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Thermal conductivity of nonequilibrium carriers

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Abstract

We present a theoretical analysis of the thermal conductivity of charge carriers in semiconductors under nonequilibrium conditions due to an applied electric field. The theory is based on a correlation-function formalism which directly relates this kinetic coefficient to four spectral densities involving carrier velocity and energy flux fluctuations. Monte Carlo calculations performed for the cases of p-Si and n-GaAs give an evidence of a strong dependence of the thermal conductivity on increasing electric fields.

Keywords: Thermal conductivity; Correlation functions; Monte Carlo Calculations; Energy transport

1. Introduction

Thermal conductivity of charge carriers represents one of the relevant kinetic coefficients resulting from the motion of carriers under the action of a temperature gradient [1]. In contrast to other kinetic coefficients, its dependence on the applied electric field has received minor attention from the semiconductor community. This can be attributed in part to a greater interest in the electrical than in the thermal properties, and in part to the difficulty in providing the experimental counterpart of the theoretical calculations due to the prevailing contribution of the lattice over that of the charge carriers. It must be stressed however that a detailed analysis of energy flux phenomena in semiconductors is a mandatory issue of to-date small-device modelling: as a matter of fact quite different electrical characteristics have been predicted according to the specific model used for the nonequilibrium thermal conductivity [2].

The most straightforward method to obtain kinetic coefficients consists in modelling the linear response of the system to weak external perturbations such as electric field, gradient of temperature, gradient of chemical potential, magnetic field, etc. On the other hand, one can take advantage of the fluctuation–dissipation relation [3] to obtain these coefficients from the knowledge of an appropriate set of correlation functions without including

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the external perturbation. While for the case of the electrical conductivity the generalization to the nonequilibrium regime of the fluctuation–dissipation relation was provided more than 30 years ago [4], it has not been the case for thermal conductivity, where nonequilibrium calculations have been addressed by making use of phenomenological generalizations of the Wiedemann–Franz law using relaxation–time approximations [2].

2. Theory

To evaluate the thermal conductivity $\kappa(E,\omega)$ of nonequilibrium carriers as a function of electric field E and angular frequency ω we use the expression proposed in Ref. [5]:

$$k(E,\omega) = \frac{n}{K_B T_x^2(E,\omega)} \times \frac{I_{v-v}(E,\omega) I_{v\varepsilon-v\varepsilon}(E,\omega) - I_{v-v\varepsilon}(E,\omega) I_{v\varepsilon-v}(E,\omega)}{I_{v-v}(E,\omega)}, \quad (1)$$

where n is the carrier concentration, K_B the Boltzmann's constant, I_{x-y} the spectral densities involving the fluctuations of single carrier velocity v and energy flux $v\varepsilon$ and T_x an appropriate temperature associated with the nonequilibrium stationary condition of the carrier system. Actually, the two plausible choices for T_x are: (i) the electronic temperature T_e associated with the average carrier energy, or (ii) the noise temperature T_n (by analogy with the well-known Price relation [4]). The different spectral densities entering Eq. (1) can be computed by Fourier transforming the corresponding correlation functions obtained from a standard Monte Carlo simulation of the nonequilibrium system at the given field.

3. Results

We have performed Monte Carlo calculations for the case of p-Si and n-GaAs, respectively. Being directly related to the time integration of the corresponding correlation function, the dependence of the low-frequency value of each spectral density on field results from the competition between the change in the associated variance (where the trend is to increase with field) and the change in the correlation time (where the trend is to decrease with field). It must be noted that in the case of GaAs the increase of the variances is significantly slowed down when a significant fraction of carriers start to populate higher valleys. Moreover, for both materials the nonequilibrium correlation functions exhibit in general a quite complicated (i.e. nonexponential) behavior reflecting the presence of several time scales (velocity, energy, etc.). The spectral density I_{v-v} at low frequency (basically the diffusion coefficient) decreases with field for both materials, thus revealing the dominant effect of the decrease in the correlation time. An analogous behavior is also found for the cross-correlation spectral density $I_{v-v\varepsilon}$ which is associated with the response of the energy flux to an initial stochastic fluctuation of velocity. However, while I_{v-v} is always a positive quantity under far nonequilibrium conditions $I_{v-v\varepsilon}$ can become negative. The other couple of spectral densities, $I_{v\varepsilon-v\varepsilon}$ and $I_{v\varepsilon-v}$, exhibits similar behaviors, both being related to the response of the system to an initial stochastic fluctuation of the energy-flux. At low fields both increase, thus revealing the dominant effect of the increase in the variance. This behavior persists in the high-field region for the case of Si. On the contrary, in GaAs, for fields higher than the threshold value for negative differential mobility, the two spectral densities decrease due to the predominant influence of the shortening of the correlation time.

