A generalized Scharfetter–Gummel scheme for degenerate and non-isothermal semiconductors

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***Abstract*—We present a highly accurate generalization of the Scharfetter–Gummel scheme for the discretization of the current densities in degenerate semiconductors under non-isothermal conditions. The underlying model relies on the Kelvin formula for the Seebeck coefficient, which has the intriguing property that the ∇T-term in the electrical current density expressions vanishes exactly when passing to the drift-diffusion form – even though the thermoelectric cross-coupling is fully taken into account.**

I. Introduction

Many challenges faced in modern semiconductor devices are related to heating phenomena [1]. The on-going miniaturization of devices and the reduction of their feature size leads to higher power loss densities inside the device structure. As a consequence, self-heating phenomena such as thermal breakdown, snapback phenomena, thermal lensing or the thermal gain rollover in semiconductor lasers become important effects, which decisively limit the device performance. Moreover, there is growing interest in thermoelectric technologies for environmentally friendly conversion of heat directly into electric energy using thermoelectric generators. The accurate numerical simulation of such devices requires a consistent description of the thermoelectric cross-effects on both the continuous and discrete level.

II. The energy-drift-diffusion system and the Kelvin formula for the Seebeck coefficient

The transport of charge and heat in semiconductors is self-consistently described by the energy-drift-diffusion system [2]:

$$-\nabla\cdot\varepsilon\nabla\phi = q\left(C+p-n\right), \tag{1}$$

$$\partial_t n - \frac{1}{q}\nabla\cdot\mathbf{j}_n = -R, \tag{2}$$

$$\partial_t p + \frac{1}{q}\nabla\cdot\mathbf{j}_p = -R, \tag{3}$$

$$c_V\partial_t T - \nabla\cdot\kappa\nabla T = H. \tag{4}$$

The electrostatic potential ϕ generated be the electron density n and the density of holes p is described by Poisson's Eq. (1). Here, q is the elementary charge, ε is the dielectric permittivity and C is the built-in doping profile. The transport and recombination dynamics of the electron-hole-plasma is given by the continuity Eqs. (2)–(3), where R is the (net-)recombination rate. The transport and generation of heat is modeled by Eq. (4), where T denotes the (lattice) temperature, κ is the thermal conductivity, c_V is the volumetric heat capacity and H is the heat generation rate. Taking thermoelectric cross-effects into account, the electrical current densities are modeled as

$$\mathbf{j}_n = -\sigma_n\left(\nabla\phi_n + P_n\nabla T\right), \tag{5a}$$

$$\mathbf{j}_p = -\sigma_p\left(\nabla\phi_p + P_p\nabla T\right), \tag{5b}$$

where $\phi_{n/p}$ are the quasi-Fermi potentials and $P_{n/p}$ denote the Seebeck coefficients, which couple the current densities to temperature gradients. The electrical conductivities read $\sigma_n = qM_n n$ and $\sigma_p = qM_p p$ (with mobilities $M_{n/p}$). Following Ref. [2], the heat transport Eq. (4) and the self-consistent heat generation rate H are derived from fundamental principles of linear irreversible thermodynamics.

We make a special choice for the Seebeck coefficients, that yields solely the "classical" self-heating terms (recombination heating, Joule heating and Thomson–Peltier heating) and no additional – possibly artificial – heat sources. The corresponding expressions for the Seebeck coefficients are found to be given by the *Kelvin formula* [3, 4], i.e., the partial derivative of the entropy density s with respect to the carrier density:

$$P_n = -\frac{1}{q}\frac{\partial s\left(n,p,T\right)}{\partial n}, \qquad P_p = +\frac{1}{q}\frac{\partial s\left(n,p,T\right)}{\partial p}. \tag{6}$$

