PHYSICAL REVIEW B VOLUME 51, NUMBER 23 15 JUNE 1995-I

Improved hydrodynamical model for carrier transport in semiconductors

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(Received 6 October 1994; revised manuscript received 23 January 1995)

A set of closed hydrodynamiclike equations is derived from Boltzmann's transport equation (BTE) describing charge transport in semiconductors. The production terms are modeled as relaxation terms consistently with the Onsager reciprocity principle. Stationary and homogeneous solutions are explicitly treated. The form of the production terms is checked by applying the Grad method of moments to the BTE. Finally the model is compared with Monte Carlo simulations for silicon.

I. INTRODUCTION

The increasing miniaturization of modern electric devices requires an accurate modeling of energy transport in semiconductors. This is of paramount importance in order to be able to describe such phenomena as hot electrons, impact ionization, and heat generation in the bulk material.[1]

The standard drift-diffusion equations currently used in the device simulation programs do not include the carriers energy as a dynamical variable.[2] Therefore, short of a direct numerical integration of the full Boltzmann transport equation for carriers in semiconductors (which would require a heavy and somewhat unwarranted computational cost), it is usual to resort to an augmented set of equations usually referred to as hydrodynamical models.[1-20] Simpler models, usually referred to as energy transport models, can be recovered from the hydrodynamical-like equations by an appropriate limiting process.[13] Hydrodynamical models are obtained from the moment equations of the Boltzmann transport equation suitably truncated at a certain order N. The truncation procedure requires solving the following two important problems: (i) the closure problem, and (ii) the modeling of the production terms.

The closure problem consists of finding an appropriate expression for the $(N+1)$th moment which appears under the divergence operator of the Nth moment equation. Likewise, modeling the production terms consists of expressing them as suitable functions of the first N moments. In Refs. 14–16 Anile and co-workers proposed a solution to the closure problem which, contrary to the previous treatments, was not *ad hoc* but was based on the application of the entropy principle within the framework of extended thermodynamics.[21,22] The production terms, however, were modeled as in the Baccarani and Wordeman model,[5] and this leads to some difficulties in the framework of irreversible thermodynamics, as we shall see in the sequel.

In this paper we take a fresh look at this problem and model the production terms consistently within the framework of extended thermodynamics: as pointed out by Hänsch and Miura-Mattausch,[7] modeling the production terms is crucial in order to obtain a proper description of phenomena like saturation velocity. We also support our approach by comparing the results with (i) approximate solutions of the Boltzmann transport equation by applying Grad's expansion method, and (ii) Monte Carlo simulations for silicon in a stationary and homogeneous state.

The plan of the paper is the following: in Sec. II we set up the general formalism for the Boltzmann transport equation for semiconductors, and derive the moment equations assuming a single-band and effective-mass approximation. In Sec. III we define the states of partial and global thermal equilibrium for the system and apply the entropy principle of extended thermodynamics in order to find a closure for the unknown moments. We remark that, within this approach, the heat-flow vector is flux limited. In Sec. IV we point out the difficulties in modeling the production terms *vis a vis* the Onsager reciprocity principle. We show how to circumvent this difficulty in a satisfactory way. In Sec. V we show that our model gives rise in a natural way to velocity saturation. In Sec. VI we introduce the concept of the Maxwellian iteration in order to obtain constitutive equations for the heat flow and viscous stresses. In Sec. VII we apply Grad's method in order to find explicit expressions for the production terms. In Sec. VIII we describe the Monte Carlo simulation for silicon, and compare the results with the previous ones. Finally, in Sec. IX we draw conclusions about the validity of the proposed model.

II. GENERAL FORMALISM

We start from the semiclassical Boltzmann transport equation for electrons in the conduction band of semiconductors,[1]

$$\frac{\partial f}{\partial t}+\mathbf{v}(\mathbf{k})\cdot\nabla f-qE\cdot\nabla_{\mathbf{k}}f=Q\ , \tag{1}$$

for the one-particle distribution function $f(\mathbf{x},t,\mathbf{k})$, where q is the absolute value of the electron charge, $\mathbf{k}$ is the electron momentum, $\mathbf{k}\in B$ (where B is the first Brillouin zone), and $\mathbf{v}(\mathbf{k})$ is the electron group velocity given by

$$\mathbf{v}(\mathbf{k})=\nabla_{\mathbf{k}}\mathcal{E} \ .$$

For convenience we shall use units such as Planck's constant $\hbar=1$. The electron energy $\mathcal{E}(\mathbf{k})$ is defined by the band structure of the crystal, and Q is the collision term

$$Q=\int d\mathbf{k}'[w(\mathbf{k},\mathbf{k}')(1-f)f'-w(\mathbf{k}',\mathbf{k})f(1-f')] \ , \tag{2}$$

with $f'=f(\mathbf{x},t,\mathbf{k}')$.

The scattering rate $w(\mathbf{k},\mathbf{k}')$ is given by

$$w(\mathbf{k},\mathbf{k}')=2\pi|m_{\mathbf{k}-\mathbf{k}'}|^2\{n_B(\omega_{\mathbf{k}-\mathbf{k}'})\delta(\mathcal{E}_{\mathbf{k}}-\mathcal{E}_{\mathbf{k}'}-\omega_{\mathbf{k}-\mathbf{k}'}) + [n_B(\omega_{\mathbf{k}-\mathbf{k}'})+1]\delta(\mathcal{E}_{\mathbf{k}}-\mathcal{E}_{\mathbf{k}'}+\omega_{\mathbf{k}-\mathbf{k}'})\}+2\pi|V_{\mathbf{k}-\mathbf{k}'}|^2\delta(\mathcal{E}_{\mathbf{k}}-\mathcal{E}_{\mathbf{k}'}) \ .$$

Here the first term represents scattering with phonons (acoustic and optical), the second with impurities, $m_{\mathbf{k}-\mathbf{k}'}$ and $V_{\mathbf{k}-\mathbf{k}'}$ are the corresponding matrix elements, and $\omega_{\mathbf{k}-\mathbf{k}'}$ is the energy transferred in the scattering with phonons.

In order to focus on the essential issues we limit ourselves to the case where the effective-mass approximation holds:[23]

$$\mathcal{E}(\mathbf{k})=\frac{\mathbf{k}^2}{2m^*} \ ,$$

$$\mathbf{v}(\mathbf{k})=\frac{\mathbf{k}}{m^*} \ ,$$

with m^* the effective electron mass.

Then, for consistency, the boundary of the first Brillouin zone is moved toward infinity, and B is approximated by $\mathcal{R}^3$.[1]

Let us define the particle density $n(\mathbf{x},t)$ as

$$n(\mathbf{x},t)=\int d\mathbf{k}\,f(\mathbf{x},t,\mathbf{k}) \ ,$$

and the mean velocity $\mathbf{u}(\mathbf{x},t)$ as

$$\mathbf{u}(\mathbf{x},t)=\frac{\int d\mathbf{k}\,\mathbf{v}(\mathbf{k})f(\mathbf{x},t,\mathbf{k})}{n} \ ;$$

then the particle flux is

$$\mathbf{J}=n\mathbf{u} \ . \tag{3}$$

By integrating Eq. (1) in $\mathbf{k}$ space we obtain, assuming as usual that $f(\mathbf{x},t,\mathbf{k})$ vanishes sufficiently fast at infinity, the particle continuity equation

$$\frac{\partial n}{\partial t}+\nabla\cdot(n\mathbf{u})=0 \ .$$

Multiplying Eq. (1) by k^i and integrating, we obtain the momentum balance equation

$$\frac{\partial(nu^i)}{\partial t}+\frac{\partial\theta^{ij}}{\partial x^j}+\frac{nqE^i}{m^*}=Q^i \ , \tag{4}$$

where

$$\theta^{ij}=\frac{\int d\mathbf{k}\,fk^ik^j}{m^{*2}} \tag{5}$$

and

$$Q^i=\frac{\int d\mathbf{k}\,Qk^i}{m^*} \ . \tag{6}$$

Multiplying Eq. (1) by k^ik^j and integrating, for the traceless part we obtain

$$\frac{\partial\theta_{\langle ij\rangle}}{\partial t}+\frac{\partial\theta_{\langle ij\rangle r}}{\partial x^r}+\frac{2nqE_{\langle i}u_{j\rangle}}{m^*}=Q_{\langle ij\rangle} \ ,$$

