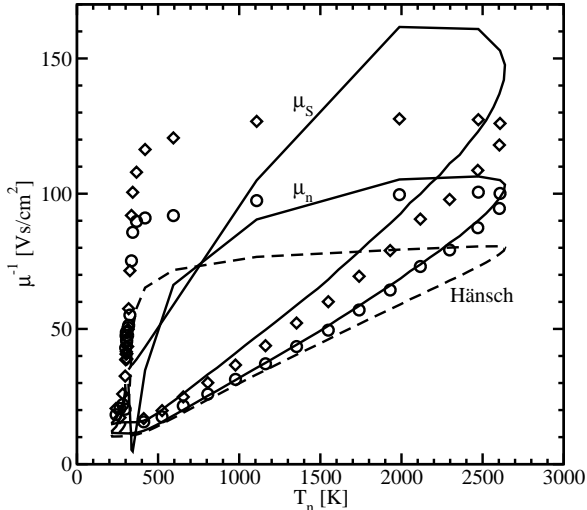


Figure 5: Mobilities required for the hydrodynamic model. The dashed line shows the results obtained by the Hänsch model.

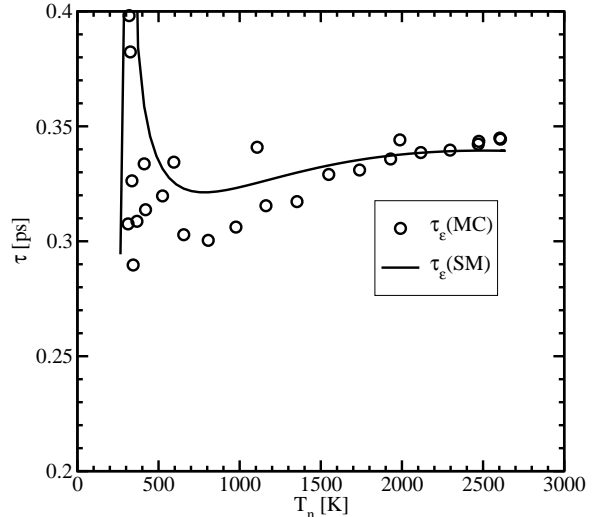


Figure 6: Relaxation times required for the hydrodynamic model.

accordingly approximated. Furthermore, if required, our approach can be easily extended to more accurate analytical models in a straight forward manner. We use the first six moments obtained from the Monte Carlo simulation to evaluate the distribution function model and the scattering integral. The resulting highly accurate mobilities and relaxation times are shown in Fig. 3 and Fig. 4 for an n^+-n-n^+ structure with $L_c = 100$ nm and a maximum electric field of $E_{\max} = 100$ kV/cm. For the channel region where $c = 0$ and no heuristic criteria are applied the error in the mobilities and relaxation times is well below 0.1%. Even in the drain region, where the bulk relation between the average of the square of the energy and the average energy is assumed to be valid, the accuracy is extremely good.

In Fig. 5 and Fig. 6 the analogous expressions for the hydrodynamic model are evaluated which clearly confirm that the resulting heated and drifted Maxwellian distribution is not well suited for the modeling of hot carrier processes. In addition, the results obtained by the Hänsch model is shown in Fig. 5 with $\tau_E = 0.33$ ps.

5 Conclusion

Modeling of physical processes in macroscopic transport models requires knowledge of the distribution function. In hydrodynamic models the distribution function is frequently assumed to be a heated and shifted Maxwellian distribution. It has been often shown that this approach is inaccurate for hot carrier processes such as impact ionization where hydrodynamic models give notoriously wrong results. This has been attributed to the fact that the heated Maxwellian distribution cannot reproduce the hot energy tail of the distribution function. Here we have demonstrated that similar limitations apply to the modeling of scattering processes occurring at lower carrier energies such as phonon and impurity scattering. Although the results

obtained with the heated Maxwellian approximation do not differ by orders of magnitude, as is the case for impact ionization, the improved quality obtained with a six moments representation is striking. We can therefore conclude that a six moment description provides not merely a marginal improvement over the conventional heated Maxwellian distribution but rather makes precise modeling of energy dependent processes possible. This is underlined by the fact that the six moments model provides sufficient information to accurately model all required transport parameters which is not the case for lower order transport models.

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