

## Thermodynamic Aspects of the Energy model of hot carrier Transport in semiconductor Devices

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### Abstract

A new treatment of the energy model of the hot carrier transport is proposed. The approach has been stimulated by a successful analysis of the drift-diffusion model which is partially based on the use of the free energy of the semiconductor device (cf. [3], [4]). Here an other thermodynamic potential is proposed for the energy model. As a consequence, the entropy density (instead of the energy or the carrier temperature) has to be chosen as a dynamic variable. Thus we are lead to a system of equations, which is equivalent to the widely accepted energy model.

The energy model or the quasi-hydrodynamical model is one of the phenomenological models which allow the simulation of carrier transport in semiconductor devices. The specific assumption which distinguishes the energy model of hot carriers from other phenomenological models is that the electrons in the conductivity band and/or the holes in the valence band of a semiconductor device can be considered as a thermodynamic subsystem with its own temperature. Moreover, but for simplicity only, we assume that electrons and holes have one carrier temperature  $\Theta$  in common and that the lattice temperature is a constant parameter  $T$ . The lattice temperature will be chosen as the unit of the carrier temperature. The aim of the paper is to present a new approach to the energy model in analogy to a successful analysis of the drift-diffusion model realized by Gajewski and Gröger (cf. [3], [4]). Although the paper is restricted to the Boltzmann statistics, essential parts of it can be extended analogously onto the Fermi-Dirac statistics.

We start from a widely accepted system of equations

$$-\text{div}(\varepsilon \text{grad } U) = f + Q(p - n),$$

$$\begin{aligned} n &= c_n \Theta^{3/2} \exp((F_n + U - E_c)/\Theta), & p &= c_p \Theta^{3/2} \exp(-(F_p + U - E_v)/\Theta), \\ \dot{n} + \text{div } j_n &= -R, & \dot{p} + \text{div } j_p &= -R, \end{aligned}$$

$$\begin{aligned} \frac{3}{2}[(n + p)\Theta] + \text{div}(j_{v_n} + j_{v_p}) &= -3\Theta R - \frac{3}{2}(n\omega_n + p\omega_p)(\Theta - 1) \\ &+ j_n \text{grad}(U - E_c) - j_p \text{grad}(U - E_v), \end{aligned}$$

$$\begin{aligned} j_n &= -A_n \text{grad } F_n - (B_n - (F_n + U - E_c)A_n/\Theta) \text{grad } \Theta, \\ j_p &= +A_p \text{grad } F_p - (B_p - (F_p + U - E_v)A_p/\Theta) \text{grad } \Theta, \\ j_{v_n} &= -\Theta B_n \text{grad } F_n - \Theta(C_n - (F_n + U - E_c)B_n/\Theta) \text{grad } \Theta, \\ j_{v_p} &= \Theta B_p \text{grad } F_p - \Theta(C_p + (F_p + U - E_v)B_p/\Theta) \text{grad } \Theta, \end{aligned} \tag{1}$$

which models the transport of hot carriers in semiconductor devices (cf. [1], [2], [5], [7], [8]). Therein  $U$ ,  $F_n$  and  $F_p$  denote the scaled electrostatic potential and the electrochemical potentials of electrons and holes, respectively. The scalars  $\varepsilon > 0$ ,  $c_n > 0$ ,  $c_p > 0$ ,  $E_c$ ,  $E_v$  and the doping profile  $f$  are given functions of the coordinates ( $Q = q^2/kT > 0$  is a constant). The netto recombination rate  $R$  is described as usually by Shockley-Read-Hall and Auger terms. The other coefficients  $\omega_n$ ,  $\omega_p$ ,  $A_n$ ,  $A_p$ ,  $B_n$ ,  $B_p$ ,  $C_n$  and  $C_p$  are considered as given material functions which may explicitly depend on the coordinates and which depend on the state variables in general. Such coefficients can be obtained either experimentally or by modelling scattering integrals in the Boltzmann equation for the distribution functions of electrons and holes.