with

$$A_{\langle ij\rangle}=\frac{(A_{ij}+A_{ji}-\frac{2}{3}\delta_{ij}A_k^k)}{2}$$

denoting the trace-free part of the tensor A_{ij}, and where

$$\theta_{ijr}=\frac{\int d\mathbf{k}\,fk_ik_jk_r}{m^{*3}} \tag{7}$$

and

$$Q_{ij}=\frac{\int d\mathbf{k}\,Qk_ik_j}{m^{*2}} \ . \tag{8}$$

For the trace part we obtain the energy balance equation

$$\frac{\partial W}{\partial t}+\nabla\cdot S+nq\mathbf{E}\cdot\mathbf{u}=Q_w \ ,$$

with

$$W=\int d\mathbf{k}\,f\mathcal{E}(\mathbf{k})$$

the energy density,

$$\mathbf{S}=\int d\mathbf{k}\,f\mathcal{E}(\mathbf{k})\mathbf{v}(\mathbf{k})$$

the energy flux, and

$$Q_w=\int d\mathbf{k}\,Q\mathcal{E}(\mathbf{k}) \tag{9}$$

the energy rate of change. Furthermore we need the energy flux equation

$$\frac{\partial S_i}{\partial t}+\frac{\partial S_{ij}}{\partial x^j}+q\left[E_j\theta_{ij}+\frac{1}{m^*}WE_i\right]=\tilde{Q}_i \ , \tag{10}$$

where

$$S_{ij}=\frac{\int d\mathbf{k}\, f\mathcal{E}(\mathbf{k})k_i k_j}{m^{*2}} ,$$
$$\tilde{Q}_i=\frac{\int d\mathbf{k}\, Q\mathcal{E}(\mathbf{k})k_i}{m^{*}} . \tag{11}$$

The tensor θ_{ij} can be decomposed into its isotropic and anisotropic parts

$$\theta_{ij}=\tfrac{1}{3}\theta_{rr}\delta_{ij}+\theta_{\langle ij\rangle} ,$$

with

$$\theta_{\langle ij\rangle}=\tfrac{1}{2}(\theta_{ij}+\theta_{ji}-\tfrac{2}{3}\theta_{rr}\delta_{ij})$$

and

$$\theta_{rr}=\frac{\int d\mathbf{k}\, fk^2}{m^{*2}}=\frac{2W}{m^{*}} .$$

Therefore Eq. (4) can be rewritten as

$$\frac{\partial(nu^i)}{\partial t}+\frac{\partial\left[\frac{2W}{3m^{*}}\delta^{ij}+\theta^{\langle ij\rangle}\right]}{\partial x^j}+\frac{nqE^i}{m^{*}}=Q^i .$$

Likewise we can decompose S_{ij} into its isotropic and anisotropic parts:

$$S_{ij}=\tfrac{1}{3}S_{rr}\delta_{ij}+S_{\langle ij\rangle} .$$

Hence Eq. (10) can be rewritten as

$$\frac{\partial S_i}{\partial t}+\frac{1}{3}\frac{\partial S_{rr}}{\partial x^i}+\frac{\partial S_{\langle ij\rangle}}{\partial x^j}+q\left[\frac{5WE_i}{3m^{*}}+E_j\theta_{\langle ij\rangle}\right]=\tilde{Q}_i .$$

III. THE CLOSURE PROBLEM AND EXTENDED THERMODYNAMICS

Let us rewrite the moments equations derived in Sec. II. They are the continuity equation

$$\frac{\partial n}{\partial t}+\nabla\cdot(n\mathbf{u})=0 , \tag{12}$$

the momentum balance equation

$$\frac{\partial(nu^i)}{\partial t}+\frac{\partial\theta^{ij}}{\partial x^j}+\frac{nqE^i}{m^{*}}=Q^i , \tag{13}$$

the stress equation for the traceless part of $\theta_{\langle ij\rangle}$,

$$\frac{\partial\theta_{\langle ij\rangle}}{\partial t}+\frac{\partial\theta_{\langle ij\rangle r}}{\partial x^r}+\frac{2nqE_{\langle i}u_{j\rangle}}{m^{*}}=Q_{\langle ij\rangle} , \tag{14}$$

the energy equation for the trace of θ_{ij},

$$\frac{\partial W}{\partial t}+\nabla\cdot S+nq\mathbf{E}\cdot\mathbf{u}=Q_w , \tag{15}$$

and the energy flux equation

$$\frac{\partial S_i}{\partial t}+\frac{\partial S_{ij}}{\partial x^j}+q\left[E_j\theta_{ij}+\frac{1}{m^{*}}WE_i\right]=\tilde{Q}_i . \tag{16}$$

It is convenient to introduce the random component $\mathbf{c}$ of $\mathbf{k}$,

$$\mathbf{k}=m^{*}(\mathbf{u}+\mathbf{c}) ,$$

and then

$$\theta^{ij}=nu^iu^j+\int d\mathbf{k}\, fc^ic^j .$$

The tensor

$$\hat{\theta}^{ij}=\int d\mathbf{k}\, fc^ic^j$$

is then split into an isotropic and traceless part

$$\hat{\theta}^{ij}=\tfrac{1}{3}\hat{\theta}^k_k\delta^{ij}+\hat{\theta}^{\langle ij\rangle} ,$$

where

$$\hat{\theta}^k_k=\int d\mathbf{k}\, f\mathbf{c}^2 .$$

Then

$$\theta^{ij}=nu^iu^j+\tfrac{1}{3}\hat{\theta}^k_k\delta^{ij}+\hat{\theta}^{\langle ij\rangle} .$$

If we define the electron temperature T as

$$\hat{\theta}^k_k=\frac{3nk_BT}{m^{*}} ,$$

then the energy density is written as

$$W=\frac{m^{*}}{2}(n\mathbf{u}^2+\hat{\theta}^k_k)=\frac{3nk_BT}{2}+\frac{nm^{*}\mathbf{u}^2}{2} . \tag{17}$$

Furthermore we can decompose the energy flow $\mathbf{S}$ as

$$\mathbf{S}=W\mathbf{u}+nk_BT\mathbf{u}+\mathbf{h}+m^{*}u_j\hat{\theta}^{\langle ij\rangle}\mathbf{e}_i , \tag{18}$$

where $\mathbf{h}$ is the heat-flow vector:

$$\mathbf{h}=\frac{m^{*}}{2}\int d\mathbf{k}\, f\mathbf{c}^2\mathbf{c} .$$

Finally the flux of energy flux S_{ij} can be written as

$$\begin{aligned}S_{ij}={}&Wu_iu_j+2nk_BTu_iu_j+\tfrac{1}{2}\mathbf{u}^2nk_BT\delta_{ij}\\&+\frac{m^{*}}{2}(2u_ru_j\hat{\theta}_{\langle ij\rangle}+2u_iu_r\hat{\theta}_{\langle jr\rangle}+\mathbf{u}^2\hat{\theta}_{\langle ij\rangle})\\&+u_jh_i+u_ih_j+u_r\hat{\theta}_{ijr}+\hat{\theta}_{ijrr} ,\end{aligned}$$

where

$$\hat{\theta}_{ijr}=\frac{m^{*}}{2}\int d\mathbf{k}\, fc_ic_jc_r ,$$

$$\hat{\theta}_{ijrs}=\frac{m^{*}}{2}\int d\mathbf{k}\, fc_ic_jc_rc_s .$$

In this section we consider only the left-hand sides of Eqs. (12)–(16) assuming the right-hand sides are known (an explicit representation for them will be discussed in Sec. IV). The variables appearing in the 13 equations (12)–(16) are the 13 variables n, u^i, T, $\hat{\theta}_{\langle ij\rangle}$, and h_i, plus $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijrr}$.

In order to obtain a closed system we need explicit expressions for $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijrr}$. One of the most commonly used models is that of Baccarani and Wordeman,[5] in which the closure problem is considered at the level of the first five equations (12), (13), and (15) representing particle number, momentum, and energy balance. The closure is achieved by assuming that the stress tensor is isotropic,

$$\hat{\theta}_{\langle ij \rangle}=0 \ ,$$

and that the heat-flow vector $\mathbf{h}$ is related to the temperature gradient by the Fourier law

$$\mathbf{h}=-\kappa \nabla T \ ,$$

with κ the thermal conduction coefficient.

