

# Phonon School

## May 21-22, 2102

### PROGRAM

#### Phonon School Registration:

Monday: 8:00-1:00 Engineering Hall Lobby  
Tuesday: 3:00-5:00 Engineering Hall Lobby  
5:30-7:30 Union South, Varsity Lounge

Technical program will be held in 1610 Engineering Hall

Breaks will be held in Engineering Hall Lobby

Reception will be held in Union South Pavilion. In case of inclement weather, it will move to Union South Varsity Hall III. See maps in back.

### Monday, May 21

#### Session M1 Chair: Li Shi

8:20-8:30 Welcome

8:30-9:30 *Measurements of thermal transport at the nanoscale using kHz and ultrafast thermal waves: the  $3\omega$  method and time-domain thermoreflectance (Plenary talk)*  
David G. Cahill  
University of Illinois at Urbana-Champaign, USA

9:30-10:15 *Thermal transport in group-IV nanostructures and superlattices based on the Boltzmann transport equation*  
Zlatan Aksamija  
University of Wisconsin - Madison, USA

10:15-10:45 Break

#### Session M2 Chair: Zlatan Aksamija

10:45-11:30 *Continuum Models of Phonons in Nanostructures*  
Michael A. Stroschio, Mitra Dutta, Banani Sen, Ke (Robin) Xu, Jun Qian, and Ke (Clare) Sun

University of Illinois at Chicago, USA

11:30-12:15 *Theory of phonon transport in nanocomposite materials*  
G. P. Srivastava  
University of Exeter, UK

12:15-1:15 Lunch

**Session M3 Chair: David Cahill**

1:15-2:15 *Phonons in Nanoelectronics (Plenary talk)*  
Kenneth E. Goodson  
Stanford University, USA

2:15-3:00 *Monte Carlo Simulation of Phonon Transport*  
Edwin B. Ramayya  
University of Wisconsin-Madison, USA

3:00-3:30 Break

**Session M4 Chair: Rob Kelsall**

3:30-4:15 *Self-Heating Effects in SOI Devices and GaN HEMTs*  
Dragica Vasileska  
Arizona State University, USA

4:15-5:00 *Electrothermal Monte Carlo Simulation of Nanoelectronic Devices*  
Toufik Sadi  
Aalto University, Finland

## **Tuesday, May 22**

**Session T1 Chair: Keivan Esfarjani**

8:30-9:30 *Thermal Transport in Graphene and other Two-Dimensional Systems (Plenary talk)*  
Li Shi  
The University of Texas at Austin, USA

9:30-10:15 *Molecular Dynamics for Thermal Transport Simulations in Solid Materials*  
Jennifer Lukes  
University of Pennsylvania, USA

10:15-10:45 Break

**Session T2    Chair: Derek Stewart**

10:45-11:30    *Thermal transport from first-principles*  
Keivan Esfarjani  
Massachusetts Institute of Technology, USA

11:30-12:15    *First-principles quantum transport modeling of thermoelectricity in nanowires and single-molecule nanojunctions*  
Branislav Nikolic  
University of Delaware

12:15-1:00    Lunch

**Session T3    Chair: Branislav Nikolic**

1:00-1:45    *An Introduction to First Principles Thermal Transport*  
Derek Stewart  
Cornell University, USA

1:45-2:30    *Phonon Transport Across Interfaces*  
Timothy Fisher  
Purdue University, USA

2:30-3:00    Break

**Session T4    Chair: Timothy Fisher**

3:00-3:45    *nanoHUB.org Tutorial: Mythbusting Scientific Knowledge Transfer in Research and Education*  
Gerhard Klimeck  
Purdue University

3:45-4:30    *The ATK platform for atomic-scale modeling*  
Kurt Stokbro  
QuantumWise A/S, Denmark

4:30-6:00    *QuantumWise and QuantumEspresso hands-on tutorials*  
*(must sign up for tutorials; sign-up sheets will be available on site)*

6:00-9:00    Reception  
Union South Pavilion, weather permitting  
In case of rain, Union South Varsity Hall III  
(see maps)

