VLSI DESIGN
2001, Vol. 13, Nos. 1–4, pp. 381–386
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Maximum Entropy Principle within A Total Energy Scheme for Hot-carrier Transport in Semiconductor Devices

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By extending the maximum entropy principle within a scheme in total average energy we obtain a closed system of hydrodynamic equations for a full nonparabolic band model in which all the unknown constitutive functions are completely determined. The theory is validated by comparing hydrodynamic calculations with Monte Carlo simulations performed for bulk and submicron Si structures at 300 K. In the general framework of the moment theory a systematic study of small-signal response functions is provided.

Keywords: Entropy maximum principle; Hydrodynamic transport; Submicron devices

1. INTRODUCTION

The basic limitations of existing MPE theories as applied to solid state physics [1–5] are in: (i) the use of parabolic energy dispersion for the single carrier, (ii) the use of a few number of macroscopic moments to be taken as constraints in the variational procedure. Both assumptions are dictated by the complexity of the analytical formulation.

The aim of this work is to overcome these limitations by reformulating the theory within a total energy scheme described by a local and isotropic maxwellian distribution in terms of an arbitrary number of generalized kinetic fields

$$\psi_A(\vec{k}) = \{\varepsilon^p, \varepsilon^p u_{i_1}, \varepsilon^p u_{\langle i_1} u_{i_2\rangle}, \ldots, \varepsilon^p u_{\langle i_1} u_{i_2} \cdots u_{i_s\rangle}, \ldots\} \tag{1}$$

where u_i is the carrier group velocity, $\varepsilon(\vec{k})$ is the single particle band energy and, in general, $u_{\langle i_1} u_{i_2} \cdots u_{i_s\rangle}$ is the traceless part of the tensor $u_{i_1} u_{i_2} \cdots u_{i_s}$ being $p = 0, 1, \ldots, N$, and $s = 1, 2, \ldots, M$ with arbitrary values for the integers N and M.

A new system of generalized hydrodynamic (HD) equations is derived with the full complexity of the band modeled in terms of a single particle with an effective mass which is a function of the

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average total energy and becomes a new constitutive function [5]. Accordingly, the present HD theory does not need other adjustable parameters but the knowledge of the elementary microscopic interactions as for the kinetic theory.

1.1. Balance Equations and Entropy Maximization

Equation (1) is the key formula since it generalizes the kinetic fields to energy dispersions of general form. With this approach, if we consider the expectation values

$$F_A = \int \psi_A(\vec{k})\mathcal{F}(\vec{k},\vec{r},t)d\vec{k} = \{F_{(p)}, F_{(p)|i_1}, F_{(p)|\langle i_1 i_2\rangle}, \ldots, F_{(p)|\langle i_1 \cdots i_s\rangle}, \ldots\} \quad (2)$$

then $N=M=1$ we find the usual physical quantities such as $n=F_{(0)}$ (*numerical density*), $W=F_{(1)}$ (*total energy density*), $nv_i=F_{(0)|i}$ (*velocity flux density*), $S_i=F_{(1)|i}$ (*energy flux density*). By contrast, for N, $M>1$ we obtain macroscopic additional variables, which in some cases correspond to fluxes of v_i and S_i. In particular all the scalar moments $F_{(p)}$ can be separated into a local equilibrium part and a non-equilibrium part $\Delta_{(p)}$ through the relationship $F_{(p)}=F_{(p)}|_E+\Delta_{(p)}$. The set of HD equations which are formally obtained within this scheme are [2–6]

$$\frac{\partial F_A}{\partial t}+\frac{\partial F_{Ak}}{\partial x_k}=-\frac{e}{\hbar}R_{Ai}E_i+P_A, \quad \text{with } A=1,\ldots,\mathcal{N} \quad (3)$$

where $\mathcal{N}$ is the number of moments used, and F_{Ak}, P_{Ai}, R_A indicate, respectively, the fluxes, the external field productions, and the collisional productions given by:

$$F_{Ak}=\int \psi_A(\vec{k})u_k\mathcal{F}(\vec{k},\vec{r},t)d\vec{k},$$

$$R_{Ai}=\int \frac{\partial\psi_A(\vec{k})}{\partial k_i}\mathcal{F}(\vec{k},\vec{r},t)d\vec{k},$$