The first assumption can be justified on the basis of Monte Carlo simulations showing that in many cases of interest the anisotropic part of the distribution function is negligible.[24] In fact, in the regime of small field ($k_B T_L \gg qE\lambda$, where λ is the mean free path of electrons and T_L is the lattice temperature) the distribution function is obviously nearly isotropic. In the regime of strong field $qE\lambda \gg \omega_{\text{op}}$ (where ω_{op} is the optical phonon energy) the distribution function is also nearly isotropic because of the strong coupling to optical-phonon scattering. Anisotropy effects could be important in the intermediate field case ($k_B T_L < qE \ll \omega_{\text{op}}$), where ballistic behavior could occur (however, this can be realized only at a sufficiently low lattice temperature).

The assumption of a Fourier law for the heat-flow vector is simply a *petitio principii* and leads to serious difficulties when a comparison is made with results arising from a direct numerical solution of the Boltzmann transport equation.[9] In particular Stettler, Alam, and Lundstrom,[9] in the simulation of the n^+-n-n^+ diode, found that the heat-flow vector $\mathbf{h}$ is not zero when the temperature gradient vanishes, and that there is a small region near the channel-drain junction where $\mathbf{h}$ actually flows against the temperature gradient.

Other authors have sought a better criterion in order to achieve a rational closure. Historically this has been based on the assumption that the distribution function could be approximated by a drifted Maxwellian,[1,4,8,20] which could be justified if the scattering among the carriers were sufficiently strong for the carrier system to be in thermal equilibrium at temperature T and drift velocity $\mathbf{u}$. There have been opposite opinions on the latter point.[1,20] The drifted Maxwellian approximation implies the following closure relations for $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijrr}$:

$$\hat{\theta}_{\langle ijk \rangle}=0 \ , \tag{19}$$

from which

$$\hat{\theta}_{ijk}=\tfrac{1}{5}(h_i\delta_{jk}+h_j\delta_{ik}+h_k\delta_{ij}) \ .$$

Moreover,

$$\hat{\theta}_{ijrr}=\frac{5n(k_B T)^2}{2m^*}\delta_{ij} \ . \tag{20}$$

The closure problem is of such paramount importance for building hydrodynamical models that its deserves a thorough investigation starting from first principles. Such an investigation has been performed by Anile and Pennisi,[14,15] and Anile, Pennisi, and Trovato[16] within the framework of extended thermodynamics. Here we report their results and comment on their relevance for the closure problem, clarifying their physical implications for a silicon device.

The critical assumption is that $\hat{\theta}_{ijr}$ *and* $\hat{\theta}_{ijrr}$ *can be considered as functions of the lower-order moments.* As it stands this is a more general and weaker assumption than that of a Maxwellian distribution function. However, it still needs to be justified and this can be done as follows.

Hänsch[1] obtained an asymptotic solution of the stationary and homogeneous Boltzmann transport equation and found that at high energy the distribution function can be approximated by an exponential (multiplied by a power law). In this asymptotic solution few parameters (≤ 13) appear, which must be determined by taking the moments of the whole distribution function. The full distribution function can be described by a thermal equilibrium Maxwellian at sufficiently low energies and the Hänsch asymptotic solution at high energies. Therefore it is reasonable to assume that the unknown parameters could be determined by the first 13 moments of the distribution function.

Also, lately Tang, Ramaswany, and Nam[18] have analyzed the n^+-n-n^+ diode using the Monte Carlo simulation, and their results imply that the flux of energy flux S^{ij} can be parametrized by the previous moments. Therefore we can reasonably assume that $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijrr}$ are functions of the 13 moments n, u^i, T, $\hat{\theta}_{\langle ij \rangle}$, and h^i. We shall assume that the production terms Q_i, Q_w, $\tilde{Q}_i$, and $Q_{\langle ij \rangle}$ are also functions of the first 13 moments. The validity of this assumption will be discussed in Sec. IV.

In order to determine $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijrr}$, Anile and Pennisi applied the methods of extended thermodynamics[22] and the entropy principle.[21] This amounts to assuming the existence of a specific entropy η and an entropy flux $\mathbf{\Phi}$, also to be considered as functions of the first 13 moments (constitutive functions in the language of continuum mechanics), such that the entropy balance law

$$\frac{\partial \eta}{\partial t}+\nabla \cdot \mathbf{\Phi}=g \tag{21}$$

holds for all solutions of the evolution equations (12)–(16) (g is the entropy production) once the dependent variables $\hat{\theta}_{ijr}$, $\hat{\theta}_{ijrr}$, Q_i, $Q_{\langle ij \rangle}$, Q_w, and $\tilde{Q}_i$ have been expressed as constitutive functions of the independent variables n, T, u_i, $\hat{\theta}_{\langle ij \rangle}$, and h_i. Furthermore the entropy production g is positive definite and vanishes only at global thermal equilibrium.

Let us introduce the vectors

$$F^A=(n,nu^i,\theta_{\langle ij \rangle},W,S^i) \ ,$$

$$F^{Aj}=(nu^j,\theta_{ij},\theta_{\langle ij \rangle r},S^j,S^{ij}) \ ,$$

$$P^A=\left[0,Q_i-\frac{nqE^i}{m^*},Q_{\langle ij \rangle}-\frac{2nq}{m^*}E_{\langle i}u_{j\rangle}\right] \ ,$$

$$Q_w-nqE_k u^k, \ \ \tilde{Q}_i-q\left[E^r\theta_{ir}+\frac{1}{m^*}WE_i\right] \ ,$$

with $A=1,2,\ldots,13$. Then Eqs. (12)–(16) can be written in compact form:

$$\frac{\partial F^A}{\partial t}+\frac{\partial F^{Aj}}{\partial x^j}=P^A . \tag{22}$$

The entropy principle states that all the smooth solutions of system (22) satisfy (21) once F^A, F^{Aj}, and P^A have been expressed as functions of the fundamental variables. According to Liu's[25] theorem this is equivalent to assuming the existence of multipliers Λ_A which are functions of the independent variables such that

$$\frac{\partial \eta}{\partial t}+\frac{\partial \Phi^j}{\partial x^j}-\sum \Lambda_A\left[\frac{\partial F^A}{\partial t}+\frac{\partial F^{Aj}}{\partial x^j}\right]=g \tag{23}$$

holds for every value of the independent variables and their first-order derivatives.

By exploiting this result it is possible to obtain differential relations[21] which yield a useful characterization for the unknown quantities $\hat{\theta}_{ijr}$, $\hat{\theta}_{ijrr}$, η, and Φ_i as functions of the fundamental variables. In particularly simple cases it is even possible to determine the constitutive functions explicitly. This is the case, for instance, of the radiation field for which the stress tensor (second-order moment) can be explicitly determined as a function of the energy density and the energy flux, thereby determining uniquely the nonlinear Eddington factor.[17] In the general case it is not possible to solve explicitly the differential relations arising from Liu's theorem. It is then mandatory to resort to approximation schemes, which should be related to the physical phenomena under investigation.

In the following we shall deal with electron conduction in an infinitely long silicon device. A Monte Carlo simulation performed for such a device (see Sec. VIII) shows that the energy relaxation time τ_w (which is the characteristic time in which the electron energy relaxes to the lattice energy) is substantially larger than the relaxation times for momentum, heat flux, and anisotropic stresses (see Fig. 1).

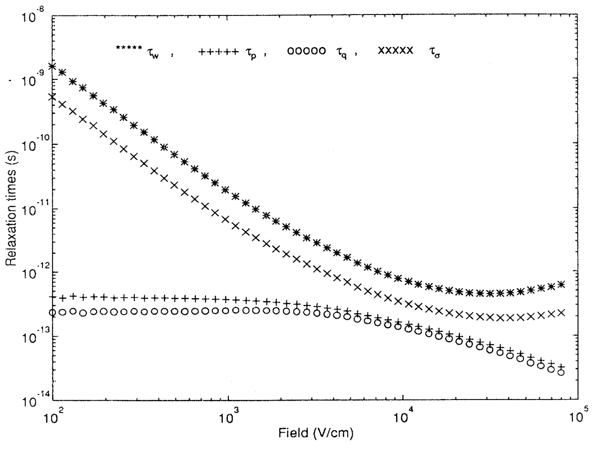

FIG. 1. Relaxation times τ_w (energy), τ_p (momentum), τ_q (energy flow), and τ_σ (shear stress) vs electric field obtained by Monte Carlo simulations for silicon.