*Plenary talk*

**Measurements of thermal transport at the nanoscale using kHz and ultrafast thermal waves: the  $3\omega$  method and time-domain thermoreflectance**

David G. Cahill

University of Illinois at Urbana-Champaign, USA

The  $3\omega$  method is a commonly used measurement technique for determining the thermal conductivity of thin layers. The  $3\omega$  method is a type of “hot-wire” approach where the self-heating of a lithographically-defined metal line generates a third harmonic voltage that serves as the thermometer in the experiment. The frequencies used are in the kHz range so that the thin film is thermally-thin and the substrate is thermally thick. Thus, the  $3\omega$  method measures the thermal resistance of the thin film in series with any interfaces in the measurement structure. Some advantages of the 3-omega method are the relatively simple equipment and high accuracy.

Time-domain thermoreflectance (TDTR) is a modulated pump-probe optical technique based on an ultrafast model-locked laser as the light source. Over the past several years, we have advanced the state-of-the-art of TDTR by improving the optical design and introducing quantitative modeling of heat transport in cylindrical coordinates for an arbitrary multilayer geometry. Some advantages of TDTR are high sensitivity to thin layers, easy sample preparation, high spatial resolution, separation of interface conductance and thin film thermal conductivity, and applicability to the study of materials under extreme conditions of high temperatures and pressures. The combination of TDTR and high pressure environments in diamond anvil cells enables powerful tests of models for heat transport in crystals, glasses, and across interfaces.

Several research groups are studying how best to model TDTR data when a significant fraction of the heat carrying phonons have mean-free-paths larger than the thermal penetration depth, i.e., when the diffusion equation is not a rigorous description of the heat transfer. We refer to the effects of these ballistic heat carriers on TDTR measurements as “frequency dependent thermal conductivity”.

# **Thermal transport in group-IV nanostructures and superlattices based on the Boltzmann transport equation**

Zlatan Aksamija

University of Wisconsin - Madison, USA

Thermoelectric (TE) refrigeration using semiconductor-based nanostructures, such as nanowires, nanoribbons, and superlattices, is an attractive approach for targeted cooling of local hotspots inside integrated circuits due to inherently no moving parts, ease of miniaturization and on-chip integration, and the nanostructures' enhanced TE conversion efficiency. TE efficiency, measured by the figure-of-merit  $ZT$ , is dictated by the ratio of electronic power factor  $S^2\sigma$  over the total thermal conductivity. Consequently, largest gains in TE conversion efficiency have come from the ability to reduce thermal conductivity. This is especially true in nanostructures, where small physical dimensions lead to reduced thermal transport due to the scattering of phonons with the nanostructure interfaces. Silicon-on-insulator (SOI) nanomembranes and membrane-based nanowires and ribbons show promise for application as efficient thermoelectrics, which requires low thermal conductivity. In this talk, we present simulation of phonon transport in ultrathin silicon nanomembranes and gated nanoribbons based on the Boltzmann transport equation. We employ a full phonon dispersion combined with a momentum-dependent model of phonon boundary scattering. We show that the thermoelectric response of Si-membrane-based nanostructures can be improved by employing the anisotropy of the lattice thermal conductivity, revealed in ultrathin SOI nanostructures due to the interplay between the anisotropy of the phonon dispersion and the strong boundary scattering. Furthermore, we explore the consequences of nanostructuring on Si/Ge and Si/SiGe alloy superlattices, and show that the drastic reduction of thermal conductivity in these structures comes from the increased interaction of lattice waves with rough interfaces and boundaries. Finally we demonstrate reduced thermal conductivity in both suspended and supported graphene nanoribbons (GNRs), which exhibit strong anisotropy due to interaction of lattice waves with line edge roughness (LER) and the competition between LER and substrate scattering. The talk will conclude with an outlook for future nanostructured thermoelectric based on nanocrystalline and nanocomposite semiconductors, and graphene.

