ROLE OF NONLINEARITY OF THE PHONON DISPERSION RELATION IN THE WAVE-TYPE PHONON HEAT TRANSPORT

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Abstract.

The heat transport in non-metallic micro- and nanostructures is predominantly due to phonon processes, and therefore it can be analysed in terms of a flow of a phonon gas. Phonons are quantized lattice vibrations characterized by wave-vectors $\boldsymbol{k}$ from the first Brillouin zone and by the $\boldsymbol{k}$ dependent frequency ω. For simplicity, a single-branch phonon model is adopted, and consequently phonon polarizations are neglected. The dispersion relation $\omega(\boldsymbol{k})$ together with the relaxation times associated with normal and resistive phonon scattering processes determine the behaviour of a phonon gas.

According to [1, 2, 3], the commonly used linear isotropic approximation of the phonon dispersion relation $\omega(\boldsymbol{k}) = c\,|\boldsymbol{k}|$ employed in the phonon gas hydrodynamics leads to the constant speeds of thermal waves propagating into the region in thermal equilibrium. This contradicts the experimental results on the second sound propagation in solids. The dependence of the second sound wave speed on the sample temperature has been analysed in [4].

The nonlinearity of the phonon dispersion relation significantly influences the thermal properties of micro- and nanostructures. Several forms of the nonlinear phonon dispersion relation $\omega(\boldsymbol{k})$ have been suggested for various structures and substrates in the literature, motivated either by empirical data or by the first-principle calculations. In micro- and nanostructures, the wave-type heat transport has been observed at low and elevated temperatures with temperature dependent propagation speeds. Hence, the phonon gas hydrodynamics employing the linear isotropic approximation of phonon dispersion relation seems to be inadequate in such cases.

The four-moment phonon gas hydrodynamics involving a nonlinear isotropic phonon dispersion relation $\omega(\boldsymbol{k}) = \omega(|\boldsymbol{k}|)$ and the maximum entropy phonon distribution function has been proposed in [1], and further developed in [5]. The governing conservation equations for energy and the quasi-momentum (understood as a vector internal state variable) are determined by the entropy function and by the additional scalar potential. Both, the entropy function and the additional potential are given by integral formulae involving the nonlinear isotropic phonon dispersion relation. Approximation of the finite domain of phonon wave-vectors by whole space R^3 eliminates the additional potential and simplifies the form of conservation equations. For this approximation, the propagation of the waves of weak discontinuity into the region in thermal equilibrium has been analysed in [6], and the dependence of the wave speeds on the temperature in a region ahead the wave front has been determined.

In order to compare predictions of the theory derived in [5, 6] with the second sound experimental data [4], the nonlinear isotropic phonon dispersion relation $|\boldsymbol{k}| = \omega\, c^{-1}\,(1+b\,\omega^2)$ proposed in [7] is adopted. For the values of the parameters c and b for NaF and Bi given in [7, 8, 9, 10], the dependence of the speed of weak discontinuity wave on the temperature ahead the wave front has been calculated and compared with the experimentally measured second sound velocity as a function of the sample temperature [4], and with the calculations based on the alternative second sound theory given in [11, 12]. Our results are in good agreement with the experimental data as well as with the predictions of [11, 12], and show that the nonlinearity of the phonon dispersion relation plays the crucial role in the effect of temperature dependence of thermal wave speeds.

In the same way, other nonlinear isotropic phonon dispersion relations proposed in the literature for specific

nanostructures can be used in the phonon gas hydrodynamics given in [5, 6]. Moreover, this hydrodynamics can be easily reformulated for two-dimensional non-metallic materials.

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