In fact most collisions are of elastic type and therefore a large number of collisions is necessary in order to relax the carrier's energy to its equilibrium value ($k_B T_L$, where T_L is the lattice temperature), while momentum, heat-flow, and anisotropic stresses relax to the equilibrium values (zero) within a shorter time. During the relaxation to *global thermal equilibrium* an intermediate state arises where the electron fluid is in its own thermal equilibrium, a state which can be called *partial thermal equilibrium.*

The state of partial thermodynamical equilibrium is characterized by $u^i=0$, $\hat{\theta}_{\langle ij\rangle}=0$, $h^i=0$, and $\Phi^i=0$ (but $T\neq T_L$) and therefore near partial thermal equilibrium u^i, $\hat{\theta}_{\langle ij\rangle}$, and h^i are first-order quantities. Therefore it is natural to expand the differential relations arising from Eq. (23) around partial thermal equilibrium (up to second order).

A crucial assumption is that the entropy density and the entropy flux do not depend upon $\mathbf{u}$. In fact $\mathbf{u}$ is the relative velocity of the electron gas with respect to the lattice; hence the entropy, being an additive quantity, cannot depend on it. It can be proved that this is also a consequence of the entropy principle applied to the mixture consisting of the lattice and the electron gas.[16]

Only with the definition and justification of the partial thermal equilibrium state can the machinery of extended thermodynamics be applied, and the following results are obtained:[14]

$$\hat{\theta}_{\langle ijk\rangle}=0 ,$$

$$\hat{\theta}_{ijrr}=\frac{5n(k_B T)^2}{2m^*}\delta_{ij} ,$$

which are exactly those [Eqs. (19) and (20)] obtained with the drifted Maxwellian assumption.

Therefore the above closure relations are completely independent of the drifted Maxwellian assumption, and hence the question of the importance of the carrier-carrier scattering is completely irrelevant in this context.

Now we prove that the above closure leads to a flux-limited heat flow $\mathbf{h}$. In fact, from Schwarz's inequality we have

$$\int d\mathbf{k}\, f|\mathbf{c}|^3=\int d\mathbf{k}\, f^{1/2}|\mathbf{c}|f^{1/2}|\mathbf{c}|^2 \le \left[\int d\mathbf{k}\, f|\mathbf{c}|^2\right]^{1/2}\left[\int d\mathbf{k}\, f|\mathbf{c}|^4\right]^{1/2} .$$

It follows that

$$|\mathbf{h}|\le 3(\tfrac{3}{2})^{1/2}c_s n k_B T ,$$

where $c_s=(5k_B T/3m^*)^{1/2}$ is the adiabatic sound speed.

IV. MODELING THE PRODUCTION TERMS AND THERMODYNAMIC RESTRICTIONS

In order to close system (12)–(16) it is necessary also to express the production terms Q^i, $Q_{\langle ij\rangle}$, Q_w, and $\tilde{Q}_i$ as functions of the fundamental variables n, T, u^i, $\hat{\theta}_{\langle ij\rangle}$, and h^i.

In most hydrodynamical models[5,8,14] the production terms are assumed to be of the relaxation type, i.e.,

$$Q^i = -\frac{nu^i}{\tau_p} , \tag{24}$$

$$Q_w = -\frac{W - W_0}{\tau_w} , \tag{25}$$

$$\tilde{Q}_i = -\frac{S_i}{\tau_q} , \tag{26}$$

$$Q_{\langle ij \rangle} = -\frac{\hat{\theta}_{\langle ij \rangle}}{\tau_\sigma} , \tag{27}$$

with τ_p, τ_w, τ_q, and τ_σ relaxation times which are functions of the temperature T (and in some cases also of the electron density n and impurities number density N_i).

Now we show that the above representation for the production terms leads to a serious inconsistency with one of the fundamental principles of linear irreversible thermodynamics, the Onsager reciprocity principle[26] (hereafter ORP). Let us assume that the distribution function is almost isotropic (which is borne out by Monte Carlo simulations[24]). Then we can safely set

$$\hat{\theta}_{\langle ij \rangle} = 0 .$$

Then the momentum Eq. (13), in the stationary limit, yields

$$\mathbf{J} = -\frac{\tau_p}{m^*}[\nabla(nk_B T) + nq\mathbf{E}] . \tag{28}$$

By introducing the quasi-Fermi potential

$$\varepsilon_F = \phi - \frac{k_B T}{q} \ln\left[\frac{n}{dT^{3/2}}\right] + \text{const} ,$$

with ϕ the electrostatic potential, $\mathbf{E} = -\nabla\phi$ and $d = (2\pi m^* k_B)^{3/2}$, Eq. (28) can be written as

$$\mathbf{J} = \frac{n\tau_p}{m^*}\left\{-q\nabla\varepsilon_F + \left[\frac{5}{2} + \ln\left[\frac{dT^{3/2}}{n}\right]\right]\nabla(k_B T)\right\} . \tag{29}$$

Likewise, near partial thermal equilibrium we can approximate

$$S^{ij} = \frac{5nk_B T}{2m^*}\delta^{ij} ,$$

and then the energy flux equation (16) in the stationary limit yields

$$\mathbf{S} = -\frac{5\tau_q}{2m^*}\{\nabla(nk_B T)^2 + qnk_B T\mathbf{E}\} ,$$

which can be rewritten in terms of the quasi-Fermi potential ε_F as

$$\mathbf{S} = \frac{5\tau_q}{2m^*}\left\{-qnk_B T\nabla\mathscr{E}_F + \left[\frac{7}{2} + \ln\left[\frac{dT^{3/2}}{n}\right]\right]nk_B T\nabla(k_B T)\right\} .$$

As discussed in the book by de Groot and Mazur,[27] Chap. XIII, Sec. 6, where electrically conducting systems are considered, the Onsager reciprocity principle relates two cross coefficients of the particle flux $\mathbf{J}$ and the total entropy flux $\mathbf{J}_{s,\text{tot}}$. It is easy to see that the total entropy flux $\mathbf{J}_{S,\text{tot}}$ to first order around thermal equilibrium coincides with the vector

$$\mathbf{H} = \mathbf{S} + q(\mathscr{E}_F - \phi)\mathbf{J} .$$

The final expression for $\mathbf{H}$ is

$$\mathbf{H} = \frac{qn\tau_p}{m^*}\left\{k_B T\left[\frac{5\tau_q}{2\tau_p} + \ln\left[\frac{dT^{3/2}}{n}\right]\right]\nabla\mathscr{E}_F + \Lambda\nabla T\right\} , \tag{30}$$

with

$$\Lambda = \frac{1}{q\tau_p}\left\{-\frac{5\tau_q}{2}\left[\frac{7}{2} + \ln\left[\frac{dT^{3/2}}{n}\right]\right]k_B T - \tau_p k_B T \ln\left[\frac{n}{dT^{3/2}}\right]\left[\frac{5}{2} + \ln\left[\frac{dT^{3/2}}{n}\right]\right]\right\} ,$$

and by comparing it with Eq. (29) we find that, in order for the ORP to hold, the following relationship must be verified:

$$\tau_p = \tau_q . \tag{31}$$

In Fig. 1 a Monte Carlo simulation for silicon shows that equality (31) is only approximately true at high energy and is violated at low energy (see also Ref. 9); in fact τ_p and τ_q differ at low energy by as much as 100%. We ascribe this discrepancy not to a failure of the ORP (because at low energy and therefore near thermal equilibrium they are a statistical consequence of microscopic irreversibility) but to an inadequate modeling of the production terms. In this case the assumption which must be abandoned is that τ_p and τ_q, in the general nonhomogeneous situation, can be modeled as functions of the temperature alone. In fact, as will be seen in Sec. VII, Grad's method of moments when applied in order to evaluate $\mathbf{Q}$ and $\tilde{\mathbf{Q}}$ near thermal equilibrium yields expressions of the more general kind, i.e.,

$$\mathbf{Q} = -(a\mathbf{J} + b\mathbf{S}) , \tag{32}$$

$$\tilde{\mathbf{Q}} = -(\tilde{a}\mathbf{J} + \tilde{b}\mathbf{S}) . \tag{33}$$

This implies that τ_p and τ_q are functions of $\mathbf{J}$ and $\mathbf{S}$ in addition to the temperature T. By utilizing the above expressions in the momentum and energy flux Eqs. (13) and (16) and proceeding as before, we finally find that the OPR is equivalent to the following relationships:

$$\tilde{a} + \tfrac{5}{2}\tilde{b}k_B T = \tfrac{5}{2}k_B T(a + \tfrac{7}{2}bk_B T) . \tag{34}$$

