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Carrier Thermal Conductivity: Analysis and Application to Submicron-Device Simulation

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Within a correlation-function (CF) formalism, the kinetic coefficients of charge carriers in semiconductors are studied under different conditions. For the case of linear response in equilibrium, the transitions from the non-degenerate to the degenerate regimes as well as from ballistic to diffusive conditions are discussed within an analytical model. Generalizing the method to high-field transport in nondegenerate semiconductors, the CFs are determined by Monte Carlo (MC) calculations for bulk silicon from which the appropriate thermal conductivity has been obtained and included into the hydrodynamic code HEIELDS. For an n^+nn^+ submicron structure the temperature and velocity profiles of the carriers have been calculated with HEIELDS.

Keywords: Kinetic coefficients, hydrodynamic transport equations, correlation functions, Monte Carlo

1. INTRODUCTION

Thermal conductivity of charge carriers is of fundamental interest in describing transport phenomena in bulk materials as well as electronic devices. To provide a microscopic theory for this coefficient, the CF approach represents a very effective method [1]. As a consequence of the fluctuation-dissipation theorem, the carrier transport coefficients may be determined by the spectrum of the fluctuations in the system. Results for the thermal conductivity available in literature are mainly based on relaxation-time approximations [2, 3]. A weighting of the single relaxation time

with a power of the energy yields a generalization of the Wiedemann-Franz law (WFL) given by

$$\kappa = \left(\frac{5}{2} + c \right) \frac{k_B^2}{q} \mu n T, \quad (1)$$

where c is the so called power law exponent, μ is the mobility and T the electron temperature. This WFL together with the energy relaxation time is usually introduced within hydrodynamic approaches [4–8].

In this paper we present the appropriate set of CFs for the cases of linear response around thermodynamic equilibrium in the ballistic and

diffusive regime under different degeneracy conditions [9], as well as the hot-carrier regime in the classical-diffusive condition [10, 11] with its applications to the simulation of an n^+nn^+ -structure.

2. LINEAR RESPONSE REGIME

In the linear regime, generalized fluxes are the response of the material to generalized externally applied forces mediated by the kinetic (or Kelvin-Onsager) coefficients $L_{\mu\nu}$ according to

$$\mathbf{j}_\mu = \sum_\nu L_{\mu\nu} \mathbf{X}_\nu \quad (2)$$

with $\mu, \nu = 1, 2$, \mathbf{j}_1 and \mathbf{j}_2 denoting the electrical current and the energy-flux densities, respectively, while \mathbf{X}_1 and \mathbf{X}_2 are the generalized driving forces. The kinetic coefficients $L_{\mu\nu}(\omega)$ in general depend on angular frequency ω and are defined by means of the Fourier-Laplace transforms $S_{\mu\nu}(\omega)$ of the respective CFs $C_{\mu\nu}(t)$ from [12]:

$$L_{\mu\nu}(\omega) = \frac{V S_{\mu\nu}(\omega)}{k_B T} \quad (3)$$

where V is the volume, k_B is the Boltzmann constant, T the absolute temperature and:

$$S_{\mu\nu}(\omega) = \int_0^\infty d\omega C_{\mu\nu}(t) \exp(-i\omega t). \quad (4)$$

Here $C_{\mu\nu}(t)$ is the symmetrized CF at thermal equilibrium

$$C_{\mu\nu}(t) = \frac{1}{2} \langle \delta \mathbf{J}_\mu(0) \delta \mathbf{J}_\nu(t) + \delta \mathbf{J}_\nu(0) \delta \mathbf{J}_\mu(t) \rangle \quad (5)$$

where the $\delta \mathbf{J}_\nu(t) = \mathbf{J}_\nu - \langle \mathbf{J}_\nu \rangle$ denote the operators of the respective observed fluctuating quantities, and $\langle \dots \rangle$ indicates averaging with respect to the stationary statistical operator. The thermal conductivity κ is given as a function of the $L_{\mu\nu}$

$$\kappa(\omega) = \frac{L_{11}(\omega)L_{22}(\omega) - L_{12}(\omega)L_{21}(\omega)}{TL_{11}(\omega)}. \quad (6)$$