$$P_A=\int \psi_A(\vec{k})Q(\mathcal{F})d\vec{k}.$$

The structure of this equation shows that there are some unknown constitutive functions $H_A=\{F_{Ak}, P_{Ai}, R_A\}$ that must be determined, in a self-consistent way, in terms of the variables F_A. Following information theory, one can determine systematically the unknown constitutive functions, by introducing the MEP in terms of generalized kinetic fields (1), and thus also an analytic expression for the non-equilibrium distribution function. The MEP is based on the assumption that the least biased distribution function assignment to a physical system is that which maximizes the entropy subject to the contrains imposed by the available *information*. For this reason we assume that the *information* expressed by a certain *fixed* number $\mathcal{N}$ of moments is sufficient to describe the thermodynamical state of hot carriers satisfactorily and we search the distribution that makes best use of this *information*. Following this approach the distribution function will have the explicit form

$$\mathcal{F}=\mathcal{F}_M \exp\left(-\sum_{s=0}^{M}\sum_{m=0}^{N}\hat{\Lambda}^{(m)}_{\langle i_1\cdots i_s\rangle}\varepsilon^m u_{\langle i_1}\cdots u_{i_s\rangle}\right) \quad (4)$$

where $\hat{\Lambda}_A$ are the nonequilibrium part of the Lagrange multipliers [2, 4, 6] and $\mathcal{F}_M$ the local maxwellian.

Now, instead of introducing a local temperature, typical for a parabolic band shape, we keep the total average electron energy [5, 6] which is a well defined quantity for any band shape [7]. To be consistent with this choice, the moments of the distribution function F_A cannot be separated into their convective and nonconvective parts and the local distribution function should be defined in terms of the total average energy of the single carrier as $\mathcal{F}_M=\gamma\exp(-\beta\varepsilon(\vec{k}))$ being $\gamma=\gamma(n,W)$ a normalization factor and $\beta^{-1}\beta^{-1}(W/n)$ an appropriate average energy. By considering an explicit energy-wave-vector relation $\varepsilon(\vec{k})$, the quantities $\{\gamma,\beta\}$, can be determined by means of the local equilibrium relationships

$$n(\vec{r},t)=\int \mathcal{F}_M d\vec{k}, \quad W(\vec{r},t)=\int \varepsilon(\vec{k})\mathcal{F}_M d\vec{k}. \quad (5)$$

By expanding around the maxwellian $\mathcal{F}_M$, both the distribution function $\mathcal{F}$ and the constitutive functions H_A can be expressed as polynomials in the non-equilibrium variables whose coefficients depend on the local equilibrium quantities $\{n(\vec{r},t), W(\vec{r},t)\}$. The explicit HD expressions obtained from Eq. (3) are detailed in [6], here numerical results are displayed for validation purposes.

1.2. Small-signal Analysis for Bulk

We consider the time evolution of a small perturbation of the single-particle moments $\tilde{F}_A = F_A/n$ under spatially homogeneous conditions. In this case the corresponding balance equations take the form:

$$\frac{\partial \tilde{F}_A}{\partial t} + \frac{e}{\hbar}\tilde{R}_{Ai}E_i + \tilde{P}_A = 0, \quad \text{with } A = 1,\ldots\mathcal{N} \quad (6)$$

By assuming that at the initial time the system of carriers is perturbed by an electric field $\delta E\xi(t)$ (where $\xi(t)$ is an arbitrary function of time satisfying $|\xi(t)| \leq 1$), we will calculate the deviations from their average values of the moments denoted respectively with $\delta\tilde{F}_A$. After linearizing Eq. (6) around the stationary state, we obtain a system of equations which can be written in the compact form

$$\frac{d\delta\tilde{F}_\alpha(t)}{dt} = \Gamma_{\alpha\beta}\delta\tilde{F}_\beta(t) - e\delta E\xi(t)\Gamma_\alpha^{(E)} \quad (7)$$

where the relaxation of the system after the perturbation of the electric field is described by the *response matrix* $\Gamma_{\alpha\beta}$. By assuming $\delta\tilde{F}_\alpha(0) = 0$, Eq. (7) has the formal solution

$$\mathbf{\Pi}(t) = -e\delta E\int_0^t \mathbf{K}(s)\xi(t-s)ds, \quad (8)$$

with $\mathbf{K}(s) = \exp(\mathbf{\Gamma}s)\mathbf{\Gamma}^{(E)}$ that can be determined through the matrix

$$\exp(\mathbf{\Gamma}t) = \mathbf{\Phi}\mathrm{diag}\{\exp(\lambda_1 t),\ldots,\exp(\lambda_{N+2}t)\}\mathbf{\Phi}^{-1} \quad (9)$$

where λ_α are the eigenvalues of $\Gamma_{\alpha\beta}$ and $\mathbf{\Phi}$ the matrix of its eigenvectors.