In a recent article,[28] the authors discussed the ORP for their hydrodynamical model. We remark that their conclusions are fallacious because they impose the ORP not on the total entropy flux vector $\mathbf{H}$ but on a different vector, for which Onsager's theorem does not apply.[27]

Another consequence of Eqs. (32) and (33) is obtained for the entropy production

$$g = g_1 + g_2 + O_3 \ ,$$

where g_1, g_2, and O_3 are terms of first-, second-, and higher-orders, respectively, in the deviation from partial thermal equilibrium:

$$g_1 = \frac{3nk_B(T-T_L)}{2Tm^*\tau_w} \ ,$$

$$g_2 = \hat{g}_2 + \frac{m^{*2}}{8nk_B T^2 \tau_\sigma} \hat{\theta}_{\langle ij \rangle} \hat{\theta}^{\langle ij \rangle} \ ,$$

with

$$\hat{g}_2 = \alpha \mathbf{J}^2 + \beta \mathbf{J} h + \gamma \mathbf{h}^2 \ .$$

The term g_1 is linear in $T-T_L$ and corresponds exactly to the rate of variation of the lattice entropy production (considering the solid as a rigid body) due to its interaction with the electron gas. The term g_2 then represents the rate of entropy production due to the dissipative nature of the interaction of the electron gas with the phonons. The coefficients of the quadratic form $\hat{g}_2$ are given by

$$\alpha = \frac{1}{2nT} \left[2a - \frac{1}{\tau_w} + 5bk_B T \right] \ ,$$

$$\beta = \frac{1}{nk_B T^2} \left[-4a - 9bk_B T + \frac{4}{5k_B T} (\tilde{a} + \tfrac{5}{2}\tilde{b} k_B T) \right] \ ,$$

$$\gamma = \frac{4}{nk_B T^2} \left[-b + \frac{\tilde{b}}{5k_B T} \right] \ .$$

The quadratic form g_2 is positive defined if $\tau_\sigma > 0$ and $\hat{g}_2$ is positive definite. The conditions for $\hat{g}_2$ to be positive definite are $\alpha > 0$, which implies

$$2\tau_w > \frac{1}{a + \frac{5}{2}bk_B T} \tag{35}$$

and

$$\beta^2 - 4\alpha\gamma < 0 \ . \tag{36}$$

A Monte Carlo simulation for silicon (see Sec. VIII) shows that these inequalities hold.

V. STATIONARY AND HOMOGENEOUS REGIME

Let us rewrite Eqs. (12)–(16) in the stationary and homogeneous case. Then we obtain

$$Q_i = \frac{nq}{m^*} E_i \ , \tag{37}$$

$$Q_w = \frac{m^*}{n} Q_i J_i \ , \tag{38}$$

$$Q_{\langle ij \rangle} = \frac{2nq}{m^*} E_{\langle i} u_{j \rangle} \ , \tag{39}$$

and, to within first order off partial thermal equilibrium,

$$\tilde{Q}_i = \tfrac{5}{2} x Q_i \ , \tag{40}$$

where $x = k_B T$.

In the case of a uniform one-dimensional semiconductor and electric field, the carrier concentration remains uniform and diffusive phenomena do not occur: as a consequence, the average velocity reduces to the drift velocity v_d. Then if we substitute Eqs. (24)–(27) in the previous equations, we can express the relaxation times τ_w, τ_p, τ_q, and τ_σ as

$$-\frac{1}{\tau_p} = \frac{qE}{m^* v_d} \ , \tag{41}$$

$$-\frac{W - W_0}{\tau_w} = qnEv_d \ , \tag{42}$$

$$-\frac{1}{\tau_q} = \frac{5}{2} \frac{nq}{m^*} k_B T \frac{E}{S} \ , \tag{43}$$

$$\frac{\|\hat{\theta}_{\langle ij \rangle}\|}{\tau_\sigma} = \frac{2nq}{m^*} \|E_{\langle i} u_{j \rangle}\| \ . \tag{44}$$

The values of the drift velocity, temperature, energy flux, and stress can be obtained by Monte Carlo calculations in steady-state conditions. With our Monte Carlo code (see Sec. VIII) we obtain the previous quantities as functions of the electric field, and also the relaxation times: in Fig. 2 we plot the percent error for the relaxation times versus the electric field. The agreement is very good for the momentum relaxation time τ_p ($\leq 0.1\%$) and reasonable for τ_w, τ_q, and τ_σ (a few percent). This shows that deviations from partial thermal equilibrium remain on the order of a few percent to within first order off partial thermal equilibrium.

Another consequence of Eq. (40) and Eqs. (32) and (33) is

$$(\tilde{a} - \tfrac{5}{2} a x)\mathbf{J} + (\tilde{b} - \tfrac{5}{2} b x)\mathbf{S} = 0 \ . \tag{45}$$

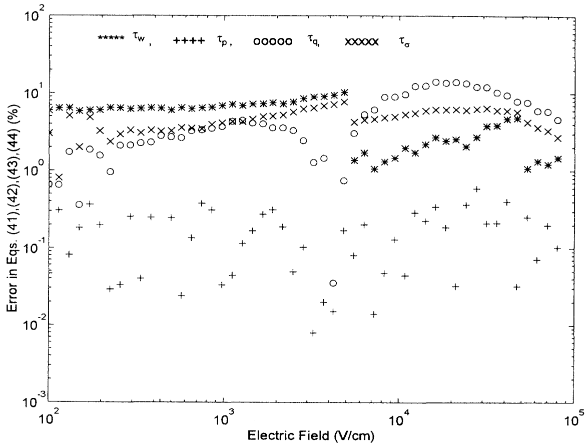

FIG. 2. Percent error between relaxation times given by Eqs. (41)–(44) and those obtained by Monte Carlo simulations for silicon vs electric field.

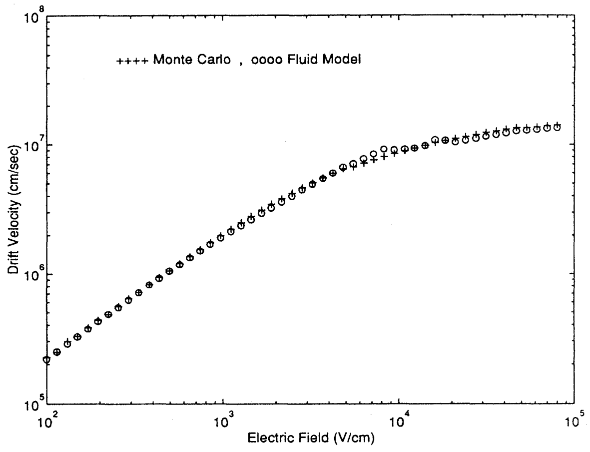

FIG. 3. Drift velocities obtained by Monte Carlo simulations for silicon and hydrodynamical model vs electric field.

From the previous equation and the definition of **S** we can express the heat flux vector (18) as follows:

$$h^i=\frac{(\tilde{a}-\frac{5}{2}ax)+\frac{5}{2}x(\tilde{b}-\frac{5}{2}bx)}{\tilde{b}-\frac{5}{2}bx}J^i\ , \tag{46}$$

and, by using Onsager's relation (34), Eq. (46) reduces to

$$h^i=-\frac{5}{2}\frac{bx^2J^i}{\tilde{b}-\frac{5}{2}bx}\ . \tag{47}$$

Now from Eqs. (32) and (37) we have

$$-a\mathbf{J}-b\mathbf{S}=\frac{nq\mathbf{E}}{m^*}\ ,$$

and by using Eq. (45) we obtain

$$\mathbf{J}=n\mu\mathbf{E}\ ,$$

where μ is the mobility:

$$\mu=\frac{q}{m^*}\frac{1}{-a+b\dfrac{\tilde{a}-\frac{5}{2}ax}{\tilde{b}-\frac{5}{2}bx}} \tag{48}$$

In Sec. VIII, with a Monte Carlo simulation, we obtain the parameters a, b and $\tilde{a}$, $\tilde{b}$, and from Eq. (48) we can evaluate the drift velocity of the fluid model: we notice that our fluid model gives the physical saturation velocity. The agreement between the Monte Carlo and the fluid drift velocity is good (see Fig. 3).

