Semicond. Sci. Technol. **12** (1997) 1511–1513. Printed in the UK PII: S0268-1242(97)84825-0

LETTER TO THE EDITOR

Hot-carrier thermal conductivity from the simulation of submicron semiconductor structures

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Received 4 June 1997, accepted for publication 9 September 1997

Abstract. We propose a novel numerical procedure to calculate the hot-carrier thermal conductivity in bulk semiconductors. The method is based on combining Monte Carlo and hydrodynamic simulations of carrier transport in submicron inhomogeneous structures. Application to a Si n^+nn^+ structure indicates a decrease over one order of magnitude of the thermal conductivity of electrons at electric fields over 10 kV cm^{-1}, in close agreement with recent results obtained within the correlation-function formalism.

The determination of hot-carrier thermal conductivity is an important issue in the modelling of submicron semiconductor devices. For this purpose, a phenomenological generalization of the Wiedemann–Franz law based on an electron temperature model and an energy-dependent relaxation time is usually introduced within hydrodynamic (HD) approaches [1–5]. However, the physical plausibility of such a phenomenological approach is questionable and the field dependence of thermal conductivity remains an open problem. Some authors [6, 7] have recently proposed a generalization of the definition of the carrier static thermal conductivity $\kappa(E)$ along the direction of the electric field $\boldsymbol{E}$ based on the correlation-function formalism which reads [7]

$$\kappa(E) = \frac{k_B n \mu_d^2(E)}{e^2} \frac{I_{11}(E)I_{22}(E) - I_{12}(E)I_{21}(E)}{I_{11}^3(E)} \qquad (1)$$

$$I_{\nu\mu}(E) = \int_0^\infty \overline{\delta j_\nu(0)\delta j_\mu(t)}\,\mathrm{d}t \qquad \nu, \mu \equiv 1, 2. \qquad (2)$$

Here k_B is the Boltzmann constant, e the electron charge, n the carrier concentration, $j_1 = v(\boldsymbol{k})$, $j_2 = v(\boldsymbol{k})\epsilon(\boldsymbol{k})$ ($v(\boldsymbol{k})$ and $v(\boldsymbol{k})\epsilon(\boldsymbol{k})$ being the carrier velocity and energy flux times unit volume along the field direction as functions of wavevector $\boldsymbol{k}$, $\mu_d(E)$ the differential mobility and $\delta j_\mu(t)$ the fluctuation of $j_\mu(t)$ around its average value). In equation (2) ergodicity is assumed so that the bar denotes time average. When applied to the case of n-Si at 300 K, the above formalism predicts for $\kappa(E)$ a dramatic decrease over one order of magnitude under hot-carrier conditions.

In the absence of direct measurements of $\kappa(E)$, the aim of this letter is to propose a numerical procedure able to evaluate this quantity from the analysis of its effects on the transport characteristics of spatially inhomogeneous structures. The comparison with the results which are independently obtained by equations (1) and (2) is taken as validation of the proposed procedure and direct confirmation of the physical reliability of calculations performed within the correlation-function formalism. For this purpose we consider a one-dimensional n^+nn^+ structure where the doping profile varies along the x direction. Under stationary conditions, velocity and energy conservation equations within the single-electron gas approximation take the form [8]

$$em^{-1}E - v\nu_v - v\frac{\partial v}{\partial x} - \frac{1}{n}\frac{\partial}{\partial x}[n\langle(\delta v)^2\rangle] = 0 \qquad (3)$$

$$evE - (\epsilon - \epsilon_{th})\nu_\epsilon - v\frac{\partial \epsilon}{\partial x} - \frac{1}{n}\frac{\partial}{\partial x}(n\langle\delta v\delta\epsilon\rangle) = 0 \qquad (4)$$

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where n, v, ϵ and E are, respectively, the profiles along the x direction of carrier concentration, average velocity, average energy and electric field; ϵ_{th} is the average carrier energy at thermal equilibrium, m^{-1} the average reciprocal effective mass, ν_v and ν_ϵ the velocity and energy relaxation rates; $\langle(\delta v)^2\rangle$ and $\langle \delta v\, \delta\epsilon\rangle$ are the velocity variance and velocity-energy covariance, respectively. While the field (or energy) dependence of m^{-1}, ν_v and ν_ϵ can be calculated from Monte Carlo (MC) simulations of the bulk material [8, 9], $\langle(\delta v)^2\rangle$ and $\langle \delta v\, \delta\epsilon\rangle$ are higher-order moments of the corresponding conservation equation which must be assigned independently and constitute the closure condition of equations (3) and (4). A reasonable closure condition is the use of the approximations $\langle(\delta v)^2\rangle \simeq \langle(\delta v)^2\rangle_0$ and $\langle \delta v\, \delta\epsilon\rangle \simeq \langle \delta v\, \delta\epsilon\rangle_0$ where $\langle\ \rangle_0$ indicates an average for the the bulk material at the given applied field (or carrier average energy) and thus directly obtainable from MC simulations [8, 9]. While $\langle(\delta v)^2\rangle_0$ can be well justified [9], $\langle \delta v\, \delta\epsilon\rangle_0$ does not account appropriately for energy-gradient effects [9]. These last are usually accounted for by adding to $\langle \delta v\, \delta\epsilon\rangle_0$ an extra term such that $\langle \delta v\, \delta\epsilon\rangle$ is written as [1]

