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Heat transport in semiconductor crystals under large temperature gradients

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ABSTRACT

We analyze and discuss the fundamental behavior of the nonlocal/nonlinear contributions to heat transport by phonons in bulk cubic semiconductor (SC) crystals subject to large temperature gradients. The calculation approach is based on solving steady-state Boltzmann-Peierls Transport Equation (BPTE) by expanding the phonon distribution function in a series of temperature gradients. We work out the modeling within the framework of the single relaxation time approximation and using modified Debye-Callaway model in which both longitudinal and transverse phonon modes are included explicitly. The SC system is treated as a continuum, elastic, isotropic and dispersionless medium. The frequency and temperature dependences of three-phonon anharmonic Normal and Umklapp scattering processes are kept the same for all SC crystals. Our model allows us to obtain compact expressions for the first three nonlocal/nonlinear thermal coefficients to which we limit our calculations. We assume these three coefficients to be the leading ones over the whole temperature range considered in our study. Their fundamental behaviors are studied by changing ambient temperature, longitudinal and transverse Grüneisen parameters as well as the mass-fluctuation parameter. In the simplest case of the grey spectrum approximation, we shed light on a very interesting result regarding the expression of the effective thermal conductivity κ_{eff} of the bulk SC crystal when the latter is subject to a space-periodic temperature profile that is typically encountered in Transient Thermal Grating (TTG) experiments. We find an expression that undoubtedly proves both nonlocality and nonlinearity to be a sound and robust explanation of the reduced measured thermal conductivity that was reported in TTG experiments.

1. Introduction

Due to the continuous development in nanotechnology and the rapid evolution in the synthesis and fabrication of different materials at a nanometer scale, understanding and controlling heat transport at very short length scales has become very crucial and challenging. Indeed, the length scales at which heat transport starts taking place in all types of conductor materials; metals, semiconductors (SC) and dielectrics, are undertaking a continuous reduction to almost approach the intrinsic characteristic microscopic lengths of the material [1,2]. For the purpose of heat transport, the main characteristic intrinsic length is the mean free path (MFP) of the energy carriers (electrons in metals and phonons in SC crystals and dielectrics) [3]. Usually, a local/linear theory of heat transport is valid as long as the MFP is short compared to the spatial variations in temperature. Nevertheless, because of the reduction of the length scales, the resulting temperature gradients due to an imposed temperature disturbance in many operation conditions can become very large, therefore setting limits to the applicability of the conventional local/linear nonequilibrium thermodynamics theory. In such case scenarios, the nonlocal/nonlinear contributions to heat transport might become of a certain importance.

The question of energy and heat transport mechanisms in solid materials at short time and length scales has been the basis of numerous theoretical and experimental papers. A part of the research has continued to exploit the conventional local/linear nonequilibrium thermodynamics theory [4–17], while the second part, has considered going beyond this theory and has investigated the nonlocal/nonlinear effects in the presence of large temperature gradients using different approaches [18–32].

The current work was inspired by the papers of Grigorenko et al. [20,21]. We follow the approach initially developed by these authors to study the nonlinear thermoelectric phenomena in metals under large temperature gradients. Despite the large thermal conductivity, that characterizes metals in general, large temperature gradients can take place in some experiments, particularly

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of surface laser heating. In their analysis, the authors applied their approach to electron transport in metals and were able to explain the Benedick's effect that was observed in some experiments [20,21]. SC crystals have a lower thermal conductivity than metals [1,2]. Hence, the onset of large temperature gradients after excitation by a certain heating source in these crystals, is even more likely than in metals. We shall apply the same approach to analyze the relevance of the nonlocal/nonlinear contributions to heat transport by phonons in SC crystals, and therefore go beyond the conventional Fourier's law in the steady-state regime. Our motivation is to present an approach within the frame work of Boltzmann kinetic theory of phonon transport using the Callaway approximation of the collision operator in order to calculate and develop compact formulas that capture the fundamental leading behavior of the first three nonlocal/nonlinear thermal coefficients which will shed light on the effect of different intrinsic and extrinsic parameters of heat conduction. It is worthwhile mentioning that a closely related approach than the one we are adopting has been worked out very recently to shed light onto the nonlinear transport of electrons [33].

We present the main steps of the theoretical modeling in Section 2. In Section 3, we discuss the results of this approach by analyzing the effect of varying different intrinsic and extrinsic parameters of bulk SC crystals. We also provide a detailed analysis, in the simplest case of the grey spectrum approximation, of the effective thermal conductivity of the bulk SC crystal when the latter is subject to a space-periodic temperature profile that is typically encountered in Transient Thermal Grating experiments [12,15]. We finish with summary and concluding remarks in Section 4.

2. Theory

In this section, we present the method that allows deriving compact expressions of the first three nonlocal/nonlinear thermal coefficients of bulk cubic SC crystals that give an insight onto the leading behavior in their responses in the steady-state regime. We assume the temperature profile to vary in only one dimension. This approximation applies well to many experimental situations and permits obtaining a flexible and rather smooth analysis, as we shall see below.

2.1. Boltzmann-Peierls transport equation

The starting point of our modeling is Boltzmann-Peierls Transport Equation (BPTE) in the framework of the single relaxation time approximation and using modified Debye-Callaway model in which both longitudinal and transverse phonon modes are included explicitly [34–36]. The SC system is assumed to have a cubic symmetry and is treated as a continuum, elastic and isotropic medium characterized by a linear (Debye-like) phonon spectrum for each phonon polarization branch. Despite its simplicity, Debye-Callaway model has been proven to be very robust and effective in the study and the prediction of the temperature behavior of the thermal conductivity of SC crystals within the conventional local/linear nonequilibrium thermodynamics theory [34–36].