Fig. 1 reports the thermal conductivity of charge carriers for the case of p-Si (a) and n-GaAs (b) calculated using the electronic temperature and the noise temperature alternatively. At the lowest fields the two temperatures coincide with that of the lattice and the equilibrium value of κ is recovered in agreement with the Wiedemann–Franz law. At the highest fields, in the case of Si, when using T_n we found a dramatic decrease of κ mainly due to the strong increase of the noise temperature associated with a tendency towards the saturation of the drift velocity. By contrast, when using T_e κ is found to slightly increase because the increase of T_e is

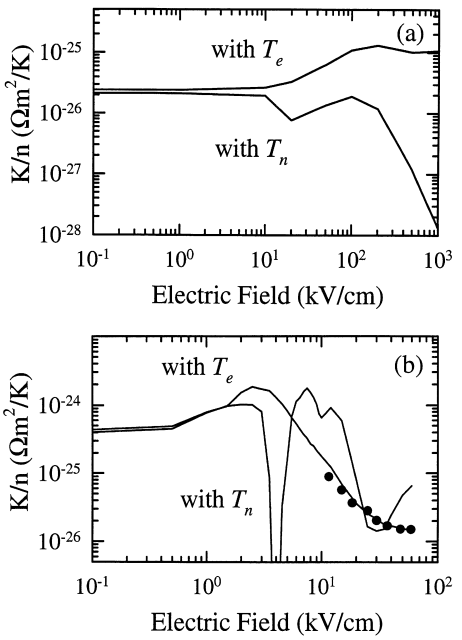

Fig. 1. Thermal conductivity calculated by a Monte Carlo simulation of p-Si (a) and n-GaAs (b) as a function of the electric field strength at $T = 300$ K and with a carrier concentration of 10^{17} cm^{-3}. The dots in Fig. 1(b) report the value of an independent calculation performed with the method of Ref. [6].

significantly weaker than that of T_n. For the case of GaAs the high field region is complicated by the presence of negative differential mobility: as a matter of fact, when approaching the threshold field the noise temperature diverges, thus leading κ to vanish. For fields higher than the threshold value the noise temperature is negative and the definition of a thermal conductivity remains an open problem. We also remark the difficulty in the numerical calculation of T_n due to a vanishing differential conductivity. In any case, the application of Eq. (1) under these extreme conditions is found to provide plausible results. Here, the use of T_e instead of T_n produces a smoother behavior of κ in the threshold region but the main features remain similar. Fig. 1(b) also reports an estimation of κ made from a microscopic analysis of an n^+nn^+ structure using the procedure developed in Ref. [6]. The excellent agreement found with the T_e model confirms the plausibility of the proposed theoretical approach.

4. Conclusions

By using the correlation function approach the main features of the nonequilibrium thermal conductivity are directly traced back to the microscopic fluctuation spectra of the velocity and energy flux of single carriers, thus overcoming too simple relaxation-time approximations. The calculated thermal conductivity shows significant deviations from its equilibrium value as a direct consequence of the strong dependence on the field exhibited by the variances and the several time scales entering these correlation functions. A problem which remains open concerns with the choice of the nonequilibrium temperature appearing in the definition of thermal conductivity. The result of an independent estimation of the thermal conductivity based on a hydrodynamic-like simulation is in good agreement with our calculation, thus confirming, in the absence of more direct experimental data, the validity of the proposed approach.

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