$$\langle \delta v\, \delta\epsilon\rangle = \langle \delta v\, \delta\epsilon\rangle_0 - \frac{\kappa_\epsilon(E)}{n}\frac{\partial \epsilon}{\partial x} \tag{5}$$

where $\kappa_\epsilon(E) = (2/3k_B)\kappa(E)$ is a carrier thermal conductivity independent of lattice heating at the given electric field measured in units of diffusivity per unit volume. Due to this phenomenological incorporation, there is no way to obtain an independent calculation of $\kappa(E)$ under hot-carrier conditions. Therefore, in recent years several authors [1–5] have developed different approaches to provide values of $\kappa(E)$ in terms of a phenomenological generalization of the Wiedemann–Franz law.

To check the reliability of the values of $\kappa(E)$ so obtained and, hence, the validity of the related assumptions, we propose the following procedure which is here applied to the case of electrons in Si at 300 K. The spatial profiles of $\langle \delta v\, \delta\epsilon\rangle$ in a submicron n^+nn^+ structure are calculated with MC simulations [10, 11]. Near the anode homojunction a local spike of $\langle \delta v\, \delta\epsilon\rangle$ associated with the strong gradient of the carrier mean energy can be related to $\kappa(E)$ via the decomposition given in equation (5). To this purpose, by using the HD approach of equations (3) and (4) with the energy-dependent parameters obtained from the MC approach, but neglecting thermal conductivity effects, we calculate the energy profile of the carriers in the structure. Then, the corresponding $\langle \delta v \delta\epsilon_0\rangle$ profile is obtained. Figures 1 and 2 report the profiles of the $\langle \delta v\, \delta\epsilon\rangle$ and $\langle \delta v\, \delta\epsilon\rangle_0$ calculated with the MC and HD simulations, respectively. From figures 1 and 2 we conclude that the presence of the local spike in $\langle \delta v\, \delta\epsilon\rangle$ at the n^+n homojunction is associated with the contribution of $\kappa(E)$ which, in turn, can be quantitatively estimated using equation (5). There, $\langle \delta v\, \delta\epsilon\rangle$ and $(1/n)\partial\epsilon/\partial x$ are obtained from MC and $\langle \delta v\, \delta\epsilon\rangle_0$ from the corresponding HD simulation.

Figure 3 reports a typical result of the present procedure for an applied voltage of 1.5 V. We notice that the region near the anode nn^+ junction, where $\partial\epsilon/\partial x$ is maximum, is the most sensitive to the effects of thermal

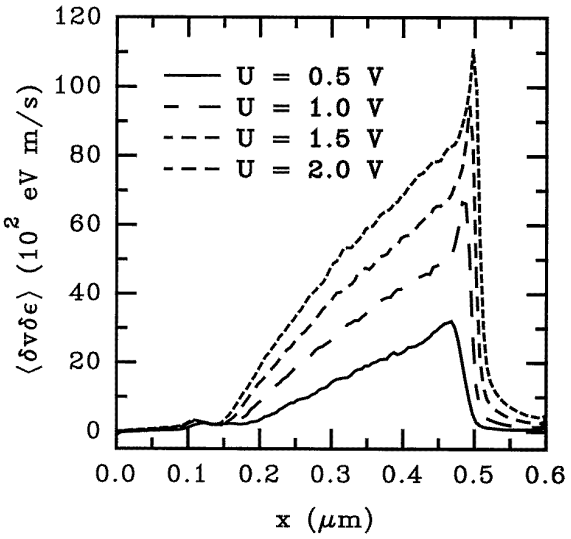

Figure 1. Spatial dependence of the covariance of the velocity–energy fluctuations calculated with a MC approach for a 0.1–0.4–0.1 μm n^+nn^+ Si structure with doping levels $n = 2 \times 10^{15}$ cm^{-3} and $n^+ = 5 \times 10^{17}$ cm^{-3} at $T = 300$ K and applied voltages of 0.5, 1.0, 1.5 and 2.0 V. Results refer to an electric field applied along the ⟨111⟩ crystallographic direction.