VI. MAXWELLIAN ITERATION AND CONSTITUTIVE EQUATIONS

In Sec. III for the moment equations we obtained a closed system (12)–(16), in the 13 variables n, u^i, T, $\hat{\theta}_{\langle ij\rangle}$, and h^i, by using the techniques of extended thermodynamics. However, the above system is still too complicated to be used for device simulation and therefore we now derive a reduced system. First we consider the stress equation (14) with (27):

$$\frac{\partial\hat{\theta}_{\langle ij\rangle}}{\partial t}+u_k\frac{\partial\hat{\theta}_{\langle ij\rangle}}{\partial x^k}+\hat{\theta}_{\langle ij\rangle}\frac{\partial u_k}{\partial x^k}+\frac{2}{5m^*}\left[\frac{\partial h_i}{\partial x^j}+\frac{\partial h_j}{\partial x^i}-\frac{2}{3}\frac{\partial h_k}{\partial x^k}\delta_{ij}\right]+\frac{nk_BT}{m^*}\left[\frac{\partial u_i}{\partial x^j}+\frac{\partial u_j}{\partial x^i}-\frac{2}{3}\frac{\partial u_k}{\partial x^k}\delta_{ij}\right]=-\frac{\hat{\theta}_{\langle ij\rangle}}{\tau_\sigma}\ . \tag{49}$$

Now we shall apply an iteration technique to Eq. (49) following Ref. 29. In Sec. III we dealt with a state of *partial thermal equilibrium* for the electron fluid, which is characterized by $u^i=0$, $\hat{\theta}_{\langle ij\rangle}=0$, and $h^i=0$, whereas u^i, $\hat{\theta}_{\langle ij\rangle}$ and h^i and first derivatives are first-order quantities: we define the zeroth iterate in the previous equilibrium state. In the left-hand side of Eq. (49) we substitute the zeroth iterate of **h**, **u**, and $\hat{\theta}_{\langle ij\rangle}$. Then the right-hand side of this equation yields the first iterate for **h**, **u**, and $\hat{\theta}_{\langle ij\rangle}$, once nonlinear terms of orders higher than the first in the deviation from partial thermal equilibrium have been neglected. It is immediate that the first iterate gives

$$\hat{\theta}_{\langle ij\rangle}=0\ .$$

Then we consider the equation for the heat flux: by taking Eqs. (12)–(16) with the closure Eqs. (19) and (20), and $\hat{\theta}_{\langle ij\rangle}=0$, we obtain a differential equation for **h**:

$$\frac{\partial h_i}{\partial t}+u^j\frac{\partial h_i}{\partial x^j}+\frac{7h_i}{5}\frac{\partial u^k}{\partial x^k}+\frac{2h_j}{5}\frac{\partial u^j}{\partial x^i}+\frac{7h^j}{5}\frac{\partial u_i}{\partial x^j}+\frac{5}{2}\frac{nk_BT}{m^*}\frac{\partial(k_BT)}{\partial x^i}$$
$$=\left[\tilde{Q}_i-m^*u^iu^jQ_j-m^*\frac{u^2}{2}Q_i-\frac{5}{6}u_i(2Q_w-m^*Q_ju^j)\right]-\frac{5}{2}k_BTQ_i\ , \tag{50}$$

where Q_w is given by Eq. (25), and Q_i and $\tilde{Q}_i$ are given by Eqs. (32) and (33). In the spherical band approximation it is possible to show that **J**, **h**, and **S** are collinear, i.e.,

$$\mathbf{S}=S\mathbf{e},\quad \mathbf{J}=J\mathbf{e},\quad \mathbf{h}=h\mathbf{e},\quad \mathbf{e}^2=1\ ,$$

and we have

$$\frac{1}{\tau_p}=a+b\frac{S}{J}\ , \tag{51}$$

$$\frac{1}{\tau_q}=\tilde{b}+\tilde{a}\frac{J}{S}\ . \tag{52}$$

Again we shall apply the previous iteration technique to Eq. (50). We obtain

$$\frac{5}{2}\frac{nk_BT}{m^*}\frac{\partial(k_BT)}{\partial x^i}=-\frac{S^i}{\tau_q}+\frac{5}{2}\frac{k_B(T-T_0)}{\tau_w}J^i+\tfrac{5}{2}k_BT\frac{J^i}{\tau_p}\ .$$

According to the Monte Carlo simulation (see Sec. VIII and Fig. 1) $\tau_p \ll \tau_w$, and therefore we can neglect the second term on the right-hand side. Also, from expression (18) for **S** we obtain

$$\frac{5}{2}\frac{nk_BT}{m^*}\frac{\partial(k_BT)}{\partial x^i}=-\frac{h^i}{\tau_q}+\tfrac{5}{2}k_BTJ^i\left[\frac{1}{\tau_p}-\frac{1}{\tau_q}\right]\ .$$

Since the three vectors **J**, **S**, and **h** are collinear, substituting from Eqs. (51) and (52) we obtain a second-order equation for h:

$$Mh^2+(PJ-G)h+NJ^2-\tfrac{5}{2}k_BTJG=0\ , \tag{53}$$

where

$$G:=\frac{5}{2}\frac{nk_BT}{m^*}\mathbf{e}\cdot\nabla(k_BT)\ ,$$

$$M:=-\tilde{b}+\tfrac{5}{2}k_BTb\ ,$$

$$N:=\tfrac{5}{2}k_BT[-\tilde{a}+\tfrac{5}{2}k_BT(a-\tilde{b})+(\tfrac{5}{2}k_BT)^2b]\ ,$$

$$P:=-(\tilde{a}+\tfrac{5}{2}k_BT\tilde{b})+\tfrac{5}{2}k_BT(a-\tilde{b})+(\tfrac{5}{2}k_BT)^2 2b\ .$$

Let us assume that Onsager's relation Eq. (34) holds: then we obtain

$$P<0,\quad N<0,\quad M<0\ ,$$

and the discriminant of Eq. (53) is non-negative. Then this equation admits two solutions.

In order to choose the sign let us analyze the case $G=0$ (i.e., constant temperature): we obtain the two solutions

$$h_+=-\tfrac{5}{2}k_BTJ\ ,$$

$$h_-=-\frac{5}{2}\frac{bx^2J}{\tilde{b}-\frac{5}{2}bx}\ .$$

The choice h_+ is not admissible because it leads to

$$\mathbf{S}=\tfrac{5}{2}k_BT\mathbf{J}+\mathbf{h}=(\tfrac{5}{2}k_BTJ+h_+)\mathbf{e}=0\ ,$$

which is not physically reasonable: the convective energy flux must depend on the scattering process.

The choice h_- leads to the same expression (47), and by continuity the correct solution of Eq. (53) is that with the minus sign:

$$2Mh=-(PJ-G)-[(P^2-4MN)J^2+G^2-2(P-5Mk_BT)JG]^{1/2}\ . \tag{54}$$

The constitutive equation (54) for h is not the usual Fourier law because it has a nonlinear dependence on the temperature gradient. For large G Eq. (54) reduces to

$$2Mh\simeq-(PJ-G)-|G|\ . \tag{55}$$

If $G>0$ then the heat flux is limited, consistent with numerical simulation;[9] if $G<0$ then h can become unbounded with G, diverging to first order in the Maxwellian iteration.

VII. GRAD'S METHOD OF MOMENTS

In previous sections we found a set of closed equations, which are consistent with the principles of irreversible thermodynamics. Now the problem arises of determining the relaxation times, which appear as unknown parameters. The above equations are valid in the single-valley case, whereas in practical situations we deal with multivalley semiconductors.[30]

Therefore these equations should be rewritten for each valley together with the coupling continuity equations, since an additional term $(\partial n/\partial t)_c$ has to be introduced in the second member of Eq. (12) to take into account the intervalley transfer. A rough but useful approximation consists of averaging all relevant quantities over all valleys of the considered band structure: by doing so, these equations can still be applied to a multivalley semiconductor. Then the relaxation times and the effective mass can be determined from a Monte Carlo simulation under steady-state conditions, and inserted into our system. Thus, at least, this method has the advantage of providing steady-state results which are exact within the band model used, since all operating parameters are analytically fitted with Monte Carlo calculations.