## **Theory of phonon transport in nanocomposite materials**

G. P. Srivastava  
University of Exeter, UK

I will present a theory of phonon transport in nanocomposite materials. This is based on a relaxation time approximation within the Boltzmann transport formalism and a model anharmonic Hamiltonian accounting for acoustic as well as optical phonons. Analytic expressions are derived for phonon scattering rates due to interface mass mixing, interface dislocation formation, and anharmonic three-phonon Normal and Umklapp processes in the presence of more than one material in a composite structure. Extensive numerical calculations, based on accurate dispersion relations for acoustic and optical phonons, of the thermal conductivity tensor are made to assess the relative importance of different phonon scattering mechanisms in explaining experimentally measured results for Si/Ge and GaAs/AlAs superlattices.

## **Continuum Models of Phonons in Nanostructures**

Michael A. Stroschio, Mitra Dutta, Banani Sen, Ke (Robin) Xu,  
Jun Qian, and Ke (Clare) Sun  
University of Illinois at Chicago, USA

This lecture will summarize the dielectric continuum model and its use in describing optical phonons and the elastic continuum model and its use in describing acoustic phonons. The talk will illustrate how to use these continuum models to describe few-phonon processes. In addition, the talk will discuss how to use these continuum results to model carrier-phonon interactions and to explain why confined phonon effects are especially important in selected classes of optoelectronic devices. The important role of sum rules for confined, interface, and half-space phonons will be emphasized. The presentation will address the use of these continuum models in describing nanoscale structures.

The general techniques for applying these continuum models to describe optical and acoustic phonons in nanostructures will be described. The application of these models will be described in several important and illuminating cases including:

- (a) phonons for bucky balls which have a "membrane" that is a single layer thick but which can be modeled accurately using the continuum approach;
- (b) optoelectronic devices where phonons play a decisive role in the proper functioning of the devices - such as the quantum cascade laser;
- (c) thermal transport through thin graphite layers where phonon confinement effects are shown to have a dramatic effect on thermal transport;
- (d) carbon-nanotube-based structures where interfacial effects play a key role in thermoelectric properties.

*Plenary talk*

## **Phonons in Nanoelectronics**

Kenneth E. Goodson  
Stanford University, USA

Nanoelectronic devices - and their constituent materials and interfaces - present some of the most promising and challenging opportunities for the study of phonon conduction. Examples include scaled and nanopillar FETs, phase change memory cells, silicon-based photonic sources and waveguides, and composite substrates for power semiconductor devices. The temperature distributions in these structures, especially those near interfaces, consume an increasing fraction of the available “thermal budget” for electronic and optoelectronic systems. While a subcontinuum phonon-based analysis is not always essential for the accurate simulation of these structures, this situation is gradually changing with continued dimensional scaling, heterogeneous materials integration, and structures targeting 2D/3D band manipulation.

This presentation describes thermal phenomena in nanoelectronic devices and materials with a focus on experiments and phonon transport. Much attention is given to interfaces, whose thermal properties are strongly influenced by multicarrier transport, electron-phonon nonequilibrium, and near-interfacial disorder. Interface transport is complicated by materials (including some of the chalcogenides relevant for phase change memory) in which electrons and phonons contribute comparably to heat conduction. The varying conductivity contributions of electrons and phonons, and their dependence on lengthscale, feature prominently in several examples including metal-semiconductor multilayers and metal interconnects with cross sectional dimensions down to 7 nm.