For momentum relaxation times which depend on a power  $\beta$  of the kinetic energy of carriers (e.g.  $\beta = -1/2$ ), one obtains

$$A_n = \mu_n \Theta^\beta n, \quad B_n = (5/2 + \beta)A_n, \quad C_n = (7/2 + \beta)B_n$$

with a material function  $\mu_n > 0$ . Unfortunately, such special momentum relaxation times are not general enough. For a better numerical simulation it will be necessary to describe properties of the coefficients more exactly. Besides measurements more qualitative descriptions are desirable. Under rather general assumptions the coefficients  $A_n$ ,  $B_n$ ,  $C_n$  depend on  $\Theta$  and on the state variable  $z_n := (F_n + U - E_c)/\Theta$ . Meanwhile  $A_n$ ,  $B_n$ ,  $C_n$  and  $D_n := C_n - B_n^2/A_n$  depend rather strongly on  $\Theta$ , these functions are expected to vary rather mildly with  $z_n$  and the quotients  $Q_n := B_n/A_n$ ,  $C_n/B_n$  are expected to depend rather weakly on the temperature too. Furthermore, the coefficients should have positive values only.

Of course, the above system of partial differential equations is to be supplemented by boundary conditions. Up to now we divide the boundary  $\partial\Omega$  of the domain  $\Omega$  in two parts  $\Gamma_D$  and  $\Gamma$ . On  $\Gamma_D$  Dirichlet data are given, but on  $\Gamma$  we choose some natural boundary conditions which include the normal derivatives  $\partial_\nu U$ ,  $\partial_\nu \Theta$  and the normal components  $\nu j_n$ ,  $\nu j_p$  etc. of current densities and which admit boundary conditions of the third kind too. Heterogeneous materials are permitted if the interfaces do not carry additional dynamic variables.

## 1 An Equivalent System

If one looks for thermodynamic potentials which might be applicable as Ljapunov functions for the evolution equations or in controlling the step width in the time discretization (cf. [3], [4]) the so-called thermodynamic potential

$$g_n + g_p = -c_n \Theta^{5/2} \exp z_n - c_p \Theta^{5/2} \exp z_p =: g(F_n, F_p, \Theta; U)$$

( $z_p = -(F_p + U - E_v)/\Theta$ ) of the two-component carrier gas in exterior potentials  $E_c - U$  or  $-E_v + U$ , respectively, is a good candidate, since the  $3 \times 3$  matrix of the second order partial derivatives is definite, meanwhile the free energy as a function of  $n$ ,  $p$ ,  $\Theta$  does not have this property. This can be proved by applying the Routh-Hurwitz criteria onto the characteristic polynomials of the corresponding matrices. The conjugate variables of  $F_n$ ,  $F_p$  and  $\Theta$  with respect to this potential are the densities  $n$ ,  $p$  and the entropy density of the two-component carrier gas. Thus we are lead to an equivalent system of equations

$$\begin{bmatrix} \dot{n} \\ \dot{p} \\ \dot{s} \end{bmatrix} + \operatorname{div} \begin{bmatrix} j_n \\ j_p \\ j_s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -\frac{3}{2}(n\omega_n + p\omega_p)(\Theta - 1)/\Theta \end{bmatrix} - R \begin{bmatrix} 1 \\ 1 \\ 3 - z_n - z_p \end{bmatrix}$$

(2)

$$-\frac{1}{\Theta} \begin{bmatrix} 0 \\ 0 \\ \nabla F_n \cdot j_n - \nabla F_p \cdot j_p + \nabla \Theta \cdot j_s \end{bmatrix}$$

instead of the particle and energy balance equations, where

$$\begin{bmatrix} j_n \\ j_p \\ j_s \end{bmatrix} = - \begin{bmatrix} A_n & 0 & B_n - z_n A_n \\ 0 & A_p & B_p - z_p A_p \\ B_n - z_n A_n & B_p - z_p A_p & \frac{(B_n - z_n A_n)^2}{A_n} + \text{frac}(B_p - z_p A_p)^2 A_p + D_n + D_p \end{bmatrix} \begin{bmatrix} \nabla F_n \\ -\nabla F_p \\ \nabla \Theta \end{bmatrix}.$$