For a finite one-dimensional conductor of length ℓ limited by ideal (i.e. completely absorbing and thermalizing) contacts, if scattering is treated within the relaxation time approximation, the thermal conductivity κ can be calculated analytically showing the transitions both from ballistic to diffusive (with increasing ℓ) and from degenerate to non-degenerate (with increasing T) conditions. The static (i.e. $\omega = 0$) limiting cases are given by [9]

$$\kappa^{ndg,bl} = \frac{nk_B^2 T}{m} \tau_T^{ndg} = \frac{n\ell k_B^{3/2} T^{1/2}}{(2\pi m)^{1/2}}, \quad (7a)$$

$$\kappa^{dg,bl} = \frac{\pi^2 nk_B^2 T}{6m} \tau_T^{dg} = \frac{2\pi^2 \ell k_B^2 T}{3h}, \quad (7b)$$

$$\kappa^{ndg,df} = \frac{3nk_B^2 T}{2m} \tau_c, \quad (7c)$$

$$\kappa^{dg,df} = \frac{\pi^2 nk_B^2 T}{3m} \tau_c. \quad (7d)$$

Here $\tau_T^{ndg/dg}$ is the carrier transit time in the ballistic (*bl*) case under non-degenerate and degenerate conditions, respectively, while in the diffusive (*df*) cases τ_c denotes the relaxation time. Figure 1 shows the behavior of $\kappa(0)$ at fixed carrier density as function of ℓ and T . The maximum value is reached in the ballistic degenerate case.

3. FAR FROM EQUILIBRIUM (HOT-CARRIER) CASE

The CFs of microscopic fluxes are calculated with respect to stationary values at the given bias point and the thermodynamic temperature T is replaced by the noise-temperature spectrum $T_n(E, \omega = 0)$ [13] associated with velocity fluctuations at the given field E , where we restrict to the stationary case ($\omega = 0$). The thermal conductivity parallel to the applied electric field, $\kappa(E, \omega = 0)$, generalized to hot-carrier conditions is thus given by Eq. (6) with the following replacement:

$$T \Rightarrow T_n(E, \omega) = \frac{V \text{Re}[S_{11}(E, \omega)]}{k_B \text{Re}[\sigma_d(E, \omega)]}, \quad (8)$$

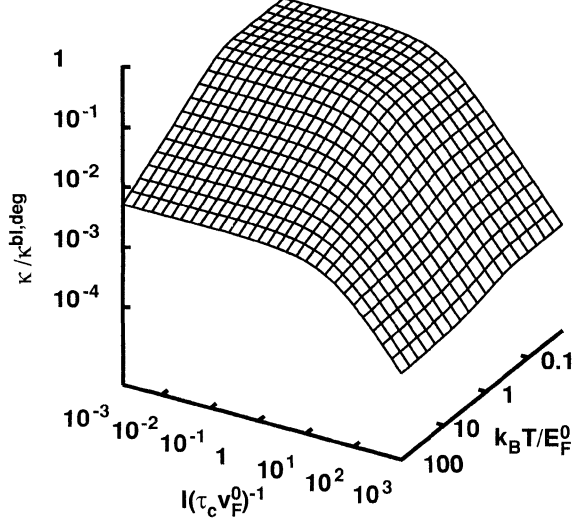


FIGURE 1 Thermal conductivity at zero frequency (normalized to its value in the ballistic degenerate case) at a fixed density n as a function of device length and temperature. $v_F^0(E_F^0)$ denote the Fermi velocity (Fermi energy) at $T=0$ K for the given density n and τ_c is the relaxation time.

where σ_d is the differential conductivity. Under thermal-equilibrium conditions (i.e. $E=0$) $T_n(\omega)=T$, and standard linear-response formalism is recovered [14]. The CFs and conductivities entering the definition of κ are calculated using MC simulations [15]. We have considered the case of extrinsic n -Si, doping concentration 10^{17} cm^{-3} , at $T=300$ K. Figure 2 from a) to d) reports the four longitudinal CFs $C_{\mu\nu}(t)$ (fluctuations of flux variable along the electric field direction) at increasing values of the electric field normalized to their respective initial values. At increasing fields the correlations decay faster. $C_{22}(t)$ shows the fastest decay, which indicates that its decay-rate is the sum of momentum and energy rates. Thus we see that even at thermal equilibrium an approach based on a single time-scale is very poor. We observe that the variances $C_{11}(0)$, $C_{22}(0)$ and $C_{12}(0)=C_{21}(0)$ increase systematically with increasing electric field, which is due to hot-carrier effects. Figure 3 reports the low frequency spectral densities $S_{\mu\nu}(E, \omega=0)$ of the respective CFs as a function of the electric field. Their different