Note that this definition differs from the often used *Heikes–Mott formula* [3]. A very intriguing consequence of the Kelvin formula is seen when passing from the "thermodynamic form" of the current densities (5) to the drift-diffusion form:

$$\mathbf{j}_n = -qM_n n\nabla\phi + qD_n\left(n,T\right)\nabla n, \tag{7a}$$

$$\mathbf{j}_p = -qM_p p\nabla\phi - qD_p\left(p,T\right)\nabla p. \tag{7b}$$

Surprisingly, the driving force related to the temperature gradient vanishes exactly – even though the thermoelectric effect is fully taken into account. The ∇T-terms are partially absorbed by the Seebeck terms in Eq. (5); the remaining parts are "hidden" in the carrier density gradients and the temperature-dependent transport coefficients. The diffusion coefficients in Eq. (7) are given via the *generalized* Einstein relations [5]

$$qD_n\left(n,T\right) = k_B T M_n g\left(n/N_c\left(T\right)\right),$$
$$qD_p\left(p,T\right) = k_B T M_p g\left(p/N_v\left(T\right)\right)$$

where the *degeneracy factor*

$$g\left(x\right) = x\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathscr{F}^{-1}\left(x\right)\right) \tag{8}$$

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gives rise to nonlinear diffusion as a consequence of Pauli-blocking. In the non-degenerate limit (Maxwell–Boltzmann statistics $\mathscr{F}(\eta) = \exp(\eta)$), the usual case of linear diffusion $g \equiv 1$ is recovered. In general, $\mathscr{F}(\eta)$ is given by, e.g., the Fermi–Dirac integral or the Gauss–Fermi integral. The effective density of states functions are denoted as $N_{c/v}(T)$.

III. Current density discretization

For the numerical simulation of charge transport in semiconductors, a naive finite difference discretization of the current densities leads to instabilities due to the typically exponentially varying carrier densities. The problem has been overcome by Scharfetter and Gummel [6], who developed a stable discretization scheme for the case of Maxwell–Boltzmann statistics and isothermal conditions. In this paper, we generalize the Scharfetter–Gummel scheme to the more general case of both degenerate materials (Fermi–Dirac statistics with arbitrary density of states) and thermoelectric cross-coupling using the Kelvin formula (6) for the Seebeck coefficients.

With the usual assumptions of constant electric field, mobility and current density along the edge $\overline{KL}$ between two adjacent nodes K and L in the grid (see Fig. 1), the discrete electron current density projection $j_{n,K,L}$ is obtained from the two-point boundary value problem (BVP):

$$\frac{k_B T(x)}{q\,\delta\phi_{K,L}} g\left(\frac{n(x)}{N_c(T(x))}\right)\frac{\mathrm{d}n}{\mathrm{d}x} = n(x) + \frac{j_{n,K,L}}{qM_n\,\delta\phi_{K,L}}, \qquad n(0) = n_K, \qquad n(1) = n_L. \tag{9}$$

The position on the edge $\mathbf{r} = x\mathbf{r}_L + (1-x)\,\mathbf{r}_K$ is described by the parameter $x \in [0,1]$. The electric potential difference reads $\delta\phi_{K,L} = \phi_L - \phi_K$. In the non-degenerate limit ($g \equiv 1$), the problem (9) can be solved exactly assuming a linearly varying temperature along the edge $T(x) = xT_L + (1-x)\,T_K$. In the degenerate case ($g \not\equiv 1$), however, no analytical solution is possible. Following Refs. [5, 7], we derive an approximate solution by "freezing" the degeneracy factor on a suitable average along the edge $g(n(x)/N_c(T(x))) \to g_{n,K,L}$. As a result, the discrete current density is obtained as

$$j_{n,K,L} = qM_n U^{T,n}_{K,L}\left(n_L B\left(\frac{\delta\phi_{K,L}}{U^{T,n}_{K,L}}\right) - n_K B\left(-\frac{\delta\phi_{K,L}}{U^{T,n}_{K,L}}\right)\right) \tag{10}$$

where $U^{T,n}_{K,L} = k_B T_{K,L} g_{n,K,L}/q$ is the edge-averaged thermal voltage, $B(x) = x/(\exp(x)-1)$ is the Bernoulli function,

$$T_{K,L} = \frac{T_L - T_K}{\log(T_L/T_K)}$$

is the logarithmically averaged temperature and the thermodynamically consistent average of the degeneracy factor is [5, 7]

$$g_{n,K,L} = \frac{\mathscr{F}^{-1}(n_L/N_c(T_L)) - \mathscr{F}^{-1}(n_K/N_c(T_K))}{\log(n_L/N_c(T_L)) - \log(n_K/N_c(T_K))}.$$

The accuracy of the scheme is investigated (i) analytically and (ii) by comparison with the numerically exact solution of Eq. (9). The latter is obtained using a shooting method combined with numerical root finding. We show that the scheme becomes exact in several limiting cases.