## **Monte Carlo Simulation of Phonon Transport**

Edwin B. Ramayya  
University of Wisconsin - Madison, USA

The silicon nanowire has been shown to have a large thermoelectric figure of merit thus making it a prime candidate for building efficient and cheap energy conversion devices. Although the reason for increased thermoelectric efficiency in nanowires is attributed to low thermal conductivity (two orders of magnitude smaller than that in bulk silicon), the theory behind the large reduction in thermal conductivity observed by experimental groups is not fully understood. In this talk I will first go over the algorithm used to calculate the thermal conductivity using the Monte Carlo technique and then go into the fine details of its implementation. I will cover the implementation of phonon-phonon, phonon-impurity, and phonon-boundary scattering in the modeling of heat flow in bulk and nanowire based semiconductors. The importance of the phonon-boundary scattering to account for extremely low thermal conductivity in thin nanowires will be addressed based on two approaches. A modified particle based treatment for the phonon-boundary scattering to account for the thermal conductivity reduction below the Casimir's limit will also be given towards the end of the lecture. I will present some of the important test cases that will help one to debug the code and test for the consistency in the simulation results. Though the presentation will be geared towards accounting for the large reduction in thermal conductivity in silicon nanowires from their bulk value, the algorithm can be easily adapted to other semiconductors with only minor modifications.

## **Self-Heating Effects in SOI Devices and GaN HEMTs**

Dragica Vasileska  
Arizona State University, USA

In this presentation an overview will be given on modeling self-heating effects in SOI devices and GaN HEMTs. The talk will begin with a motivation for this work which is immediately followed by a brief description of electro-thermal (Joule heating) and thermoelectric effects (Peltier, Seebeck and Thompson effect). The incorporation of electro-thermal effects in device simulators, such as SILVACO ATLAS and Synopsys Sentaurus, will be described. Afterwards, a brief overview of previous work done by several authors in this area will be presented. This includes the works of Majumdar, Pop, Stroschio, Waschutka, etc. Next, our electro-thermal studies on self-heating effects in SOI devices and GaN HEMTs will be elaborated. Detailed description will be given on the coupling of the energy balance solvers for acoustic and optical phonons and the Monte Carlo device simulator for the electrons. Convergence analysis of the electro-thermal solver will be discussed. Further extensions of the code to incorporate Phonon Boltzmann Equation Solver will be described at the end of the talk. Finally, summary and directions of future research will be presented.

# **Electrothermal Monte Carlo Simulation of Nanoelectronic Devices**

Toufik Sadi  
Aalto University, Finland

The current device miniaturization trend may not be sustained without dramatic consequences on the operation of next-generation nanodevices, as unrealistic power density levels and temperatures are predicted. Conserving such trend will make the operation of nanoelectronic devices impossible without significant improvements in cooling technology or fundamental changes in device designs. Hot-spots, the low thermal conductivity in thin films and nanowires, and the thermal resistance appearing at interfaces, present all a difficult challenge in guaranteeing device operation with minimized self-heating. For future technology developments, a fundamental understanding of thermal transport at the nanoscale is necessary. In this context, the development of reliable theoretical and simulation tools for coupled electron and phonon transport is essential to address all these issues. The self-heating phenomenon in nanoelectronic devices and the various physics-based models used to study the electrothermal behavior of these structures are discussed. Attention is focused on electrothermal modeling using ensemble Monte Carlo simulations. The Monte Carlo technique is very suitable for the simulation of electron transport in nanoscale semiconductor devices, as it is free from low-field near-equilibrium approximations. More importantly, the method is well-suited for electrothermal modeling, since it allows a detailed microscopic description of electron-phonon scattering which provides an inherent and direct prediction of the spatial distribution of heat generation. A demonstration of the efficiency of the simulation model is given by presenting results from the study of nanoscale field-effect devices based on silicon and compound III-V semiconductors.

*Plenary talk*

**Thermal Transport in Graphene and other Two-Dimensional Systems**

Li Shi

The University of Texas at Austin, USA

This presentation will review results from recent theoretical and experimental studies of thermal transport in graphene and other two-dimensional (2D) layered materials such as hexagonal boron nitride (h-BN) and bismuth telluride. The theoretical questions to be discussed include size-dependent thermal conductivity of 2D systems, as well as the contribution from the flexural phonon modes to the graphene thermal conductivity. Techniques based on micro-Raman spectroscopy and resistance thermometry micro-devices developed for probing thermal transport in 2D materials will be introduced and compared. The wide range of measurement results obtained from these experiments will be examined. In conjunction with theoretical analysis, these experimental results have suggested high thermal conductivity in suspended clean graphene and h-BN, as well as the apparent suppression of phonon transport in graphene by the interaction with a substrate support or polymeric medium. While the high thermal conductivity of 2D graphene and h-BN may be useful for thermal management, phonon-boundary scattering and quantum confinement of electrons in nanostructures have been investigated as possible approaches to increasing the figure of merit of thermoelectric materials including bismuth telluride, which has also been known to be a topological insulator recently. Some measured thermal and thermoelectric properties of bismuth telluride atomic layers will be presented to highlight the intriguing questions on the effects of the protected surface states on the thermoelectric power factor and dimension cross-over on lattice thermal conductivity of the quasi-2D systems.

