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Non-equilibrium boundary conditions for the Boltzmann equation and derived transport models at band edge discontinuities in semiconductor devices

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A number of models for the description of electron transport in semiconductor devices has been proposed in the literature, e.g. [1,2,3,4]. This paper addresses the problem of boundary conditions at hetero interfaces from a fundamental microscopic point of view in order to derive self-consistent boundary conditions for various transport models and to help selecting a suitable model for the consideration of interface effects.

First, a boundary condition for the Boltzmann equation is established. Based on this expression, a method of deriving boundary conditions for derived equations, namely the balance equations obtained by moments of the Boltzmann equation, is given. For simplicity, in this abstract a one-dimensional description has been taken. Because of the fundamental point of view, the paper concentrates on an "ideal" interface, neglecting the effects of additional surface charges and interface states, although these effects can be quite important. They can be included in the model proposed here in a natural way.

The following model of a heterojunction is assumed (cf. fig. 1). At $x = x_0$, two

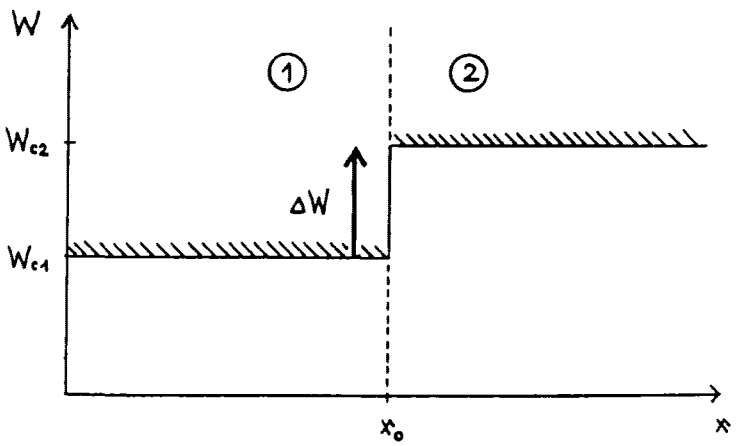

Figure 1: Energy bands at band discontinuity

different materials adjoin each other. Due to the different material specific properties a band edge discontinuity ΔW appears. Other effects influencing the band discontinuity can be incorporated by assuming ΔW as a given parameter [5].

It is supposed that the regions extend far enough that the electron dynamics for each of them can be described by effective mass theory [6], giving rise to different effective masses m_1 and m_2. Thus, this model is not suited to the description of quantum wells and 2D electron gases, where the quantum mechanical electron dynamics has to be taken into account in greater detail [7]. In this paper, the behaviour of the electrons at the interface is described in a semi-classical way.

Concerning fig. 1 this means that particles coming from the left with an energy below W_{C2} are reflected at the interface. Particles having an energy sufficient to overcome the potential barrier arrive at region 2, being slowed down [5]. All particles approaching the interface from region 2 are emitted into region 1, being accelerated.

Fig 2 depicts this situation from the (one-dimensional) phase space point of view. If k^*

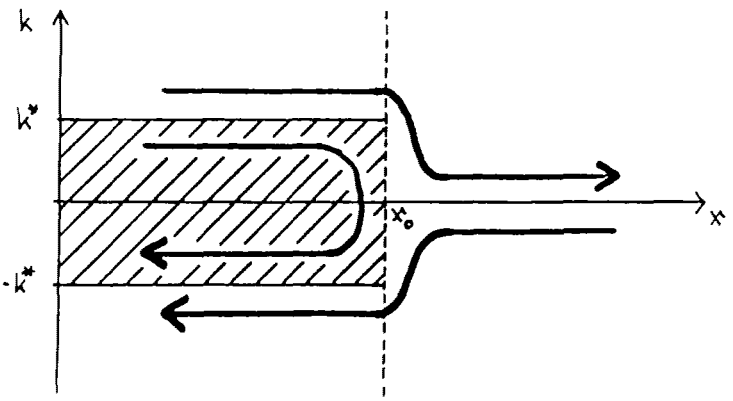

Figure 2: Particle fluxes in x-k-space

represents the value of k corresponding to the kinetic energy equal to the potential barrier, all carriers arriving at the interface with $k < k^*$ are reflected to $-k$. As depicted in fig. 2, all particles arriving with $k > k^*$ cross the interface and are slowed down, while those transcending from the right with $k < -k^*$ are accelerated.

