Moment model and boundary conditions for energy transport in the phonon gas

Abstract Heat transfer in solids is modeled in the framework of kinetic theory of the phonon gas. The microscopic description of the phonon gas relies on the phonon Boltzmann equation and the Callaway model for phonon–phonon interaction. A simple model for phonon interaction with crystal boundaries, similar to the Maxwell boundary conditions in classical kinetic theory, is proposed. Macroscopic transport equation for an arbitrary set of moments is developed and closed by means of Grad’s moment method. Boundary conditions for the macroscopic equations are derived from the microscopic model and the Grad closure. As example, sets with 4, 9, 16, and 25 moments are considered and solved analytically for one-dimensional heat transfer and Poiseuille flow of phonons. The results show the influence of Knudsen number on phonon drag at solid boundaries. The appearance of Knudsen layers reduces the net heat conductivity of solids in rarefied phonon regimes.

Keywords Phonon heat transfer · Moment method · Slip boundary conditions

1 Introduction

There has been an increasing focus in the last two decades on miniaturization, as scientists and engineers aim to utilize the benefits of micro- and nanotechnology. In order to effectively design devices at the corresponding length scales, it is important to understand the governing equations. As length scale decreases, different effects become more dominant and others might become less, such that approximations used in classical macroscopic theories loose validity. As a result, well-known relations, such as Fourier’s law for heat conduction and the Navier–Stokes equations, begin to break down in certain regimes.

Understanding temperature and heat transfer is important for determining virtually any other property in a material, such as viscosity, electrical and thermal conductivity, heat capacity, elasticity, and ductility. Furthermore, the small size of an object and its resultant tiny thermal mass combined with the relative power of lasers can lead to huge fluctuations in temperature over short periods of time. Understanding temperature and heat transport will improve the sensitivity of sensors and could also be used for more effective thermal management of miniaturized devices, including semiconductor systems [1].

Heat in a solid is caused by vibrations of particles in the crystal lattice with respect to their mean position. These vibrations can be quantized into quasiparticles known as phonons [2,3]. Macroscopic properties such as temperature, internal energy, and heat flux can be determined by analysis of the phonon properties, such as energy and quasimomentum. Heat and temperature properties of systems can be determined by tracking all phonons in a domain (i.e., by molecular dynamics), but this can be prohibitively expensive when large numbers
of phonons are present. The direct simulation Monte Carlo method (DSMC), which uses a statistical approach to groups of particles, can be used in situations where large numbers of phonons are present, but it can still be computationally expensive [4].

Another approach is to extend the classical heat transport equations—i.e., Fourier’s law—by using phonon kinetic theory to add terms and equations to the existing macroscopic equations. In the case of heat transport in solids, extended equations are necessary at larger (>0.01) Knudsen numbers, Kn, defined as the ratio of the mean free path of phonons, \( \lambda \), to the length scale, \( L \), of the system. The equations are extended by analyzing microscopic phonon kinetic theory and then integrating the properties to develop macroscopic equations. This approach was first used by Grad in kinetic theory of classical gases [5] and later extended to phonon kinetic theory [6].

Earlier moment models did not include a proper theory of boundary conditions, which limited the consideration of the extended transport models to few special cases [6]. Clearly, to render the macroscopic approach to phonon transport into a useful tool for simulation and understanding of devices, one needs reliable boundary conditions. Phenomenological boundary conditions to extended thermodynamic equations for phonons have recently been presented [7–9] for the Guyer–Krumhansl equations [10,11] that correspond to a 9-moment model.

In the present paper, in order to bridge between the microscopic and macroscopic descriptions of phonon transport, we present boundary conditions based on a microscopic analysis of model phonon–surface interactions. Three types of interactions are considered: isotropic scattering, specular reflection, and surface thermalization. The purpose of the model is to be versatile enough, so that proportions of the three types of interactions can be changed relative to each other to approximate experimental data.

The moment description of phonons in [6] was based on a simplified kinetic description of phonons, which we shall adhere to as well. The main simplifications are (a) a linear dispersion relation between phonon energy and momentum, (b) extension of the Brillouin zone to infinity, and (c) modeling of phonon interactions with the Callaway model [12], with frequency-independent collision frequencies. These simplifications allow relatively fast access to moment systems of arbitrary moment number. The resulting models describe the rarefied phonon gas in principle and offer parameters such as the relaxation times that can be used for fitting to experiments. We note, however, that these underlying assumptions are not valid for the description of systems at room temperature, where phonon dispersion is nonlinear, and the Brillouin zone cannot be extended to infinity. Hence, the present models are of limited use for application for many actual systems.

Since it is based on the same assumptions, the model of boundary conditions that we present here complements [6] in that it provides complete boundary conditions for the moment equations presented there. For self-consistency, we shall recall the model and development of the moment equations in some detail and then develop the appropriate moment boundary conditions for the moment systems. As a result, we present a framework of moment equations and boundary conditions for an arbitrary number of moments.

Detailed equations and boundary conditions are then presented and discussed for sets of 4, 9, 16, and 25 moments. The relation of the 4-moment model to Fourier’s law, and of the 9-moment model to the Guyer–Krumhansl equations is pointed out. One advantage of the moment description of rarefied gases is that one can find analytical solutions for processes in simple geometry, which is not possible for the kinetic description through the Boltzmann equation. To show the capabilities of the equations, two simple problems are solved analytically, one-dimensional heat transfer through a finite crystal, including a case with an interface within the crystal, and heat flow in a narrow conductor with adiabatic sides, where phonon flow is similar to classical Poiseuille flow. We study generic cases by considering solutions of the dimensionless equations for a variety of dimensionless parameters. The solutions agree with Fourier’s law for small Knudsen numbers, but boundary effects such as temperature jump and Knudsen layers markedly reduce overall conductivity for larger Knudsen numbers.

Our results show that the macroscopic approach to phonon transport allows the solution of boundary value problems for technically relevant processes with meaningful results. We refrain from comparison with actual experimental data, since the present kinetic model relies on too many simplifying assumptions (linear dispersion, finite Brillouin zone, constant collision frequency). While the present work proves that meaningful boundary conditions for moment systems for phonons can be derived, we believe that for accurate description of actual experiments, the model should be based on a more realistic kinetic model.

The remainder of the paper is organized as follows: In Sect. 2 we recall the basic elements of the microscopic description of phonons through the phonon Boltzmann equation with Callaway model, derive the moment equations, and use the Grad method for closure. Section 3 details the microscopic model for phonon–boundary interactions. The Grad distribution function is used to determine the appropriate boundary conditions for the...