We assume application of a temperature disturbance along the direction $\vec{x}$, In addition, we will assume local thermal equilibrium throughout, without which a temperature cannot be defined [3]. Under the relaxation time approximation, the steady-state Callaway form of the BPTE along the x axis, for a phonon distribution function $n_S(x,q,t) \equiv n_{q,S}$ is given by:

$$v_{S,q_x}\frac{\partial n_{q,S}}{\partial x} = \frac{n_{q,S}^{\lambda_S} - n_{q,S}}{\tau_{q,S}^{N}} + \frac{n_{q,S}^{0} - n_{q,S}}{\tau_{q,S}^{R}} \tag{1}$$

where $n_{q,S}^{0} = \left(e^{\hbar\omega_S(q)/k_BT} - 1\right)^{-1}$ is the equilibrium phonon Planck distribution function to which resistive phonon scattering processes (all scattering processes that change the total phonon wave vector: Umklapp, boundary, defects, imperfections) tend to return the phonon system with a single relaxation time $\tau_R(q,S)$. $\omega_S(q)$ is the dispersion relation of the phonon in state (q, S), k_B and T are the Boltzmann constant and the absolute local temperature, respectively. On the other hand, the distribution function, which is stationary for N-processes (scattering processes that don't change the total phonon wave vector) is not $n_{q,S}^{0}$ but rather $n_{q,S}^{\lambda_S} = \{\exp[(\hbar\omega_S(q) - \lambda_S q)/k_BT] - 1\}^{-1}$. N-processes lead the phonon system to a displaced (*drifted*) Planck distribution function $n_{q,S}^{\lambda_S}$ with a single relaxation time $\tau_N(q,S)$, where λ_S has the dimension of a velocity times Planck constant $\hbar$ [34–36]. Here we assume the heat transport to be in the same direction as the applied temperature disturbance.

Following the approach of Grigorenko et al. [20,21], we expand $n_{q,S}$ in a series of temperature gradients:

$$n_{q,S} = n_{q,S}^{0} + \sum_{i\geqslant 1} g_{q,S}^{(i)} \tag{2}$$

As it is customary in Callaway analysis [34–36], the λ_S is assumed to have a very small module. Then, to first order in λ_S, the Taylor's series expansion of $n_{q,S}^{\lambda_S}$ such that $O(\lambda_S^2)$ is neglected, gives:

$$\begin{cases} n_{q,S}^{\lambda_S} \equiv n_{q,S}(\lambda_S) \cong n_{q,S}(0) + f_{q,S}^{(1)} \\ f_{q,S}^{(1)} = \lambda_S\left(\frac{\partial n_{q,S}(\lambda_S)}{\partial \lambda_S}\right)_{\lambda_S=0} = \frac{(\lambda_S q)T}{\hbar\omega_{q,S}}\frac{dn_{q,S}^{0}}{dT} \end{cases} \tag{3}$$

where $\lambda_S = -\hbar\beta_S v_{S,q_x}^2(\partial T/\partial x)/T$ and β_S is Callaway parameter that has the dimension of a relaxation time [34–36].

Since we are dealing with Debye-like phonon dispersion relation, so that one considers heat transport due only to acoustic phonons, we have [34–36]:

$$\lambda_S q = -\hbar\omega_{q,S}\beta_S v_{S,q_x}\left[\frac{\partial T/\partial x}{T}\right] \tag{4}$$

It is worthwhile mentioning here that even though, the expression of the drift velocity $\lambda_S/\hbar$ of a phonon (q, S) is proportional to $(\partial T/\partial x)/T$, the proportionality constant is too small over almost the whole temperature range considered in our study. This is due to the smallness of Callaway pseudo-relaxation time β_S [34,35]. Therefore, there is no need to use higher orders in the Taylor's expansion of $n_{q,S}^{\lambda_S}$ even for very high values of $(\partial T/\partial x)/T$. By multiplying the latter with the effective MFP of the phonon l_{eff}, one obtains a dimensionless parameter $\xi = l_{eff}(\partial T/\partial x)/T$ that can be used as a measure of the deviation from local equilibrium [20,21].

Now we insert Eqs. (2) and (3) into Eq. (1) and we compare the terms of the same order in both parts of the expression. After some algebra, we obtain the following hierarchical system of differential equations in which we keep terms up to the third order. We assume these terms to be the leading ones over the whole temperature range considered in our study:

$$\begin{cases} v_{S,q_x}\frac{\partial n_{q,S}^{0}}{\partial x} = -\frac{g_{q,S}^{(1)}}{\tau_{q,S}^{C}} + \frac{f_{q,S}^{(1)}}{\tau_{q,S}^{N}} \\ v_{S,q_x}\frac{\partial g_{q,S}^{(1)}}{\partial x} = -\frac{g_{q,S}^{(2)}}{\tau_{q,S}^{C}} \\ v_{S,q_x}\frac{\partial g_{q,S}^{(2)}}{\partial x} = -\frac{g_{q,S}^{(3)}}{\tau_{q,S}^{C}} \end{cases} \tag{5}$$

where $(\tau_{q,S}^{C})^{-1} = (\tau_{q,S}^{R})^{-1} + (\tau_{q,S}^{N})^{-1}$ is the "combined" relaxation time [34–36].