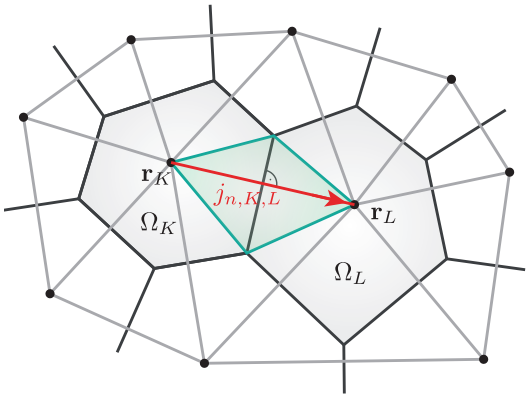

Fig. 1. The system (1)–(4) is discretized using the finite volume method with Voronoï boxes as control cells [8]. A stable expression for the discrete current density $j_{n,K,L}$ between two adjacent cells K and L is provided by Eq. (10).

IV. Summary

We have developed a generalized Scharfetter–Gummel scheme for the discretization of the current densities in degenerate semiconductors under non-isothermal conditions. The underlying thermoelectric transport model relies on the Kelvin formula for the Seebeck coefficient, which has several appealing consequences. The discretization of the electrical current density exploits the surprising feature of exactly vanishing ∇T-related driving forces in the continuous expression. A detailed comparison with the numerically exact solution of the corresponding two-point boundary value problem shows that the new scheme is highly accurate and becomes exact in several limiting cases.

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References

[1] D. M. Rowe, ed., *Thermoelectrics Handbook: Macro to Nano*. Boca Raton: CRC Press, Taylor & Francis Group, 2006.

[2] G. K. Wachutka, "Rigorous thermodynamic treatment of heat generation and conduction in semiconductor device modeling," *IEEE Trans. Comput.-Aided Design Integr. Circuits Syst.*, vol. 9, pp. 1141–1149, 1990.

[3] M. R. Peterson and B. S. Shastry, "Kelvin formula for thermopower," *Phys. Rev. B*, vol. 82, p. 195105, 2010.

[4] Y. Apertet, H. Ouerdane, C. Goupil, and P. Lecoeur, "A note on the electrochemical nature of the thermoelectric power," *Eur. Phys. J. Plus*, vol. 131, no. 4, p. 76, 2016.

[5] T. Koprucki, N. Rotundo, P. Farrell, D. H. Doan, and J. Fuhrmann, "On thermodynamic consistency of a Scharfetter–Gummel scheme based on a modified thermal voltage for drift-diffusion equations with diffusion enhancement," *Opt. Quantum. Electron.*, vol. 47, pp. 1327–1332, 2015.

[6] D. L. Scharfetter and H. K. Gummel, "Large-signal analysis of a silicon Read diode oscillator," *IEEE Trans. Electron Devices*, vol. 16, no. 1, pp. 64–77, 1969.

[7] M. Bessemoulin-Chatard, "A finite volume scheme for convection-diffusion equations with nonlinear diffusion derived from the Scharfetter–Gummel scheme," *Numer. Math.*, vol. 121, no. 4, pp. 637–670, 2012.

[8] P. Farrell, N. Rotundo, D. H. Doan, M. Kantner, J. Fuhrmann, and T. Koprucki, "Drift-diffusion models," in *Handbook of Optoelectronic Device Modeling and Simulation: Lasers, Modulators, Photodetectors, Solar Cells, and Numerical Methods* (J. Piprek, ed.), vol. 2, ch. 50, pp. 733–771, Boca Raton: CRC Press, Taylor & Francis Group, 2017.