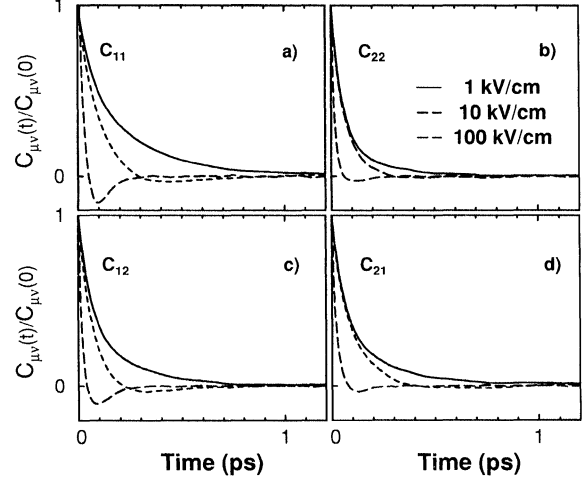


FIGURE 2 Longitudinal CFs normalized to their initial value for extrinsic n -Si with doping concentration $n=10^{17} \text{ cm}^{-3}$ at 300 K and increasing electric-field strengths of 1, 10, and 100 kV/cm.

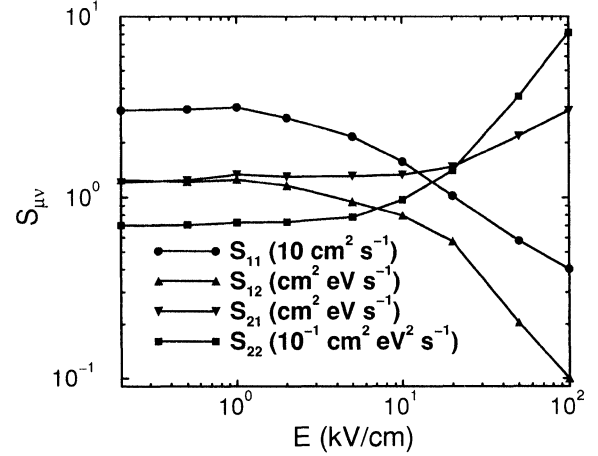


FIGURE 3 Spectral densities of the CFs of Figure 2; at $\omega=0$ as a function of electric-field strength.

behaviors are the result of the competitive effect between shortening time-scales and increasing variances of the corresponding CFs at increasing fields. The carrier thermal-conductivity at low frequency calculated from Eq. (6) is shown in Figure 4. It is compared to the values obtained from a parameterized WFL (1), for different values of the power law exponent. As can be noticed, the

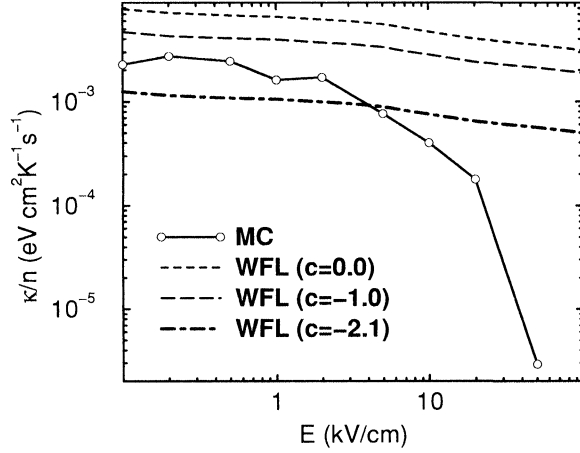


FIGURE 4 Thermal conductivity per unit concentration in n -Si at 300 K as a function of electric-field strength. The different curves are obtained by setting $c=0.0$, $c=-1.0$ and $c=-2.1$ in the WFL and by using the CF approach together with MC.

strong decrease at high fields may not be reproduced by a parameterized WFL.