The vector function $\mathbf{K}(t)$ determines the linear response of the moments $\tilde{F}_A$ to an arbitrary perturbation of the electric field. For example, with $K_{\tilde{w}}(t)$, $K_v(t)$ and $K_{\tilde{s}}(t)$ we denote the *response functions*, respectively for the fluctuations of: mean energy, velocity, and energy flux.

2. NUMERICAL RESULTS

In this section the theory of moments is applied to the case of n-Si where full-band effects are described by introducing an effective mass as a function of the electron total energy [5]. For the collisional processes, scattering with phonons of *f*- and *g*-type are considered. MC simulations are performed using full-band model [8] and analytic nonparabolic-band model [9]. The MC with analytic-band model and the HD calculations make use of the same physical scattering parameters [9].

2.1. Bulk with an Arbitrary Number of Moments (Linear Expansion)

Figure 1 shows the HD values for $\{v, \tilde{W}, \tilde{S}\}$ as a function of the electric field, calculated for $N=1$, $N=3$, $N=5$ and $M=1$ both in the parabolic and nonparabolic case. For the velocity, energy, and energy flux we report the MC values of full-band simulations [8] (open circles) and analytic nonparabolic-band simulations [9] (crosses); for the velocity we report also the experimental data. We note that the HD calculations exhibit small variations (at most within 10%) from the number of moments used. In any case the numerical results converge for $N=5$ both in the parabolic and nonparabolic case. The convergence is particularly evident for the velocity-field curves which are in closer agreement with experimental data.

Figure 2 reports the time-dependence of the linear response function (in the non-parabolic case) of the first scalar $\{K_{\tilde{w}}(t), K_{\tilde{F}_{(2)}}(t), K_{\tilde{\Delta}_{(2)}}(t)\}$ and vectorial moments $\{K_v(t), K_{\tilde{s}}(t), K_{\tilde{F}_{(2)|i}}(t)\}$ for

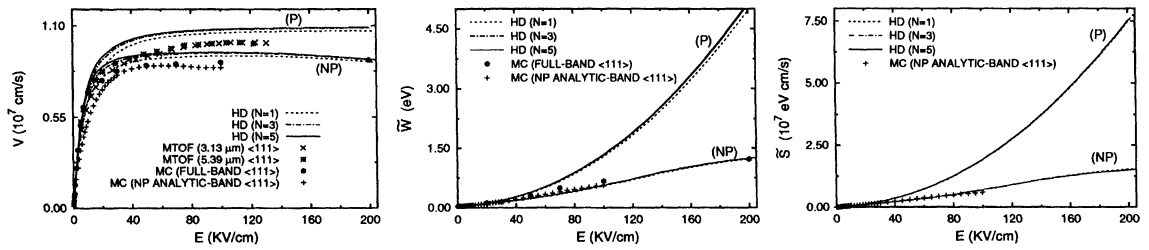

FIGURE 1 Drift velocity v, average total-energy $\tilde{W}$, and energyflux $\tilde{S}$ *vs.* electric field for electrons in Si at $T_0 = 300$ K. Lines refer to present parabolic (P) and nonparabolic (NP) HD calculations with $N = 1$ (dashed lines), $N = 3$ (dash-dotted lines) $N = 5$ (solid lines). Open circles refer to full-band MC simulations performed along ⟨111⟩ crystallographic directions [8]. Crosses refer to analytical NP band MC simulations performed along the ⟨111⟩ crystallographic direction [9]. For the drift velocity we report also the experimental data obtained with the microwave time-of-flight technique (MTOF) along the ⟨111⟩ crystallographic direction [10].