The system of equations reveals the symmetry of Onsager's relations. The coefficient matrix in the system of current equations is definite such that the leading terms in the nonlinear system of equations define a nice operator from the mathematical point of view. The terms on the right-hand side of the entropy balance equation can naturally be interpreted. In particular the third term is the nonnegative entropy production of the carrier and entropy current. It can be written with the coefficient matrix of these currents in a very symmetric way.

## 2 The Thermodynamic Potential for a Gas with a Consistent Potential

We have to modify the thermodynamic potential  $g$  in such a way that it becomes the thermodynamic potential of the two-component carrier gas with a consistent electrostatic potential. The necessary modifications become more accessible if we consider the Legendre transform of  $g$  which is defined by

$$u(n, p, s; U) := nF_n - pF_p + \Theta s + g(F_n, F_p, \Theta; U).$$

The transform turns out to be the more familiar energy

$$u(n, p, s; U) = \frac{3}{2}(n + p)\Theta + n(E_c - U) - p(E_v - U).$$

The potential  $U = U_{ext} + U_{int}$  is split up in the sum of an exterior potential and an interior potential. The exterior potential is determined by the bias voltages and by the doping profile. Let us denote  $V_n := E_c - U_{ext}$  and  $V_p := E_v - U_{ext}$ . The interior potential  $U_{int} = \mathbf{P}(p - n)$  is the solution of the Poisson equation  $-\text{div}(\epsilon \text{grad } U) = Q(p - n)$  with homogeneous boundary conditions. The energy density of the two-component carrier gas is

$$u = \frac{3}{2}(n + p) + nV_n - pV_p + \frac{1}{2}(p - n) \cdot \mathbf{P}(p - n).$$

In accordance with this modification the thermodynamic potential is

$$g = -(n + p)\Theta - \frac{1}{2}(p - n) \cdot \mathbf{P}(p - n).$$

Since the additional term contains an integral operator  $\mathbf{P}$ , the thermodynamic relations can no longer be formulated in the language of the densities of state variables and their partial derivatives, but functional derivatives must be considered. Let us consider e. g.

$$G(F_n, F_p, \Theta) = - \int \left[ (n+p)\Theta + \frac{1}{2}(p-n) \cdot \mathbf{P}(p-n) \right] dx.$$

The functional derivative  $\partial_{F_n} G$  may be defined as a Fréchet or Gâteaux derivative, i. e. as a linear functional on a function space like

$$V := H_0^1(\Omega \cup \Gamma) = \left\{ v \in H^1(\Omega) : v|_{\Gamma_D} = 0 \right\}.$$

A special class of functionals on this space are defined with functions  $n \in L_r(\Omega)$  ( $r > 1$  in two dimensions or  $r > 6/5$  in three dimensions) by  $\int n v dx$ . In the sense

$$\langle \partial_{F_n} G, v \rangle = - \int n v dx \quad (3)$$

In this sense the thermodynamic relation  $\partial_{F_n} G = -n$  can be derived. Additional difficulties arise from the fact that the functional dependence  $G = G(F_n, F_p, \Theta)$  cannot be described explicitly. Indeed, the dependence of  $n$  and  $p$  upon  $F_n$ ,  $F_p$  and  $\Theta$  is given only implicitly by the state equations

$$\begin{aligned} n &= c_n \Theta^{3/2} \exp((F_n + \mathbf{P}(p-n) - V_n)/\Theta), \\ p &= c_p \Theta^{3/2} \exp(-(F_p + \mathbf{P}(p-n) - V_p)/\Theta). \end{aligned} \quad (4)$$

