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Consistent Treatment of Carrier Emission and Capture Kinetics in Electrothermal and Energy Transport Models

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Abstract

The quasi-static approximation usually employed to model the reaction kinetics of electrons, holes, and impurities in semiconductor devices is critically re-examined. It is shown that in the case of high trap concentrations, hot carriers, low temperature operating conditions or wide-gap devices the commonly used balance equations for particle and energy flow must be supplemented by additional terms in order to correctly include the emission and capture kinetics of the free carriers.

1. Introduction

In semiconductor device modeling the reaction kinetics of carrier emission and capture by the action of impurities is usually described within the so-called quasi-static approximation. For shallow impurities, local thermal and chemical equilibrium between donors and electrons or acceptors and holes, respectively, is assumed. So, for instance, incomplete ionization is modeled with the implicit supposition that the lattice temperature T_L and the electrochemical potential of the donors μ_D are equal to the electron temperature T_n and the electron quasi-Fermi level $-q\Phi_n$, respectively, and with the analogous assumption for acceptors and holes ($T_L = T_p$ and $\mu_A = -q\Phi_p$).

Trapping and generation-recombination processes through deep centers are described by a steady-state quasi-equilibrium Gibbs distribution

$$f_{tp}^{(o)} = \left(1 + g_{tp}\, exp\left((E_{tp} - \mu_{tp})/kT_L\right)\right)^{-1} \tag{1}$$

leading to the well-known Shockley-Read-Hall net reaction rate $(G - R)_{SRH}$. Here the underlying assumption is that the relaxation time τ_{tp} of the transient occupation number $f_{tp}(t)$ is much faster than the time scale relevant to the electric and thermal device operation.

Considering the operating conditions of lifetime-tailored power devices with a high concentration of complex recombination centers, highly integrated circuits with hot carriers, low temperature devices or novel wide-gap silicon carbide or diamond devices, the above-mentioned assumptions seem questionable and, therefore, have been subjected to critical reexamination.

2. Consistent Completion of the Governing Equations

Applying thermodynamic methods, the composite system of (possibly hot) electrons and holes, host lattice, donors, acceptors, and deep centers can be treated in a consistent way. It turns out that, indeed, the basic equations constituting the drift-diffusion-model, the electrothermal model [1] or the hydrodynamic [2] or energy transport models [3],[4],[5] have to be supplemented and completed by additional terms.

On the right-hand side of the current continuity equations (6) and (7), the time-derivatives of the ionized donor and acceptor concentrations, $\partial N_D^+/\partial t$ and $\partial N_A^-/\partial t$, respectively, have to be added. Even within the quasi-static approximation, where we assume instantaneous ionization and neutralization of the shallow impurities on the electrical and thermal time scale of interest, these terms must not be neglected, because N_D^+ and N_A^- may quasi-stationarily vary with time through the temporal evolution of temperature and quasi-Fermi levels according to

$$\frac{\partial N_D^+}{\partial t} = \left(\frac{\partial N_D^+}{\partial \Phi_n}\right)_{T_L} \frac{\partial \Phi_n}{\partial t} + \left(\frac{\partial N_D^+}{\partial T_L}\right)_{\Phi_n} \frac{\partial T_L}{\partial t} \tag{2}$$

and the analogous equation for $\partial N_A^-/\partial t$. Omitting these contributions from the particle balances may lead to a serious violation of charge conservation, as has been demonstrated in [6]. By the same token, the charge of the ionized deep centers must not be neglected on the right-hand side of Poisson's equation (8) when low temperatures or high trap densities are considered. Moreover, as it has been discussed in [7], recombination via donors and acceptors may become significant in VLSI bipolar devices. To model this effect, the shallow impurity net generation-recombination rates $(G-R)_A$ and $(G-R)_D$ (see eq. (2) in [7]) have to be substituted for $\partial N_D^+/\partial t$ and $\partial N_A^-/\partial t$, respectively, the two rates adding to that of recombination via the deep centers.

Furthermore, in each of the balance equations (6), (7), (9), (10) and (12) the Shockley-Read-Hall net generation-recombination rate $(G-R)_{SRH}$ has to be replaced by the individual non-steady-state electron and hole reaction rates $(\partial n/\partial t)_{tp}$ and $(\partial p/\partial t)_{tp}$, respectively, if the relaxation time τ_{tp} of the transient occupation number $f_{tp}(t)$ becomes comparable or longer than the electrical or thermal rise and fall times. In this case, the system of dynamic equations has to be augmented by eq. (14) in order to determine $f_{tp}(t)$ consistently. Here it is important to recognize that, dependent on capture cross sections [8], injection levels and temperature, the trap relaxation time

$$\tau_{tp} = (e_n + e_p + c_n n + c_p p)^{-1} \tag{3}$$

varies over many orders of magnitude ($0.1ps$ - $1ms$). Evidently it depends on the specific situation considered (device structure and operating conditions) whether or not the steady-state occupation number $f_{tp}^{(o)}$ (cf. eq.(1)) is an acceptable approximation of the true value $f_{tp}(t)$.