The advantages of the hydrodynamic simulation with respect to a Monte Carlo one are short CPU usage and results without noise: these are very important aspects for industrial purposes. However, this procedure has the defect that if we change the characteristics of the device (i.e., number of dopants, external bias, type of semiconductor) another Monte Carlo simulation is needed. Thus it is of great interest to obtain information about the relaxation times by analytic methods.

What can be done is to develop the distribution function for electrons around the state of global thermal equilibrium, where the electrons, in the material, lie close to the bottom of the conduction band. We shall assume that the electron gas is not degenerate, such that the collision term Q linearizes:

$$Q=\int d\mathbf{k}'[w(\mathbf{k},\mathbf{k}')f'-w(\mathbf{k}',\mathbf{k})f]\ ,$$

with $f'=f(\mathbf{x},t,\mathbf{k}')$.

According to a well-known procedure due to Grad,[31] we expand the distribution function $f(\mathbf{x},t,\mathbf{k})$, in Hermite polynomials:

$$f = f_{\mathrm{eq}} \sum_{r=0}^{\infty} \frac{1}{r!} a^{(r)}_{i_1,\dots,i_n} H^{(r)}_{i_1,\dots,i_n}(y) , \tag{56}$$

where

$$f_{\mathrm{eq}} = \frac{n}{(2\pi m^* k_B T_0)^{3/2}} e^{-\varepsilon/k_B T_0} ,$$

$$\mathbf{y} = \frac{\mathbf{k}}{(m^* k_B T_0)^{1/2}} .$$

Then we insert Eq. (56) into the Boltzmann equation (1) and moments (3), (5), and (7) by using the orthogonality properties of Hermite polynomials and the quasi-isotropy of the distribution function.[24] We obtain

$$f = \alpha + k_i \beta^i ,$$

$$\alpha = f_{\mathrm{eq}} \left[1 + \left[\frac{T}{T_0} - 1 \right] \left[\frac{\varepsilon}{k_B T_0} - \frac{3}{2} \right] \right] ,$$

$$\beta_i = \frac{f_{\mathrm{eq}}}{n k_B T_0} \left[J_i \left[\frac{7}{2} - \frac{\varepsilon}{k_B T_0} \right] + \frac{1}{5} \frac{S_i}{k_B T_0} \left[\frac{2\varepsilon}{k_B T_0} - 5 \right] \right] .$$

Now from Eqs. (24)–(26) and the approximate expression for the distribution function, we can determine the relaxation times if we know the scattering rates.

In the following we shall deal with silicon at room temperature ($T_0 = 300$ K) and, for the sake of simplicity, we shall consider only phonon scattering (acoustical and optical). The band structure of silicon is such that electrons which contribute to charge transport, even at high electric field, are those in the six equivalent ellipsoidal valleys along $\langle 100 \rangle$ directions at about $0.85(2\pi/a)$ (where a is the lattice constant) from the center of the Brillouin zone.[30]

Electrons in silicon are subject to intravalley elastic scattering with acoustic phonons and inelastic intervalley scattering with nonpolar scattering with optical phonons (of types f, i.e., between perpendicular valleys, and g, i.e., between parallel valleys). According to selection rules, intravalley nonpolar scattering for optical phonons is forbidden, whereas anelastic intervalley scatterings of types f and g is allowed; the matrix elements of such processes, in the approximation of spherical valleys, can be found in Ref. 30. Since we consider spherical valleys in homogeneous conditions, the six valleys can be considered equivalent: we approximate the material with a single valley and the intervalley scattering reduces to intravalley scattering.

With such a hypothesis we obtain

$$\tau_w = 3.82 \times 10^{-12} \text{ s} ,$$

$$\frac{1}{\tau_p} = a + b \frac{S}{J} , \tag{57}$$

$$\frac{1}{\tau_q} = \tilde{b} + \tilde{a} \frac{J}{S} , \tag{58}$$

where

$$b = 42.8 \text{ ps}^{-1}, \quad a = 1.07 \text{ (eV ps)}^{-1} ,$$

$$\tilde{a} = -0.0589 \text{ eV ps}^{-1}, \quad \tilde{b} = 6.178 \text{ ps}^{-1} .$$

These results will be compared with a Monte Carlo simulation in Sec. VIII.

For a quasi-isotropic distribution function the deviatoric stress tensor vanishes and therefore τ_σ is not defined. We note that τ_w is constant and this due to the fact that the Grad expansion holds near thermal equilibrium.

Similar equations are obtained by Hänsch[1] by expanding moments in a power series of energy. That is not admissible because the distribution function $f \in L^1$, and it is not possible to expand it in a convergent power series of energy.

VIII. MONTE CARLO SIMULATION AND COMPARISON WITH GRAD'S RESULTS

The Monte Carlo solutions of the Boltzmann equation have been well investigated over the years. The Monte Carlo method provides an accurate description of carrier transport in submicron semiconductor devices, even under highly nonequilibrium conditions, because various scattering mechanisms and band-structure models are considered.[32,33]

In order to evaluate the production terms Q_i, Q_w, $\tilde{Q}_i$, and $Q_{\langle ij \rangle}$ we observe that they are defined as moments over the right-hand side of the Boltzmann equation (1) [see Eqs. (6), (8), (9), and (11)]. According to the definition of the collisional operator Eq. (2), the production terms can be evaluated via Monte Carlo simulations:

$$Q_i = \frac{1}{N_{\mathrm{coll}}} \sum_{\mathrm{coll}} \frac{\delta v_i}{\delta t} ,$$

$$Q_w = \frac{1}{N_{\mathrm{coll}}} \sum_{\mathrm{coll}} \frac{\delta \varepsilon}{\delta t} ,$$

$$\tilde{Q}_i = \frac{1}{N_{\mathrm{coll}}} \sum_{\mathrm{coll}} \frac{\delta(\varepsilon v_i)}{\delta t} ,$$

$$Q_{\langle ij \rangle} = \frac{1}{N_{\mathrm{coll}}} \sum_{\mathrm{coll}} \frac{\delta(v_{\langle i} v_{j \rangle})}{\delta t} ,$$

where $\delta(\ )$ indicates the variation of the quantity ( ) after and before the collision, δt is the time between two collisions, the summation runs over all scattering events, and N_{coll} is the number of collisions. We observe that, in order to avoid transient effects, we gather statistics for times greater than picoseconds and we run the simulation until a static and steady-state regime is reached.

The relaxation times for energy, momentum, heat flow, and shear are then obtained from Eqs. (24)–(27), and these are the standard definitions.[18,34] In order to compare the analytic results of Sec. VII we develop a Monte Carlo code for this purpose. We consider a parabolic band structure and acoustic-phonon and optical nonpolar scatterings for silicon at room temperature, as in Sec. VII.

In this work a homogeneous electric profile, frozen in the material along the x direction (1–80 000 V cm^{-1}) is

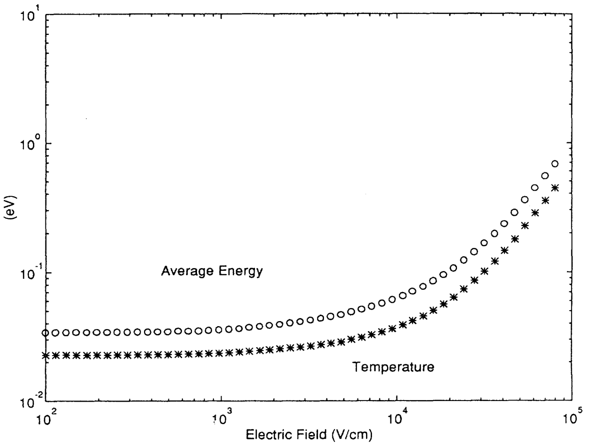

FIG. 4. Average energy and temperature obtained by Monte Carlo simulations for silicon vs electric field.