Now these processes must be put into equations. The idea is to adapt the content of the Boltzmann equation, namely the particle conservation in phase space, from volume elements to interfaces. To keep the expressions simple, a single parabolic band is assumed.

The number of particles crossing the interface from material 1 having wave vector k_1 is proportional to $f_1(x_0, k_1)$ times the volume element $v_1(k_1)\Delta t \Delta k_1$ in $x - k$-space [8]. Analogously, the number of particles leaving the interface to the right in material 2 is proportional to $f_2(x_0, k_2)v_2(k_2)\Delta t \Delta k_2$. If k_1 and k_2 are related such that the deceleration is described correctly, the number of particles arriving at the interface are equal to those which leave the interface on the other side. This gives rise to the expression

$$v_1 f_1(k_1)\Delta k_1 = v_2 f_2(k_2)\Delta k_2. \tag{1}$$

The relation of k_1 and k_2 is determined by the conservation of energy

$$W_{kin1} = \Delta W + W_{kin2}, \tag{2}$$

where W_{kin} is the carrier energy counted from the respective band edge. Using the abbreviation

$$k^* = \sqrt{\frac{2m_1}{\hbar^2}\Delta W}, \tag{3}$$

this yields

$$k_1 = \pm\sqrt{\frac{m_1}{m_2}k_2^2 + k^{*2}}. \tag{4}$$

The sign in (4) has to be taken equal to the sign of k_2.

Eqs. (1) and (2) are valid for the acceleration of electrons crossing the interface from left to right, too. Inserting (4) into (1) and solving for f_1 yields as a boundary condition for the Boltzmann equation

$$f_1(x_0, k_1) = f_2\left(x_0, \pm\sqrt{\frac{m_2}{m_1}(k_1^2 - k^{*2})}\right) \qquad |k_1| > k^*. \tag{5}$$

In the case of $W_{kin1} < \Delta W$, the electrons are assumed to be specularly reflected at the potential barrier. Hence, the RHS of (1) has to be replaced by the LHS with k_1 reversed. This gives

$$f_1(x_0, k_1) = f_1(x_0, -k_1) \qquad |k_1| < k^* \tag{6}$$

as a boundary condition for the respective k-values.

Eqns. (5) and (6) constitute the required boundary conditions for the distribution function at a band edge discontinuity. It is emphasized that no equilibrium assumptions have been made deriving (5 - 6).

Throughout the derivation $\Delta W > 0$ has been presupposed. The case of negative ΔW must be treated by an appropriate transformation.

Most often in semiconductor device analysis, simplified transport models as e.g. the drift-diffusion model are utilized which can be derived from the Boltzmann equation by the method of moments [2,3]. In these models, the distribution function is replaced by certain integrals of itself with respect to k. The particle concentration n, the particle current density s, the kinetic energy density w and the energy flow density q are given by respective moments of the distribution function [2]. Transport equations are derived by taking the moments of the Boltzmann equation [2,4]. Analogously, self-consistent boundary conditions can be derived by taking moments of the boundary condition (5-6). This gives for a moment of arbitrary order n

$$\int_{-\infty}^{\infty} dk_1\ {k_1}^n\ f_1(x_0, k_1) = (-1)^n \int_{-k^*}^{k^*} dk_1\ {k_1}^n\ f_1(x_0, k_1)$$

$$+\ \sqrt{\frac{m_1}{m_2}}^{n+1} \int_{-\infty}^{\infty} dk_2\ (sgn\ k_2)^{n-1}\ k_2 \sqrt{k_2^2 + \frac{m_2}{m_1}k^{*2}}^{n-1} f_2(x_0, k_2). \tag{7}$$

The integration variable of the second integral on the RHS has been changed to k_2 using (4).