## **Molecular Dynamics for Thermal Transport Simulations in Solid Materials**

Jennifer Lukes  
University of Pennsylvania, USA

This talk will provide a basic introduction to molecular dynamics simulation techniques for modeling thermal transport in solid materials. First, the key features common to all molecular dynamics simulations will be discussed, including intermolecular potential functions, system initialization, application of boundary conditions, and integration algorithms. Next, equilibrium, nonequilibrium, and homogeneous nonequilibrium methods for calculating thermal conductivity will be presented. A technique for computing thermal interfacial resistance will also be covered, as will the wavepacket approach for phonon transport and scattering. Selected results generated using the above computational methods will be presented, and current challenges in the field will be outlined.

## **Thermal transport from first-principles**

Keivan Esfarjani

Massachusetts Institute of Technology, USA

A popular way of modeling thermal transport in bulk and nanostructures is to use equilibrium or non-equilibrium molecular dynamics (MD). Interaction potentials used in the simulations are however empirical with little accuracy especially as far as the third derivatives are concerned. The latter are crucial in determining the phonon lifetimes to which the thermal conductivity is proportional. We have developed a method to compute from first-principles density functional theory (FPDFT) calculations in a supercell, the second, third and fourth derivative of the total energy with respect to atomic displacements. These force constants allow us to calculate the phonon dispersion and their lifetimes using Fermi's Golden rule (FGR). These are the main ingredients for the calculation of the lattice thermal conductivity within the relaxation time approximation. Furthermore, the force constants can be used in defining an interatomic interaction based on the Taylor expansion of the potential energy with respect to atomic displacements. We have shown that this classical potential is of similar accuracy to the true forces from a FPDFT calculation. The phonon linewidths extracted from the atomic trajectories are in very good agreement with the FGR calculation. This potential has the advantage to be able to include alloying effects and anharmonicity to higher orders. It is thus a very valuable tool for investigating and understanding thermal transport at high temperatures.

## **First-principles quantum transport modeling of thermoelectricity in nanowires and single-molecule nanojunctions**

Branislav Nikolic  
University of Delaware, USA

This lecture will overview nonequilibrium Green function combined with density functional theory (NEGF-DFT) approach to modeling of elastic phononic and electronic quantum transport in nanoscale thermoelectrics. The NEGF-DFT results for phonon thermal conductance will be contrasted with NEGF combined with semi-empirical models using examples drawn from the studies of graphene nanoribbons (GNR) or single- molecule nanojunctions with GNR electrodes. Hands-on examples using Matlab and GPAW scripts will be provided. Finally, possible directions for the inclusion of inelastic processes will be discussed.

## **An Introduction to First Principles Thermal Transport**

Derek Stewart  
Cornell University, USA

A clear understanding of thermal transport due to phonons is crucial for several fields, including thermoelectrics, heat mitigation, and even the thermodynamics of planetary cores. However, developing an accurate theory of lattice thermal conductivity in materials has remained a long-standing problem. This is primarily due to the difficulty of determining accurate interatomic force constants and the challenge of properly addressing phonon-phonon scattering in materials. In this talk, I will present a new *ab-initio* framework that accurately predicts thermal transport in both materials and nanostructures. This approach uses density functional theory to calculate harmonic and where necessary anharmonic force constants between atoms. These *ab-initio* force constants provide the foundation for two separate techniques to model diffusive and ballistic phonon transport.