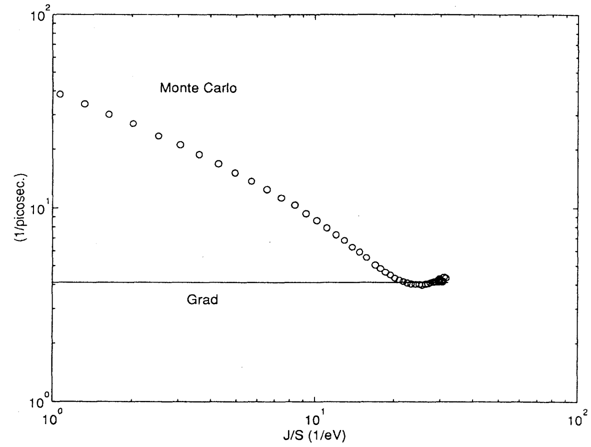

FIG. 6. $1/\tau_q$ vs J/S obtained by Monte Carlo simulations for silicon and Eq. (58) obtained by the Grad method.

considered, and the test device is unbounded. In Fig. 1 we show the relaxation times τ_w, τ_p, τ_q, and τ_σ as functions of energy, obtained with our Monte Carlo simulator: we notice that $\tau_p \ll \tau_w$, and that momentum is relaxed faster than energy. In Fig. 3 we plot the drift velocity obtained by the Monte Carlo simulation and the fluid model, and in Fig. 4 the average energy and temperature versus the electric field. In Eq. (17) the kinetic energy is negligible in comparison to the thermal energy ($\frac{3}{2}nk_BT$).

In Fig. 5 we plot $1/\tau_p$ versus S/J and in Fig. 6 $1/\tau_q$ versus J/S: these plots are not linear (although some authors claim they are[12]), i.e., in Eqs. (51) and (52) a, b and $\tilde{a}$, $\tilde{b}$ are not constant but they should be functions of T and N_i. Grad's method evaluates these quantities around global thermal equilibrium: the straight lines given by Eqs. (57) and (58) are tangent to the Monte Carlo data (Figs. 5 and 6).

A fitting of $1/\tau_p$ and $1/\tau_q$ can be obtained in this way:

$$\frac{1}{\tau_p} = a_0 + a_1\frac{T}{T_0} + a_2\frac{T^2}{T_0^2} + \left[b_0 + b_1\frac{T}{T_0} + b_2\frac{T^2}{T_0^2} \right] \frac{S}{J}, \tag{59}$$

$$\frac{1}{\tau_q} = \tilde{b}_0 + \tilde{b}_1\frac{T}{T_0} + \tilde{b}_2\frac{T^2}{T_0^2} + \left[\tilde{a}_0 + \tilde{a}_1\frac{T}{T_0} + \tilde{a}_2\frac{T^2}{T_0^2} \right] \frac{J}{S}, \tag{60}$$

where, if $J/S \leq 6.568\ \text{eV}^{-1}$,

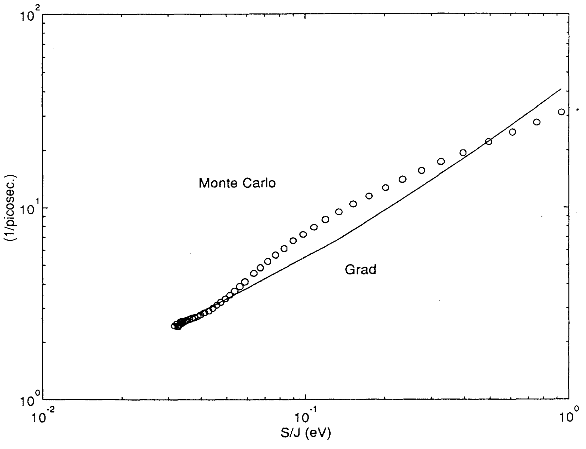

FIG. 5. $1/\tau_p$ vs S/J obtained by Monte Carlo simulations for silicon and Eq. (57) obtained by the Grad method.

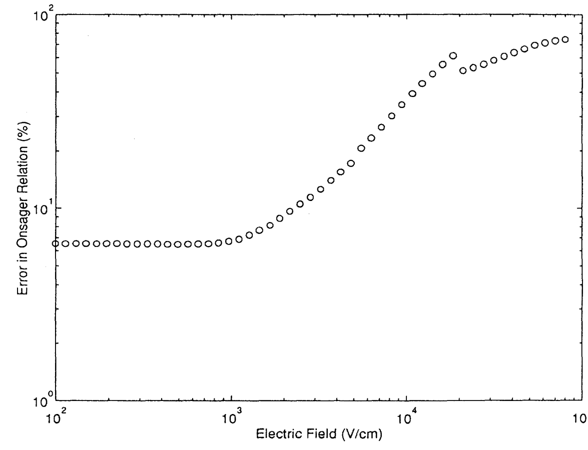

FIG. 7. Percent error in Onsager relation Eq. (34) obtained by Monte Carlo simulations for silicon vs electric field.

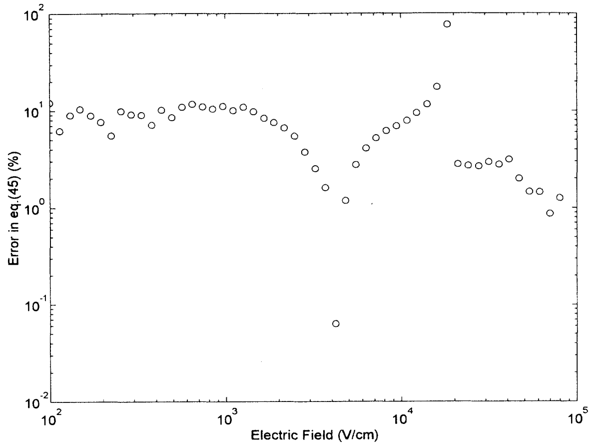

FIG. 8. Percent error in Eq. (45) obtained by Monte Carlo simulations for silicon vs electric field.

$$\tilde{a}_0=-0.6721,\quad \tilde{a}_1=2.4533,\quad \tilde{a}_2=0\ ,$$

$$\tilde{b}_0=-27.3229,\quad \tilde{b}_1=1.1622,\quad \tilde{b}_2=0\ .$$

Otherwise

$$\tilde{a}_0=-0.8712,\quad \tilde{a}_1=3.3903,\quad \tilde{a}_2=-2.581\ ,$$

$$\tilde{b}_0=-33.1229,\quad \tilde{b}_1=36.9863,\quad \tilde{b}_2=1.6339\ .$$

For the other coefficients, if $S/J \leq 0.1346$ eV, then

$$a_0=-11.0807,\quad a_1=33.7494,\quad a_2=-21.5443\ ,$$

$$b_0=-185.8055,\quad b_1=204.6364,\quad b_2=24.8215\ .$$

Otherwise

$$a_0=2.3104,\quad a_1=-6.4247,\quad a_2=0\ ,$$

$$b_0=163.2724,\quad b_1=-0.6763,\quad b_2=0\ .$$

The units of a_i and $\tilde{b}_i$ are in ps^{-1}, b_i in (ps eV)$^{-1}$, and $\tilde{a}_i$ in (eV ps^{-1}); T_0 is the room temperature.

With Eqs. (59) and (60) we checked the Onsager relation Eq. (34): in Fig. 7 we plot the percent error versus the electric field. We observe that the OPR is fulfilled only at low fields (≤ 5000 V/cm). In Fig. 8 we plot the percent error for Eq. (45): since this error is less than 10%, our fluid model is given by Eqs. (12)–(16). The closure Eqs. (19) and (20) and the relaxation times (59) and (60) and those for τ_w and τ_σ are self consistent.

IX. CONCLUSIONS

In this paper we have constructed a hydrodynamical model for electron transport in silicon which is consistent with the principles of linear irreversible thermodynamics. The details are as follows.

(i) The closure of the moment equations (at the level of the flux of the heat flux) is achieved by imposing the entropy principle and not by assuming any specific *ad hoc* expression for the distribution function.

(ii) The form of the production terms of the momentum, energy, and energy flux is such that at low energies the Onsager reciprocity principle is obeyed. Furthermore the conditions for the thermodynamical stability of the partial thermal equilibrium state are also satisfied.

(iii) The resulting system of partial differential equations (PDE's) is therefore equivalent to a symmetric hyperbolic one, and enjoys nice mathematical properties.[21]

The model we have constructed is consistent with (a) the results obtained by applying the Grad method near global thermal equilibrium, and (b) Monte Carlo simulations for silicon under stationary and homogeneous conditions.

In order to be a viable model for device calculations, our model must be tested against Monte Carlo simulations in nonstationary and inhomogeneous cases. Furthermore the model must be extended to cover the bipolar case (electrons and holes) according to the methods expounded in Ref. 16. Work along these lines is in progress and will be presented elsewhere.

ACKNOWLEDGMENTS

The authors wish to thank Dr. M. V. Fischetti for helpful discussion and comments. This work was partly supported by a contract with CORIMME (SgS-Thomson and University of Catania).

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