4. DEVICE SIMULATIONS

To study the role of thermal conductivity in device simulation, the transport in a Si submicron n^+-n-n^+ structure has been analyzed by means of the hydrodynamic device simulator HFIELDS [16]. The simulated structure is the same n^+-n-n^+ diode analyzed in [17]: the high doped n^+ -regions have length $0.1\mu\text{m}$ and doping concentration $5 \times 10^{17}\text{cm}^{-3}$, the lower doped n -region has length $0.4\mu\text{m}$ and doping concentration $2 \times 10^{15}\text{cm}^{-3}$.

The electron mobility $\mu(\varepsilon)$ and energy-relaxation time $\tau_\varepsilon(\varepsilon)$ as a function of the mean electron energy ε , required in the hydrodynamic simulator, are calculated from the velocity and energy versus field curves obtained from MC simulations.

For the thermal conductivity both the models obtained from the results of MC simulations and from the parameterized WFL are adopted. In Figure 5 the velocity profile along the device obtained with different models of the thermal conductivity are shown. When the WFL (1) is applied, the spike in the electron velocity curve can

be remarkably reduced by setting the value of the power law exponent to $c=-2.1$; at the same time the velocity profiles is smoothed with respect to the MC solution presented in [17] for the same structure. This can be ascribed to the slow decrease of the WFL thermal conductivity with increasing electric field. The CF approach yields to a stronger dependence of the thermal conductivity on the electric field, which allows to obtain a better comparison with MC data. The carrier temperature profile is shown in Figure 6: also in this case the WFL approach tends to smooth the

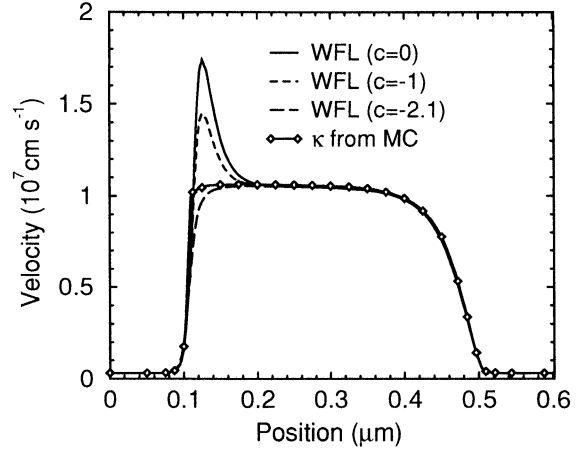


FIGURE 5 Velocity profile of the n^+-n-n^+ device calculated with four different thermal conductivities as shown in Figure 4.

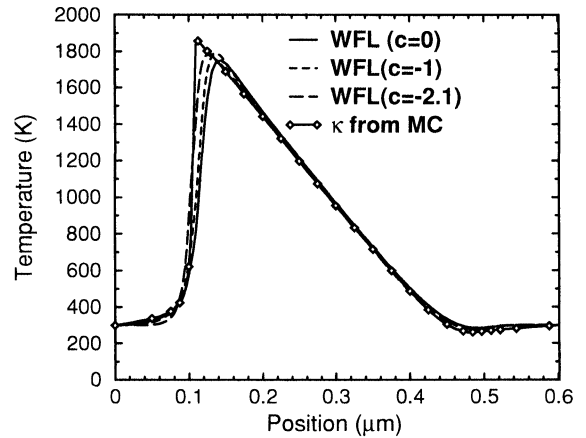


FIGURE 6 Temperature profile of the n^+-n-n^+ device for the cases as shown in Figure 5.

profile with respect to the case when the results of the CF method are applied.

5. CONCLUSION

We have shown that the CF formalism provides an effective method for calculating electronic transport parameters in different transport regimes. These parameters, calculated in the case of non-equilibrium and incorporated into the hydrodynamic simulator fields, allow for a description of the electronic behavior of submicron structures in agreement with the results of more sophisticated microscopic approaches.

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Tilman Kuhn, born 1959 in Alpirsbach (GERMANY), graduated in physics in 1984 and received the Ph.D. in physics from the University

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Paola Golinelli, born 1969 in Rivoli (ITALY), received the Dr. in Physics degree in 1995 from Modena University. Her main research activity has been the generalization of charge carrier thermal conductivity to hot-carrier conditions.