With the view to energy transport modeling, the right-hand sides of the electron and hole energy balance equations (9) and (10) must be supplemented by the terms

$$(w_{tp} - w_n)(\partial n/\partial t)_{tp} + (w_D - w_n)\,\partial N_D^+/\partial t \tag{4}$$

and

$$-\,(w_{tp} + w_p)(\partial p/\partial t)_{tp} + (w_A - w_p)\,\partial N_A^-/\partial t \tag{5}$$

respectively, which account for the energy lost or gained by the hot carrier subsystems due to carrier emission or capture by the impurity subsystems. For deep centers and/or heated carrier distributions, the respective energy transfer per particle $w_{tp} - w_n$ etc. can easily attain half or more of the band gap energy. Therefore the additional contributions to the heat exchange rate in the electron and hole temperature equations (9) and (10) may become substantial not only for fast transient processes, but also under quasi-static conditions in device regions where trap-assisted generation-recombination dominates.

The additional terms in (9) and (10) originate from the fact that under non-equilibrium conditions, the electrochemical potentials of the impurities, μ_D, μ_A and μ_{tp}, and the carrier quasi-Fermi levels, $-q\Phi_n$ and $-q\Phi_p$, differ each from the other, as well as the respective temperatures. Thus, for instance, we may regard the expressions $(w_D - w_n)\,\partial N_D^+/\partial t$ and $(w_A - w_p)\,\partial N_A^-/\partial t$ as corrections of the invalidated assumption of local thermal and chemical equilibrium between donors and electrons or acceptors and holes, respectively (which can be attained under global isothermal conditions solely).

Finally, our analysis also brings up some consequences for the formulation of the electric and thermal boundary conditions. In particular, it shows that inconsistencies arise in the widely used model of an "ideal ohmic contact", because the postulates of local thermodynamic equilibrium and charge neutrality are in contradiction to charge conservation and the energy balance equations.

3. Summary

The completed set of basic equations for particle and energy transport in semiconductor devices reads as follows:

particle balance equations

$$\frac{\partial n}{\partial t} = \frac{1}{q}\, div\, \vec{J}_n + \frac{\partial N_D^+}{\partial t} + \left(\frac{\partial n}{\partial t}\right)_{tp} + (G-R)_{else} \qquad (6)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\, div\, \vec{J}_p + \frac{\partial N_A^-}{\partial t} + \left(\frac{\partial p}{\partial t}\right)_{tp} + (G-R)_{else} \qquad (7)$$

($(\partial n/\partial t)_{tp}$ and $(\partial p/\partial t)_{tp}$: electron and hole reaction rate with deep centers)

Poisson's equation

$$div(\epsilon\nabla\psi) = q\,(n - p + N_A^- - N_D^+ - (z^{emp}(1-f_{tp}) + z^{occ} f_{tp})N_{tp}) \qquad (8)$$

(f_{tp} : trap occupation number; z^{emp} and z^{occ}: electric charge number of empty and occupied trap, respectively; N_{tp} : total trap concentration).

energy balance equations for hot carriers

$$c_n \frac{\partial T_n}{\partial t} = div\,(\kappa_n \nabla T_n + L_n \vec{J}_n) + H_n^{(old)} + (w_{tp} - w_n)\left(\frac{\partial n}{\partial t}\right)_{tp} + (w_D - w_n)\frac{\partial N_D^+}{\partial t} \qquad (9)$$

$$c_p \frac{\partial T_p}{\partial t} = div\,(\kappa_p \nabla T_p + L_p \vec{J}_p) + H_p^{(old)} - (w_{tp} + w_p)\left(\frac{\partial p}{\partial t}\right)_{tp} + (w_A - w_p)\frac{\partial N_A^-}{\partial t} \qquad (10)$$

where

$$w_\alpha \;:=\; \mu_\alpha - T_\alpha \left(\frac{\partial \mu_\alpha}{\partial T_\alpha}\right)_{f_\alpha} \tag{11}$$

(μ_α : electrochemical potentials of electrons, holes, donors, acceptors and traps, respectively)

heat flow equation for lattice

$$c_L \frac{\partial T_L}{\partial t} \;=\; div\,(\kappa_L \nabla T_L) \;+\; H_L \tag{12}$$

with

$$\begin{aligned} H_L \;=\;& q \left[T_p \left(\frac{\partial \phi_p}{\partial T_p}\right)_{n,p} - T_n \left(\frac{\partial \phi_n}{\partial T_n}\right)_{n,p} + \phi_n \;-\; \phi_p \right] (G-R)_{else} \\ & + \frac{3}{2}\, k\, n \,\frac{T_n - T_L}{\tau_{nL}} \;+\; \frac{3}{2}\, k\, p\, \frac{T_p - T_L}{\tau_{pL}} \end{aligned} \tag{13}$$

rate equation for trap occupation number

$$\frac{\partial f_{tp}}{\partial t} \;=\; -(e_n + e_p + c_n n + c_p p) f_{tp} + e_p + c_n n \tag{14}$$

(e_α, c_α : emission and capture coefficients of electrons and holes, respectively)

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