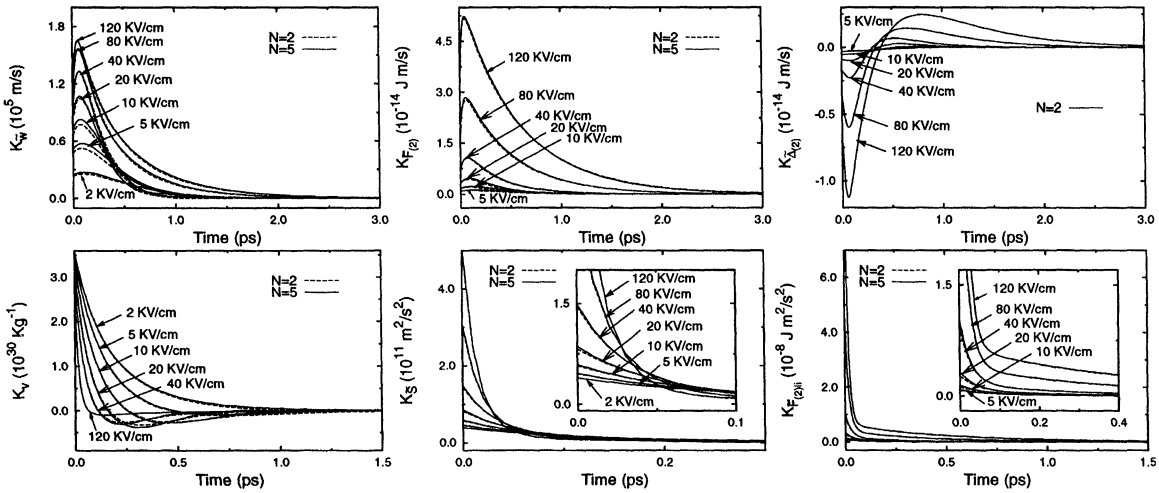

FIGURE 2 Response functions $\{K_{\tilde{w}}, K_{\tilde{F}_{(2)}}, K_{\tilde{\Delta}_{(2)}}\}$ and $\{K_v, K_{\tilde{s}} K_{\tilde{F}_{(2)|i}}\}$ (associated respectively to scalar $\{\tilde{w}, \tilde{F}_{(2)}, \tilde{\Delta}_{(2)}\}$ and vectorial $\{v_i, \tilde{S}_i, \tilde{F}_{(2)|i}\}$ moments) *vs.* time for electrons in Si in the case of a NP band model at $T_0 = 300$ K and increasing electric fields. The dashed and the continuous lines refer to $N = 1$ and to $N = 5$ respectively.

$\{N = 2,\ N = 5\}$ at increasing electric fields. As a general trend, from Figure 2 we notice that the increase in the number of moments yields small differences in the shape of the response function at any field value. The decay with time of the response functions is controlled essentially by the momentum and energy relaxation rates. The presence of the electric field couples the two relaxations processes [6], thus provoking a non-exponential shape of the decay. We note that $K_{\tilde{s}}$, $K_{\tilde{F}_{(2)|i}}$ and all vectorial moments decays similarly but faster than K_v.

2.2. Structures with the First 13 Moments (Nonlinear Expansion)

Figure 3 reports v, $\tilde{w}$ and $\tilde{S}$ for three n^+nn^+ Si structures with channel lengths of 0.2, 0.3 and 0.4 μm and an applied voltage of 1.5 V and 2 V, respectively. For the HD calculations both parabolic and nonparabolic band models are reported. For the longer structure MC results of the analytical nonparabolic model with the same scattering parameters used in the HD calculations are also reported. When compared with MC

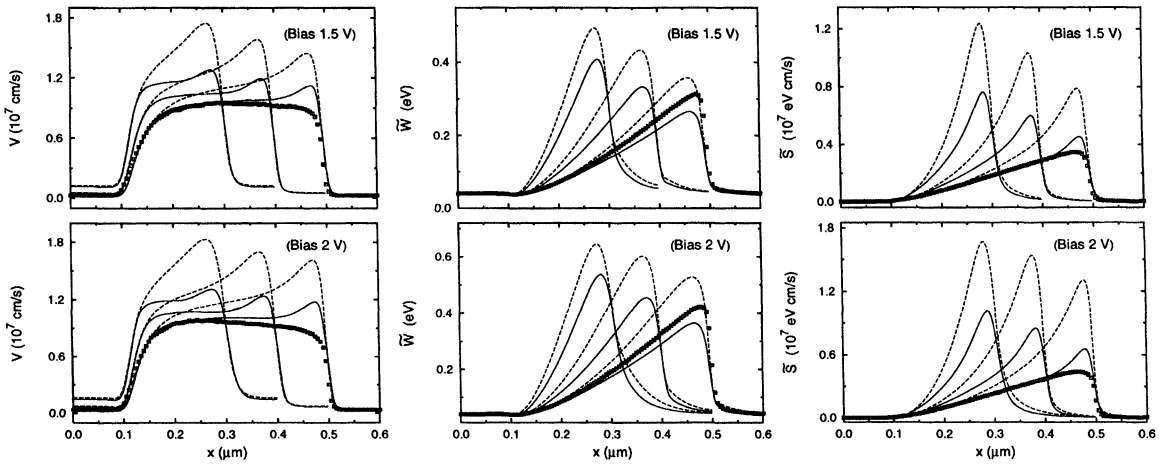

FIGURE 3 Velocity v, average total-energy $\tilde{W}$, and energy flux $\tilde{S}$ for a n^+nn^+ Si structure with a channel length of 0.2, 0.3 and 0.4 μm, respectively, with $n^+ = 5 \times 10^{17}\,\mathrm{cm}^{-3}$ and $n = 2 \times 10^{15}\,\mathrm{cm}^{-3}$ for an applied voltage of 1.5 V and 2 V at 300 K. Sharp homojunctions are considered. Continuous (dotted) curves refer to present NP (P) HD calculations, respectively. Points refer to MC simulations with a NP analytical model.