In the case of odd n, (7) can be solved immediately since the first term on the RHS vanishes due to (6). For the first and third moment, this gives

$$s_1 = s_2 \tag{8}$$

$$q_1 = q_2 + \Delta W\ s_2, \tag{9}$$

thus establishing continuity of particle and energy flow at the interface. Eq. (9) expresses the energy loss (or gain) of electrons crossing the potential step ΔW.

The even moments yield additional conditions for the particle and energy densities. Yet in this case, (7) cannot be solved entirely in terms of the moments. As for the collision integral in the Boltzmann equation, a self-consistent solution can be computed by making

an ansatz for the distribution function which contains the transport quantities as parameters [2]. As an example, in this paper only the ansatz of McAndrew *et al.* [4] shall be considered for brevity:

$$f(x,k) = e^{-\frac{1}{kT}\left[\frac{\hbar^2 k^2}{2m} + W_c - \Phi_n\right]} \left[1 - \frac{\tau}{kT}\frac{\hbar k}{m}\left(grad\ \Phi_n + \left(\frac{\hbar^2 k^2}{2m} + W_c - \Phi_n\right)\frac{1}{T}\ grad\ T\right)\right]. \tag{10}$$

Particle concentration and energy is expressed by quasi-Fermi level Φ_n and electron temperature T, respectively. Inserting (10) into (7) gives

$$h_n(\infty) - h_n\left(\sqrt{\frac{\Delta W}{kT_1}}\right) = \left[h_n(\infty) - h_n\left(\sqrt{\frac{\Delta W}{kT_2}}\right)\right]\sqrt{\frac{T_2}{T_1}}^{n+1} e^{-\frac{W_{c1}-\Phi_{n2}}{kT_2} + \frac{W_{c1}-\Phi_{n1}}{kT_1}}, \tag{11}$$

where $h_n(x) = \int dx\ x^n\ e^{-x^2}$ has been used. Eq. (11) is satisfied for arbitrary even n if

$$\Phi_{n1} = \Phi_{n2} \tag{12}$$

$$T_1 = T_2 \tag{13}$$

holds, expressing continuity of quasi-Fermi level and electron temperature at the interface. Thus the implicit use of (12) for non-equilibrium in simulations of hetero structures [9] has been justified for the McAndrew model by a rigorous derivation.

In conclusion, a boundary condition for the Boltzmann distribution function at band edge discontinuities has been given, and a method for the derivation of analogous self-consistent boundary conditions for arbitrary transport models using the method of moments has been suggested. As an example, the method has been applied to a recently proposed transport model [4].

References

[1] G. Baccarani and M.R. Wordeman. An investigation of steady-state velocity overshoot in silicon. *Solid State Electron.*, 28, p.407, 1985.

[2] W. Hänsch and M. Miura-Mattausch. The hot-electron problem in small semiconductor devices. *J. Appl. Phys.*, 60, p.650, 1986.

[3] K. Bløtekjær. Transport equations for electrons in two-valley semiconductors. *IEEE Trans. Electron Devices*, ED-17, p.38, 1970.

[4] C.C. McAndrew, E.L. Heasell, and K. Singhal. A comprehensive transport model for semiconductor device simulation. *Semicond. Sci. Technol.*, 2, p.643, 1987.

[5] J.Y. Tang and K. Hess. Theory of hot electron emission from silicon into silicon dioxide. *J. Appl. Phys.*, 54, p.5145, 1983.

[6] J. Callaway. *Quantum theory of the solid state.* Academic Press, 1974.

[7] K. Hess and G.J. Iafrate. Hot electrons in semiconductor heterostructures and superlattices. In L. Reggiani, editor, *Hot-electron transport in semiconductors*, page 201, Springer, 1984.

[8] E. Spenke. *Elektronische Halbleiter* Springer, 1965.

[9] M S. Lundstrom and J. Schuelke. Numerical analysis of heterostructure semiconductor devices. *IEEE Trans. Electron Devices*, ED-30, p.1151, 1983.