By using these force constants in an iterative solution to the phonon Boltzmann transport equation, we can predict thermal conductivities for materials (i.e. Si, Ge, diamond) in excellent agreement with experiment and without the use of adjustable parameters. This Boltzmann approach is also well suited for examining nanocomposite thermoelectrics, such as *nanoparticle embedded in alloy thermoelectric* (NEAT) materials for low nanoparticle concentrations.

Nanostructures present unique opportunities for heat mitigation and thermoelectric applications. However, nanoscale thermal transport is dominated by ballistic phonons and requires a different simulation approach. By using a Green's function approach that incorporates *ab-initio* interatomic force constants, we can study how disorder affects nanoscale thermal transport in the cases of defects in carbon nanotubes as well as phonon scattering from isotopes in boron nitride nanotubes and graphene.

## **Phonon Transport Across Interfaces**

Tim Fisher  
Purdue University, USA

Phonons are the principal carriers of thermal energy in semiconductors and insulators, and they serve a vital role in dissipating heat produced by scattered electrons in semiconductor devices. Despite the importance of phonons, rigorous understanding and inclusion of phonon dynamics in simulations of modern electronic devices is very challenging, particularly because spatial confinement tends to complicate their dispersion, or frequency-wavelength, characteristics. This lecture will first provide a foundational description of phonon dynamics using a simple 1D atomic chain as a beginning example. Then, a parallel treatment of phonon dynamics using an atomistic Green's function (AGF) approach will be presented to demonstrate its ability to replicate canonical results, particularly for heterogeneous interfaces. Results from the AGF method applied to heterogeneous atomic chains, planar interfaces, and superlattices will be presented to illustrate the utility of the approach in more practical situations. The lecture will include interactive examples that utilize tools on [nanoHUB.org](http://nanoHUB.org) and its focused group, [thermalHUB](http://thermalHUB.org).

## **nanoHUB.org Tutorial: Mythbusting Scientific Knowledge Transfer in Research and Education**

Gerhard Klimeck  
Purdue University, USA

By serving a community of over 201,000 users annually with an ever-growing collection of 3,000+ resources, including 230+ simulation tools, nanoHUB.org has established itself as “the world’s largest nanotechnology user facility”. nanoHUB.org is driving significant knowledge transfer among researchers and speeding transfer from research to education, quantified with usage statistics, usage patterns, collaboration patterns, and citation data from the scientific literature. Over 850 nanoHUB citations in the literature resulting in a secondary citation h-index of 41 prove that high quality research by users outside of the pool of original tool developers can be enabled by nanoHUB processes. Cumulatively, over 14,000 students in over 760 formal classes in over 185 institutions have used nanoHUB simulations proving that research codes can be transferred systematically into class room use without major code rewrites. In addition to high-quality content, critical attributes of nanoHUB success are its open access, ease of use, utterly dependable operation, low-cost and rapid content adaptation and deployment, and open usage and assessment data. This tutorial will overview usage scenarios, typical web-deployed tool expectations, and nanoHUB impact on research and education.

## **The ATK platform for atomic-scale modeling**

Kurt Stokbro  
QuantumWise A/S, Denmark

Atomistix ToolKit (ATK) from QuantumWise is a platform for atomic-scale modeling that provides an user-friendly interface to a wide variety of state-of-the-art simulation codes, including DFT, tight-binding and classical potential methods developed by QuantumWise, as well as external software packages.

The platform has a modular structure which allows for development of third-party plugins for extended and customized functionality. This makes the platform extremely versatile and efficient for working on a broad class of nano-scale problems.

In this presentation I will demonstrate the tool and discuss applications such as:

- Calculation of electrical currents at the atomic scale using the NEGF method[1].
- Calculation of properties of graphene and metal-organic interfaces[2].
- Properties of single electron transistors[3].
- How to use ATK as an interface to GPAW, VASP and other academic codes.
- Support for classical potentials, and our new project with the SCAI Fraunhofer Institute in the area of classical MD and thermal properties of materials.
- Our advanced atomic geometry builder, with extensive functionality for building surfaces, interfaces, and graphene devices.