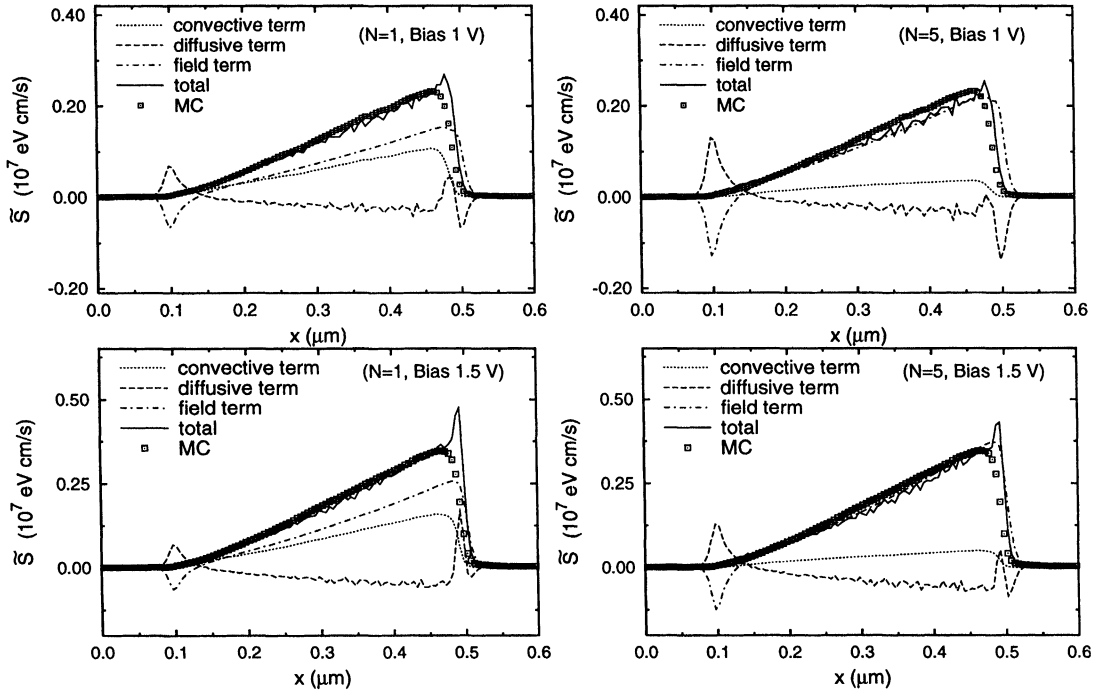

FIGURE 4 Spatial profile of energy flux $\tilde{S}$ for a n^+nn^+ Si structure with a channel length of 0.4 μm, $n^+ = 5 \times 10^{17}\,\mathrm{cm}^{-3}$, $n = 2 \times 10^{15}\,\mathrm{cm}^{-3}$ and applied voltages of, respectively, 1 V, and 1.5 V. Symbols refer to an explicit evaluation of the energy flux making use of data obtained from NP MC simulations. Curves refer to results obtained from the constitutive functions (dotted lines for the convective term, dashed lines for the diffusive term, dashdotted lines for the field term and continuous lines for the total) by substituting in the appropriate expressions the values of the average moments and electric field obtained from MC data of the Si structure.

results, HD calculations are found to agree satisfactorily apart from some discrepancy near the anode region. These discrepancies are associated with the strong gradient of the electric fields which need to account for other moments in the development of the analytical approach. As second step, we consider the contribution of higher moments and in Figure 4 we report a relevant subset of a complete series of data showing the spatial profiles of $\tilde{S}$ for the n^+nn^+ structure calculated for an increasing number of moments with $M=1$, $N=1$ and $N=5$ at increasing applied voltages. Overall, the agreement between the HD and MC results is considered to be satisfactory, thus validating the constitutive relations found here.

Acknowledgements

Drs. M. V. Fischetti, T. Gonzalez and M. J. Martin are thanked for providing the MC data. Partial support from the MADESS II project of the Italian CNR is gratefully acknowledged.

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