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Yuan Dong

Dynamical Analysis of Non-Fourier Heat Conduction and Its Application in Nanosystems

Doctoral Thesis accepted by
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To my family,
for their unconditional love
and firm support

Supervisor's Foreword

Heat conduction is a traditional subject that can be traced back to 1822, the year Fourier's conduction law was established. Through nearly two centuries the application of the theory of heat conduction has been immensely developed in the fields of energy, electronics, material processing, environment protection, as well as human health. The heat conduction research based on Fourier's conduction law usually focuses on how to transfer heat efficiently for heating or cooling objects. However, in the past three decades, with the development of short pulse laser and fabrication of nanomaterials, the validation of Fourier's law has been challenged. It was pointed out in the mid-twentieth century that Fourier's law implies an infinite heat propagation speed, a physically unacceptable notion. In studies on ultrafast laser heating on materials from the 1980s, it is observed that the temperature response on laser heating exhibits the behavior of lagging, relaxation, or delay, which indicates the failure of Fourier's conduction law. On the other hand, in low-dimensional materials such as carbon nanotube and graphene, as well as nanosized semiconductors, the heat conduction shows a size-dependent behavior. The limited size of materials can either provide ultrahigh heat conductivity, which sheds light on the heat management of large-scale Integrated circuits, or much-suppressed heat conductivity, which can enhance the figure of merit of thermoelectric devices. These applications provide potential solutions to the emergent needs raised by modern engineering. However, the scientific understanding and modeling of heat conduction in these extreme conductions are far from satisfactory.

In the present work by Dr. Dong, non-Fourier heat conduction is investigated through various perspectives. The basic idea originates from the thermomass theory, which was established by our research group since 2005. In the thermomass theory, based on the mass–energy equivalence of Einstein, thermal energy is regarded as a weighable fluid flowing through the porous mediums, which is different from the caloric theory of the eighteenth century. As a result, a general heat conduction law was presented to describe the relationship between the heat flux and the temperature gradient by use of principle of fluid dynamics, which degenerates to Fourier's conduction law or other non-Fourier heat conduction models under different simplifications. Dr. Dong's work first studies the microscopic foundation of thermomass theory in the dielectric medium, where the main heat carriers are phonons. Based on the phonon Boltzmann theory, he revealed the connection between the phonon quasi-momentum and the real momentum of phonon gas. In this way, the momentum balance equation of phonon gas can be formulated, which then leads to the general heat conduction law beyond Fourier's conduction law. The general heat conduction law is similar to the phonon hydrodynamics model proposed in the 1960s, with a new term corresponding to the convection effect of phonon gas. The author proves that this difference comes from the higher order expansion of the phonon distribution function. This derivation bridges the microscopic and macroscopic theories. It not only provides a microscopic explanation for the thermomass theory, but also clarifies the hierarchy for many non-Fourier models.

Second, the thermomass theory enables one to analysis the irreversible thermodynamics from a perspective of fluid mechanics. By distinction of the reversible and irreversible effects in the general heat conduction law, this work claims that irreversibility in non-Fourier heat conduction is induced only by the friction force rather than the driving force. Thus the traditional expression of entropy production has to be modified. Like the analysis of the extended irreversible thermodynamics, the proposed general entropy production avoids the negativity paradox in non-Fourier heat conduction processes. The modification of entropy production naturally causes the revision of the entropy and temperature in thermodynamics. Using the approach of compressible fluid dynamics, the author announces the static temperature and total temperature in non-Fourier heat conduction, which are the static and total pressures of the phonon gas. The distinction between these two temperatures is comprehensively investigated through the thermodynamic laws, as well as the phonon Boltzmann equation. The by-product of the above analysis is that the generalized forces and fluxes in the entropy production should be the real forces and fluxes of the thermomass flow. With this discovery, the long-existing problem in the derivation of Onsager reciprocal relation, namely the generalized fluxes cannot be expressed by the time derivatives of state variables, is solved. The author shows that the time derivative term in Onsager's derivation should be the inertia force of heat conduction. Thus the state variables are formulated as the "displacement of heat," which is the average displacement of transported quantities during fluctuation. The author further provides a macroscopic derivation of the Onsager reciprocal relation based on the principles of Galilean invariance and the third law of Newtonian dynamics.