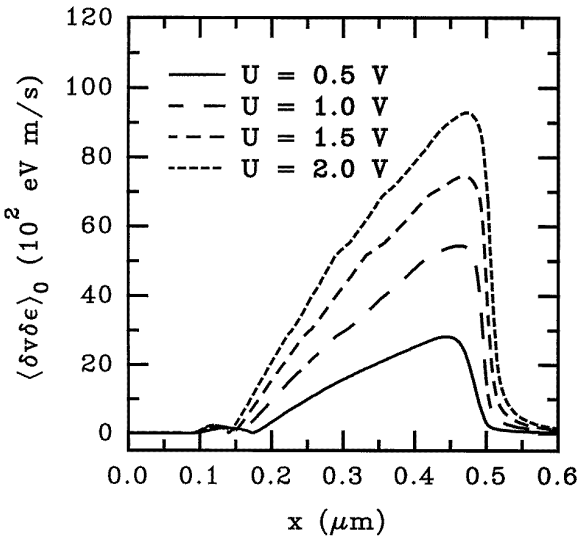

Figure 2. Spatial dependence of the covariance of the velocity–energy fluctuations calculated with a HD approach which neglects thermal conductivity effects for the same structure and conditions as figure 1.

conductivity, thus allowing one to pick up a local value of $\kappa(E)$. Accordingly, the value of the electric field at this point is associated with the value of $\kappa(E)$ and the field dependence is obtained by repeating the procedure at various applied voltages. The comparison between the values of $\kappa(E)$ obtained from equations (1) and (2) and those calculated from the above simulative procedure is reported in figure 4. Here we show results for the two orientations ⟨100⟩ and ⟨111⟩ of the electric field with respect to the crystallographic directions where anisotropic

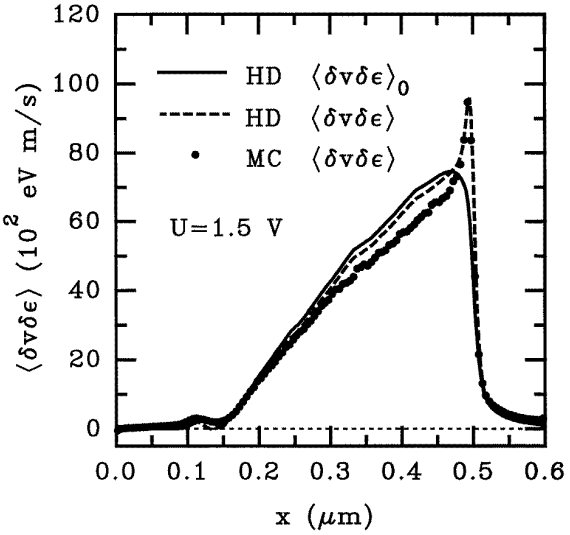

Figure 3. Spatial dependence of the covariance of the velocity–energy fluctuations calculated with HD ($\langle \delta v\, \delta\epsilon \rangle_0$), MC ($\langle \delta v\, \delta\epsilon \rangle$) and HD plus thermal-conductivity corrections. Calculations refer to the same structure and conditions as figures 1 and 2 and an applied voltage of 1.5 V.

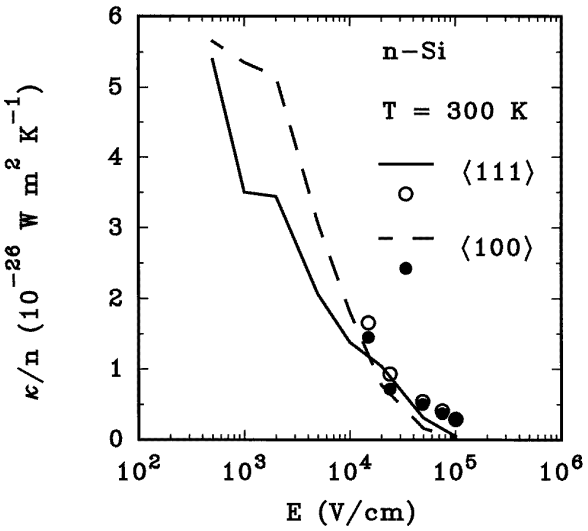

Figure 4. Longitudinal thermal conductivity per unit concentration of electrons in Si at T = 300 K as a function of electric-field strength. Curves refer to calculations performed for electrons in bulk Si using the correlation function formalism; points represent results obtained with the mixed MC–HD calculations applied to an n^+nn^+ structure and using equation (5). The full curve and open circles, and the dashed curve and full circles refer to the electric field applied along the ⟨111⟩ and ⟨100⟩ crystallographic directions, respectively.

characteristics, associated with the many-valley conduction band of Si, are expected. By requiring a strong energy gradient, the present procedure enables us to obtain values of $\kappa(E)$ only in the high field region above 10 kV cm^{-1}. Here, calculations show evidence of a dramatic decrease over one order of magnitude of $\kappa(E)$, which is found to compete with the sharp increase in the local energy gradient. Furthermore, anisotropic effects are found to play a minor role. At the highest fields the correlation function formalism predicts a negligible value of $\kappa(E)$ since here the drift velocity saturates. The non-smoothing of the curves in figure 4 illustrates the numerical uncertainty, which we estimate to be within a factor of two at worst. Overall the agreement is considered to be satisfactory and such as to validate the numerical procedure suggested here and to confirm the theoretical results predicted by the correlation-function formalism.

This work has been performed within the Lithuanian Project 'Research and Development Cooperation in Submicron Electronics' supported by the Italian Foreign Ministry. Partial support from the NATO networking linkage grant HTECH.LG 960931 and the Comisión Interministerial de Ciencia y Tecnología through the project TIC95-0652 is gratefully acknowledged.

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