A Two-Fluid Model for Carrier Transport in Semiconductors

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Modern electron devices require an even more accurate modeling of carrier transport in semiconductors in order to be able to describe high-field phenomena such as impact ionization and gate injuction probability.

Such phenomena are due to the hot electrons which constitute only a small portion of the whole carrier system.

Current calculations using Monte Carlo methods are extremely CPU intensive and therefore not practical for design applications.

For this reason several authors [**?**], [**?**], [**?**] have introduced new fluidodynamical models in which macroscopic quantities relative to the so-called tail electrons appear as new fundamental variables.

These models, which are precisely called tail electron hydrodynamic models (TEHD) present undetermined transport parameters which are obtained by using Monte Carlo simulation results, which is an undesirable feature of the models.

In this paper we propose a closure method which allows to obtain both the constitutive fluxes and the production terms as functions of the fundamental variables, without resorting to M.C simulations.

The starting point is the semiclassical Boltzmann equation (BTE) which, coupled to the Poisson equation for the electric potential, describes electron transport in semiconductors

$$\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} - \frac{e\,E_i}{\hbar}\frac{\partial f}{\partial k_i} = Q(f) \tag{1.1}$$

$f(\vec{x}, t, \vec{x})$ is a one-particle distribution function with $\vec{k}$ crystal momentum belonging to the first Brillouin zone B, $\vec{E}$ electric field and

$$\vec{v} = \nabla_{\vec{k}}\epsilon$$

group velocity of the electrons which depends on the electron energy in the conduction band.

We will use the parabolic band approximation for which

$$\epsilon = \frac{\hbar^2\,k^2}{2\,m^*} \qquad\qquad B = \Re^3$$

m^* being the electrone effective mass.

Q is the collision operator which in the non-degenerate case has the form [**?**]

$$Q(f) = \int d\vec{k'} \left[w(\vec{k}, \vec{k'})\, f(\vec{k'}) - w(\vec{k'}, \vec{k}) f(\vec{k}) \right]$$

$w(\vec{k}, \vec{k'})$ representing the electron scattering rate from a state with momentum $\vec{k'}$ to one with momentum $\vec{k}$.

Introducing a threshhold energy, ϵ_{thr}, for the electrons, which usually is the threshold energy of impact ionization, and considering the kinetic quantities: $1, \vec{v}, \epsilon, \epsilon\, \vec{v}$, one can define the number density, average velocity, energy and energy flux of electrons having energy less than and greater than ϵ_{thr} respectively

$$\begin{cases} n_1 = \int_{\tilde{\Delta}} f\, d\vec{k} & n_1\, \vec{u_1} = \int_{\tilde{\Delta}} \vec{v} f\, d\vec{k} \\ n_1\, W_1 = \int_{\tilde{\Delta}} \epsilon f\, d\vec{k} & n_1\, \vec{S_1} = \int_{\tilde{\Delta}} \epsilon \vec{v} f\, d\vec{k} \end{cases} \tag{1.2}$$

$$\begin{cases} n_2 = \int_{\Delta} f\, d\vec{k} & n_2\, \vec{u_2} = \int_{\Delta} \vec{v} f\, d\vec{k} \\ n_2\, W_2 = \int_{\Delta} \epsilon f\, d\vec{k} & n_2\, \vec{S_2} = \int_{\Delta} \epsilon \vec{v} f\, d\vec{k} \end{cases} \tag{1.3}$$

with $\Delta = \left\{ \vec{k} : \epsilon(\vec{k}) \geq \epsilon_{thr} \right\}$ and $\tilde{\Delta} = \Re^3 - \Delta$, the quantities with the subscript 2 referring to the hot electrons.

¿From the BTE one can obtain the following evolution equations for these macroscopic quantities:

$$\begin{cases} \frac{\partial n_2}{\partial t} + \frac{\partial n_2\, u_2^i}{\partial x_i} - e\, E_i\, N^i = C_{n_2} \\ \frac{\partial n_2\, u_2^j}{\partial t} + \frac{\partial n_2\, K_B\, T_2^{ij}}{\partial x_i} - e\, E_i\, U^{ji} + e\, E^j\, n_2 \frac{1}{m^*} = C_{u_2^j} \\ \frac{\partial n_2\, W_2}{\partial t} + \frac{\partial n_2\, S_2^i}{\partial x_i} - e\, \epsilon_{thr} E^i\, N_i + e\, E_i\, n_2\, u_2^i = C_{W_2} \\ \frac{\partial n_2\, S_2^j}{\partial t} + \frac{\partial n_2\, S_2^{ij}}{\partial x_i} - e\, \epsilon_{thr} E_i\, U^{ji} + e\, E_i\, n_2\, K_B\, T_2^{ij} + e\, E^j\, n_2 \frac{W_2}{m^*} = C_{S_2^j} \end{cases} \tag{1.4}$$

