ME Seminar

Atomistic Simulations and Machine Learning Driven Exploration of Extreme Thermal Conductivity Materials and Nanostructures

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ABSTRACT

The recent decades have witnessed an increased effort for discovering materials that can help to push efficiencies of renewable energy sources beyond known limits and mitigate the rising thermal challenges imposed by next generation electronic devices and artificial intelligence applications. Such efforts involve finding bulk materials and nanostructures with extreme properties such as thermal conductivity (k_{th}). High k_{th} materials are crucial in thermal management of vertically integrated circuits (ICs) for the next generation computing devices. On the opposite end of the spectrum, designing ultra-low k_{th} materials is essential for improving thermal barrier coatings in turbines and creating high performance thermoelectric devices for waste heat harvesting. In my research work, I identify binary superlattice nanostructures with extreme thermal transport properties and explore the underlying phonon and photon transport mechanisms. My approach follows two main avenues for evaluating potential candidates: (a) high fidelity atomistic simulations such as molecular dynamics simulations, and (b) Machine Learning driven rapid property prediction and nanostructure design optimization. The insight gained into the governing physics enables us to theoretically predict new materials for specific applications requiring high or low k_{th}, propose accelerated optimization pathways which can significantly reduce design time and cost, and advance the general understanding of energy transport regimes in semiconductors and dielectric materials.

ABOUT THE SPEAKER

Dr. Prabudhya Roy Chowdhury is an AI Hardware and Modeling Engineer at IBM Research, Albany. His research interests and expertise include developing thermal test hardware and simulation models for advanced semiconductor technologies, developing thermal management strategies, thermo-mechanical analysis, multi-scale multi-physics modeling (thermal, mechanical, electrical) of energy transport in materials and devices, machine learning (ML) and materials informatics (MI) methods for accelerated materials discovery. Prior to joining IBM, Prabudhya earned his B. Tech and M. Tech degrees in Mechanical Engineering from the Indian Institute of Technology, Kharagpur, India. He then received his PhD in Mechanical Engineering from Purdue University, where his research focused on atomistic modeling and machine learning driven investigation of thermal transport in nanomaterials and nanoscale heterostructures such as binary superlattices. At Purdue, Prabudhya was the recipient of multiple prestigious fellowships such as the Ross Fellowship and the Bilsland Dissertation Fellowship. He has published in leading journals including Nano Energy, Advanced Optical Materials, Physical Review B, Nature Communications, ACS Applied Materials and Interfaces and Computational Materials, as well in as top-tier conferences such as IEEE Electronic Components and Technology Conference (ECTC) & IEEE Transactions on Electron Devices. Prabudhya also holds multiple patents in the fields of semiconductor device design and process, electronics packaging, thermal management, and reliability.

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