

GRAD-TYPE EXPANSION ABOUT NONEQUILIBRIUM STATES FOR THE RELAXATION-TIME APPROXIMATION OF THE BOLTZMANN-PEIERLS EQUATION

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Summary A new type of heat transport equations for transient processes under high thermal loads is 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 kinetic equation. The proposed new type of the expansion about nonequilibrium states conforms to the time scales of the phonon gas relaxation processes and admits arbitrarily large heat fluxes.

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 kinetic equation governing the phonon distribution function (i.e., the phase density or the number density of phonons) with the commonly used Callaway's relaxation time approximation of the collision term. It involves the relaxation time τ_R of resistive processes (i.e., scattering processes which do not conserve quasi-momentum and which tend to return the phonon gas to an equilibrium Planck distribution function) and the relaxation time τ_N of normal processes which conserve quasi-momentum and which lead to a nonequilibrium anisotropic Planck distribution function, also called a drifting distribution. These two relaxation times determine natural time scales for the flow of a phonon gas and, in general, three regimes of the phonon gas flow can be distinguished, namely, the ballistic, hyperbolic, and diffusive regimes.

Our objective is to obtain the approximate description of the phonon gas flow in the time scale of the order of τ_N , in the hyperbolic regime. Moreover, we aim at the theory admitting virtually arbitrarily large values of the heat flux vector components. Thus, the use of the expansion of the phonon distribution function about a nonequilibrium anisotropic Planck distribution function and the enlargement of the set of independent gas-state variables through the introduction of higher-order moments of the distribution function suggest themselves.

In order to derive the evolution equations for the gas-state variables, we propose to generalize the classical method of Grad in the sense that, instead of the local equilibrium distribution function, we take the known specific nonequilibrium distribution function as a base for the expansion. Hence, we aim at modifying the classical Grad-type expansion for the phonon gas about the local equilibrium Planck distribution function, derived in [1,2], by employing the nonequilibrium anisotropic Planck distribution given in [3] in terms of the energy density and the heat flux vector. For the classical gas, a similar idea of expanding the distribution function about the (nonequilibrium) anisotropic Gaussian was employed in [4] but not in the form of a systematic Grad-type expansion and without any justification in the relaxation processes.

For simplicity, no distinction is made between longitudinal and transverse phonons. Also, linear isotropic dispersion relation $\Omega = c |\mathbf{k}|$ is assumed (c is the constant Debay speed) and the components of the wave vector \mathbf{k} are assumed to range from $-\infty$ to $+\infty$. Since emphasis is placed on the flow time scale of the order of τ_N , we assume that τ_N depends on \mathbf{k} while τ_R remains independent of \mathbf{k} .

Our reasoning is the following. First, we set up a weighted Hilbert space for the expansion with the aid of the formula for the kinetic entropy of a phonon gas. Subsequently, we define an orthogonal basis in this Hilbert space. 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 results in a closed system of the evolution equations for the moments. In this way, a hierarchy of closed systems can be obtained, such that each system involves two relaxation times τ_N and τ_R , is nonlinear in energy density and heat flux, and depends linearly on the higher-order moments of the distribution function. These higher-order moments are fast variables that decay to their values corresponding to the nonequilibrium drifting distribution after a short relaxation time τ_N , so that our approach seems to be particularly useful if $\tau_N \ll \tau_R$.

The first system in this hierarchy is the nine-moment system which involves the deviatoric part of the flux of the heat flux as the only fast variable. For this system, explicit closed-form expressions for the moment fluxes and productions are obtained. It is expected that this nine-moment system can describe more adequately transient processes under high thermal loads than the previous theories which treat the heat flux in a perturbative manner.

Acknowledgment

This work was supported by the State Committee for Scientific Research (KBN) through the grant No 5 T07A 046 24.

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