$$\begin{cases} \frac{\partial n_1}{\partial t} + \frac{\partial n_1\, u_1^i}{\partial x_i} = C_{n_1} - e\, E_i\, N^i \\ \frac{\partial n_1\, u_1^j}{\partial t} + \frac{\partial n_1\, K_B\, T_1^{ij}}{\partial x_i} + e\, E^j\, n_1 \frac{1}{m^*} = C_{u_1^j} - e\, E_i\, U^{ji} \\ \frac{\partial n_1\, W_1}{\partial t} + \frac{\partial n_1\, S_1^i}{\partial x_i} + e\, E_i\, n_1\, u_1^i = C_{W_1} - e\, \epsilon_{thr} E^i\, N_i \\ \frac{\partial n_1\, S_1^j}{\partial t} + \frac{\partial n_1\, S_1^{ij}}{\partial x_i} + e\, E_i\, n_1\, K_B\, T_1^{ij} + e\, E^j\, n_1 \frac{W_1}{m^*} = C_{S_1^j} - e\, \epsilon_{thr} E_i\, U^{ji} \end{cases} \tag{1.5}$$

with

$$N^i = \frac{1}{\hbar} \int_{\Sigma} f\, \nu^i d\sigma \quad U^{ji} = \frac{1}{\hbar} \int_{\Sigma} v^j f\, \nu^i d\sigma \tag{1.6}$$

$$n_2\, K_B\, T_2^{ij} = \int_{\Delta} v^i\, v^j\, f\, d\vec{k} \quad n_2\, S_2^{ij} = \int_{\Delta} \epsilon\, v^i\, v^j\, f\, d\vec{k}$$

$$
\begin{aligned}
&n_1\, K_B\, T_1^{ij} = \int_{\tilde{\Delta}} v^i\, v^j\, f\, d\vec{k} \quad n_1\, S_1^{ij} = \int_{\tilde{\Delta}} \epsilon\, v^i\, v^j\, f\, d\vec{k} \\
&C_{n_2} = \int_{\Delta} Q\, d\vec{k} \quad C_{u_2^j} = \int_{\Delta} v^j Q\, d\vec{k} \quad C_{W_2} = \int_{\Delta} \epsilon Q\, d\vec{k} \quad C_{s_2^j} = \int_{\Delta} \epsilon v^j Q\, d\vec{k} \\
&C_{n_1} = \int_{\tilde{\Delta}} Q\, d\vec{k} \quad C_{u_1^j} = \int_{\tilde{\Delta}} v^j Q\, d\vec{k} \quad C_{W_1} = \int_{\tilde{\Delta}} \epsilon Q\, d\vec{k} \quad C_{S_1^j} = \int_{\tilde{\Delta}} \epsilon v^j Q\, d\vec{k}.
\end{aligned}
$$

where $\Sigma = \left\{ \vec{k} : \epsilon(\vec{k}) = \epsilon_{thr} \right\}$, $\vec{\nu}$ the inner normal to Σ.

The first set of equations is found by integrating the BTE, while the second set is derived by substituting the first one into the usual moment equations.

The preceeding equations have the same form as those of the conventional HD model [?] except for the surface terms which represent the increasing rate of the corresponding macroscopic quantity due to the net migration of carriers from one energy zone to the other owing to the driving electric field.

In order to obtain a closed system of equations we need to express the quantities (??) as functions of the fundamental variables (??), (??).

To this aim we used the asymptotic distribution function obtained by Majorana and Liotta [?] as distribution function for the hot electrons and that one derived by means of the Maximum Entropy Principle [?], [?], [?] as distribution function for electrons with energy less than ϵ_{thr}.

Substituting these expressions into (??), we found the constitutive equations for these quantities .

As collision operator we have considered that describing the scattering between electrons and acoustical and optical phonons.

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