

## WAVE AND DIFFUSIVE PHONON HEAT TRANSPORT IN DIELECTRICS AND SEMICONDUCTORS UNDER HIGH THERMAL LOADS

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**Abstract** The new types of heat transport equations for transient processes in dielectrics and semiconductors under high thermal loads are derived from the microscopic, kinetic-theory description of a phonon gas. The modified Grad expansion method is applied to the relaxation time approximation of the Boltzmann-Peierls equation in order to derive a wave hyperbolic nine-moment system. The diffusive parabolic four-moment system is obtained by means of a similar modification of the Chapman-Enskog expansion method applied to the same kinetic model. Both modifications are based on expansions of the phonon distribution function about a nonequilibrium anisotropic Planck distribution, thereby admitting arbitrarily large heat fluxes and conforming to the time scales of the phonon gas relaxation processes.

In many modern technological applications, high transient thermal loads are applied to dielectric and semiconducting materials. It is well recognized that, in those cases, neither the classical Fourier law nor the Maxwell-Cattaneo-Vernotte heat wave equation accurately predict the thermal response of the material. Since the heat transport by phonons (quanta of a crystal vibrational energy) predominates in dielectrics and semiconductors, the suitable heat transport equations should be derived in some way from the microscopic, kinetic-theory description of a phonon gas. Hence, we consider the Boltzmann-Peierls equation governing the phonon distribution function and assume the commonly used Callaway's relaxation time approximation of the collision term. The latter involves the relaxation time  $\tau_R$  of resistive processes that conserve energy, and the relaxation time  $\tau_N$  of normal processes that conserve additionally the quasi-momentum and lead to a nonequilibrium anisotropic Planck distribution, also called a drifting distribution. These two relaxation times determine natural time scales for the flow of a phonon gas.

Our objective is to obtain the approximate description of the phonon gas flow in the time scale of the order of  $\tau_N$ , in both wave and diffusive regimes. We aim at the theory admitting arbitrarily large values of the components of the heat flux vector and taking into account the relaxation times  $\tau_R$  and  $\tau_N$ , since fast thermal phenomena are considered. We adopt a physically justified assumption that  $\tau_N$  is much smaller than  $\tau_R$ . Clearly, during the first time period, normal processes make the phonon gas approach the displaced Planck distribution, and then during the longer time period, resistive processes return it to the equilibrium Planck distribution. Hence, the use of the respective expansions of the phonon distribution function about a nonequilibrium anisotropic Planck distribution function, expressed in terms of the energy density and the heat flux [1], for the derivation of the sought hydrodynamic descriptions of the phonon gas flow suggests itself. Commonly used simplifications in the phonon kinetic model are employed. Namely, no distinction is made between longitudinal and transverse phonons, linear isotropic phonon dispersion relation  $\Omega = c|\mathbf{k}|$  is assumed ( $c$  is the constant Debay speed), the components of the wave vector  $\mathbf{k}$  are assumed to range from  $-\infty$  to  $+\infty$  and the relaxation times  $\tau_N$  and  $\tau_R$  are assumed to be constant.

In order to derive the hyperbolic evolution equations for the phonon gas state variables, we generalize the method of Grad in the sense that, instead of the local equilibrium Planck distribution, we take the nonequilibrium anisotropic Planck distribution as a base for the

expansion [2,3]. Our reasoning is as follows: Firstly, we set up a weighted Hilbert space for the expansion with the aid of the formula for a kinetic entropy of the phonon gas. Secondly, we define an orthogonal basis in this Hilbert space. Then, the expansion coefficients are determined and the relations between those coefficients and the moments of the distribution function are established. Substitution of the truncated expansion into the corresponding system of moment equations leads to a system of the evolution equations for the moments. In this way, a hierarchy of closed systems is obtained. Each system contains the relaxation times  $\tau_N$  and  $\tau_R$ , is nonlinear in the energy density and the heat flux, and depends linearly on the higher-order moments of the distribution function. The first system of the hierarchy is the nine-moment system which includes the deviatoric part of the flux of the heat flux as a gas state variable.

A similar modification of the Chapman-Enskog method is employed for the derivation of the diffusive heat transport equations. Namely, the expansion in gradients of the energy density and the drift velocity of the phonon distribution function about a nonequilibrium displaced Planck distribution is assumed as a solution of the Boltzmann-Peierls equation. The relaxation time  $\tau_N$  plays the role of the expansion parameter. The zeroth-order terms in  $\tau_N$  yield the hyperbolic system for the energy density and the drift velocity, equivalent to that derived in [1]. The first-order terms result in turn in the second-order quasilinear parabolic system of equations for the same unknowns. The relaxation time  $\tau_R$  appears in the production term on the right hand side of an equation for the drift velocity, whereas the relaxation time  $\tau_N$  appears in the expression for the deviatoric part of the flux of the heat flux. The coefficients of the system, interpreted as the transport coefficients, are nonlinear functions of the energy density and the drift velocity. It is demonstrated that this parabolic system is consistent with the second law of thermodynamics, i.e., it enables us to define a macroscopic entropy density as a function of hydrodynamic variables which satisfies the balance equation with a non-negative production due to both resistive and normal processes. Finally, a comparison of the obtained four-moment parabolic system with the result of parabolisation of the nine-moment hyperbolic system [4] is presented. It is expected that the nine-moment quasilinear hyperbolic system and the four-moment quasilinear parabolic system can describe more adequately wave and diffusive heat transport under the rapidly varying high thermal loads than the previous theories which treat the heat flux in a perturbative manner.

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