Remember that these are the familiar state equations with  $U = U_{ext} + \mathbf{P}(p-n)$ . The relation  $n = N(\cdot, F_n, F_p, \Theta)$  which assigns the density  $n$  to the functions  $F_n$ ,  $F_p$ , and  $\Theta$  is not a Nemickij operator as in the case of an exterior potential. Unfortunately, here is not space enough to derive (3) from (4) even in a naive way, which would, however, illuminate the correct mathematical treatment too. Let  $\tilde{F}_n, \tilde{F}_p, \tilde{\Theta} \in H^1(\Omega)$ ,  $0 < a < \tilde{\Theta}$ , represent the Dirichlet data of functions  $(F_n, F_p, \Theta) \in (\tilde{F}_n, \tilde{F}_p, \tilde{\Theta}) + V^3$ . We consider

$$\tilde{G}(F_n, F_p, \Theta) := G(F_n, F_p, \Theta) - G(\tilde{F}_n, \tilde{F}_p, \tilde{\Theta})$$

and

$$\tilde{U}(n, p, s) := \int [n(F_n - \tilde{F}_n) - p(F_p - \tilde{F}_p) + s(\Theta - \tilde{\Theta})] dx + \tilde{G}(F_n, F_p, \Theta),$$

where  $n$ ,  $p$ ,  $s$ ,  $F_n$ ,  $F_p$ , and  $\Theta$  are coupled by (4) and by

$$s := \frac{5}{2}(n+p) - n \cdot \log(n/c_n \Theta^{3/2}) - p \cdot \log(p/c_p \Theta^{3/2}).$$

### 3 A Ljapunov Function

Let us consider  $\tilde{U}[n(t), p(t), s(t)]$  for a solution of the transient problem (2) with initial values  $n^0$ ,  $p^0$ ,  $s^0$  and let  $F_n(t)$ ,  $F_p(t)$ ,  $\Theta(t)$  denote the corresponding functions. Then we have

$$\frac{d}{dt} \tilde{U}[n(t), p(t), s(t)] = \int \left\{ \dot{n}(t)[F_n(t) - \tilde{F}_n] - \dot{p}(t)[F_p(t) - \tilde{F}_p] + \dot{s}(t)[\Theta(t) - \tilde{\Theta}] \right\} dx \quad (5)$$

since the other terms which arise in differentiating like  $\int n \dot{F}_n dx$  and

$$\langle \partial_{F_n} \tilde{G}, F_n \rangle = \langle \partial_{F_n} G, F_n \rangle = - \int n \dot{F}_n dx$$

cancel each other. Because  $F_n(t) - \tilde{F}_n, \dots \in V$ , the equation (2) in its variational form can be applied to (5). The aim of further analysis might be to derive estimates of the "energy norm"  $\tilde{U}[n(t), p(t), \Theta(t)]$  of a solution by means of the initial value  $\tilde{U}(n^0, p^0, s^0)$  and by estimating the arising right-hand sides. To illustrate this perspective, we consider boundary values  $\tilde{\Theta} = \bar{\Theta} = 1$ ,  $\tilde{F}_n = \bar{F}_n = \text{const}$ ,  $\tilde{F}_p = \bar{F}_p = \text{const}$ , which are compatible with a partial equilibrium (only constant values  $\bar{F}_n = \bar{F}_p = \bar{F}$  are compatible with the equilibrium). For such boundary values we get the estimate