Lastly, the thermomass theory is used in up-to-date applications, i.e., the nanoscale non-Fourier heat conduction. The size dependence of the effective thermal conductivity in nanosystems is induced by the boundary scattering of heat carriers. In this work, the boundary effect is modeled by the additional boundary friction term raised by the phonon gas viscosity, in analogy to the Brinkman extension for the porous flow. On the other hand, the confined structure also causes the rarefaction effect which reduces the effective viscosity of phonon gas. By accounting for both the viscosity and rarefaction effects the author builds prediction models for the effective thermal conductivity of nanosystems, which agree well with the experiments. Moreover, a ballistic-diffusive model is proposed for the cross-plane thermal conductivity of nanofilms. The author shows that the different heat conduction directions will cause size-dependent heterogeneity of thermal conductivity, which is led by the different geometry confinement mechanisms.

This work manifests the excellent analysis skill, physical insights, and broad knowledge of the author, from the condensed physics to thermodynamics, from fundamental theory to cutting edge applications. It received unanimous high praise from the thesis reviewers. As the supervisor of Dr. Dong, I am glad to recommend this thesis to readers, particularly those specialized or interested in the heat conduction theory, nanotechnology, and thermodynamics.

Beijing, China Prof. Zengyuan Guo
August 2015

Abstract

Heat conduction cannot be characterized by Fourier's law in extreme conditions such as ultrafast transient heating or nanoscale heat conduction, which is called non-Fourier heat conduction. Based on Einstein's mass–energy equivalence, Guo et al. proposed that thermal energy has its equivalent mass, namely thermomass. Heat conduction is actually the motion of thermomass, which obeys Newton's law of motion. Therefore, the non-Fourier heat conduction can be analyzed from a dynamical viewpoint, which establishes the general heat conduction law with a clear macroscopic physical picture.

Phonons are the main thermal energy carriers in dielectric solids. This work obtains the microscopic foundation of general heat conduction law through the phonon Boltzmann equation. The transient and spatial inertial terms of thermomass come from the first and second orders of expansion of the phonon distribution function, respectively. Neglecting all the high order expansions of the phonon distribution is equivalent to neglecting the inertia terms of thermomass, and reduces the general heat conduction law to Fourier's law. The inertial effect of thermomass cannot be neglected in ultrasmall time or spatial scales, causing non-Fourier heat conduction.

The entropy production in irreversible thermodynamics is the product of generalized forces and fluxes. The classical expression of entropy production is non-positive definite in non-Fourier heat conduction, which violates the second law of thermodynamics. This work defines the real forces and fluxes in heat conduction based on the thermomass theory, instead of the phenomenological generalized forces and fluxes. The forces in entropy production should be the friction forces rather than the driving forces. Therefore, the general expression of entropy production is obtained and is compatible with the non-Fourier heat conduction.

The definition of temperature needs to be modified in non-Fourier heat conduction. This work derives the expressions of static and stagnant temperatures based on the Bernoulli equation of thermomass flow. The static temperature is the true state variable and is consistent with the nonequilibrium temperature in extended irreversible thermodynamics. The internal energy and entropy should be expressed with the static temperature.

The linear regression of fluctuation is assumed in the proof of the Onsager reciprocal relation. It requires that the generalized fluxes are the time derivative of state variables, which is hardly satisfied by usually defined fluxes. This work proves that the linear regression of fluctuation is the balance of inertia and friction forces of the thermomass, which is a non-Fourier heat conduction process. The corresponding state variable of heat flux is the average displacement of thermomass during fluctuation.

The boundaries impose additional resistances on heat conduction in nanosystems, causing the size effect of the effective thermal conductivity. This work adds a viscous term of thermomass in the general heat conduction law to describe the boundary resistance. The in-plane effective thermal conductivities of nanofilms and nanowires are predicted by considering both the nonuniform heat flux profile in the cross section due to phonon gas viscosity and the rarefaction of phonon gas. For cross-plane effective thermal conductivity of nanofilms, a ballistic-diffusive model is built based on the Boltzmann equation regarding the nonequilibrium distribution in near boundary region. These models agree well with the experimental and numerical simulation results.

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