PhD Thesis Defense

Department of Mechanical Engineering
Indian Institute of Science, Bangalore

Uncovering unconventional heat flow in semiconductors through predictive first-principles calculations

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MS Team link to join online: PhD Thesis Defense (Nikhil Malviya)

ABSTRACT

Heat conduction in solids is traditionally described by Fourier's law, which assumes diffusive transport. However, in materials with ultrahigh thermal conductivity (κ), particularly at micro-to-nanoscale length scales, this classical description can break down, giving rise to unconventional heat flow regimes ranging from quasiballistic and ballistic transport to hydrodynamic (second sound) transport. Developing a fundamental understanding of these heat flow mechanisms and predicting the conditions under which they emerge, are essential for the thermal design of next-generation electronic and quantum devices. In this context, first-principles computations have played a pivotal role in uncovering novel heat flow regimes in ultrahigh-κ materials. In my Ph.D. research, I have advanced these state-of-the-art first-principles computational approaches to predict the materials and experimental conditions under which such unconventional heat flow regimes can be realized.

My research focuses primarily on semiconductors, where heat is predominantly carried by collective lattice vibrations known as phonons. The transport of these heat carriers is governed by the Peierls-Boltzmann transport equation (PBE), which provides a fundamental microscopic description of heat flow in these materials. I use the linearized form of the PBE (LPBE) to describe linear temperature dynamics, as observed in most experimental settings. In this context, motivated by the principal component decomposition of linear dynamical systems, I have developed a computationally efficient low-rank solution to the LPBE that remains accurate even in regimes where macroscopic equations break down. This approach enables a seamless exploration of Fourier and non-Fourier heat flow within the same first-principles computational framework. Furthermore, I have established a direct correspondence between this microscopic description of phonon transport and the macroscopic equations governing temperature dynamics, which are often used to describe unconventional, non-Fourier heat-flow regimes. This correspondence has enabled the identification of materials and experimental conditions under which these non-Fourier heat flow regimes can be experimentally observed. Subsequently, I explored different approximate models of the LPBE to predict steady-state κ and transient temperature dynamics, and found them to be suitable for low-to-moderate κ materials in diffusion-dominated heat flow regimes. Thus, through this thesis, I have presented a comprehensive study of thermal phonon dynamics and transport in the linear regime.

ABOUT THE SPEAKER



Nikhil Malviya is a PhD scholar in the Department of Mechanical Engineering at the Indian Institute of Science (IISc), Bangalore, working with Dr. Navaneetha Krishnan Ravichandran. He completed his B.Tech. in Mechanical Engineering from Motilal Nehru National Institute of Technology (MNNIT), Allahabad, in 2020 and thereafter joined IISc in October 2020. His research focuses on heat conduction in ultrahigh-κ materials at micro- to nanoscale length scales, where conventional laws are challenged.