$$\begin{aligned} \frac{d}{dt} \bar{U}[n(t), p(t), s(t)] &= \int \left[ \dot{n} (F_n - \bar{F}_n) - \dot{p} (F_p - \bar{F}_p) + \dot{s} (\Theta - 1) \right] dx = \\ &= \int \left[ j_n \nabla (F_n - \bar{F}_n) - R (F_n - \bar{F}_n) - j_p \nabla (F_p - \bar{F}_p) + R (F_p - \bar{F}_p) + \right. \\ &\quad \left. + j_s \nabla (\Theta - 1) - \frac{3n\omega_n + p\omega_p}{2\Theta} (\Theta - 1)^2 - R(3 - z_n - z_p)(\Theta - 1) \right] dx - \\ &\quad - \int \frac{1}{\Theta} (j_n \nabla F_n - j_p \nabla F_p + j_s \nabla \Theta) (\Theta - 1) dx \leq \\ &\leq - \int R \left[ 3\Theta - 3 + \frac{F_n - E_c - F_p + E_v}{\Theta} - \bar{F}_n + E_c + \bar{F}_p - E_v \right] dx. \end{aligned}$$

## 4 The Equilibrium

The system (2) should describe at least the equilibrium in an unique way. We remark that there is a solution of the equilibrium. Indeed,  $\Theta = 1$ ,  $F_n = F_p = \bar{F}$  and a solution  $\bar{U}$  of the nonlinear Poisson equation in which

$$p - n = c_p \exp(-\bar{F} - U + E_v) - c_n \exp(\bar{F} + U - E_c)$$

was substituted is a solution of (2). Now we assume that there would be still an other solution  $F_n, F_p, \Theta, n, p, s, U$  with  $\Theta > 0$ . Then the stationary version of (2) in the variational form for special test functions  $F_n - \bar{F}, \dots \in V$  provides

$$\begin{aligned} 0 &= \int [j_n \nabla (F_n - \bar{F}) - R (F_n - \bar{F}) - j_p \nabla (F_p - \bar{F}) + R (F_p - \bar{F}) + j_s \nabla (\Theta - 1) - \\ &\quad - \frac{3n\omega_n + p\omega_p}{2\Theta} (\Theta - 1)^2 - R(3 - z_n - z_p)(\Theta - 1)] dx - \\ &\quad - \int \frac{1}{\Theta} (j_n \nabla F_n - j_p \nabla F_p + j_s \nabla \Theta) (\Theta - 1) dx \leq \\ &\leq - \int R \left[ 3\Theta - 3 + \frac{F_n - E_c - F_p + E_v}{\Theta} + E_c - E_v \right] dx. \end{aligned} \tag{6}$$

The equilibrium is uniquely determined by the system (2) (in a suitable function space), if the integral on the right-hand side is nonnegative and vanishes for  $\Theta = 1$ ,  $F_n = F_p = \bar{F}$  only. We introduce the usual recombination term

$$\begin{aligned} R &= r_0 (np - \bar{n}\bar{p}) = c_n c_p r_0 \left[ \Theta^3 \exp \frac{F_n - E_c - F_p + E_v}{\Theta} - \exp(E_v - E_c) \right] \\ &= r \left[ \Theta^3 \exp \left( \frac{F_n - E_c - F_p + E_v}{\Theta} + E_c - E_v \right) - 1 \right] \end{aligned}$$

with positive coefficients  $r_0$ ,  $r$  which may depend on the coordinates and on state variables. In this case, unfortunately, the integrand on the right-hand side of (6) is not "quite" definite.

## 5 Conclusion

The various forms of the energy model are in some sense decisively more complicate than the drift-diffusion model. The single equations are coupled by terms which contain not only the unknown functions, but its derivatives too. Furthermore, the lower order terms contain the gradients of the sought functions quadratically such that the existence of solutions is a mathematical question for which there is no ready-made answer in the theory of partial differential equations. We consider it worthwhile to study the various equivalent systems numerically as well as from the point of view of the mathematical analysis. In the moment we are concerned with implementing the first version in close analogy to the two-dimensional semiconductor analysis package TOSCA, but I would like to hint that the second version of the model offers us quite another iteration strategy which seems to be close to the Gummel scheme.

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