ME 697R: Computational Methods for Nanoscale Energy Transport

Chapter 1: Introduction

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Applications of Nanoscale Energy Transport

- Thermal management of electronics
- Thermal interface materials for packaging

http://warrenkwok.blogspot.com/2007_03_01_archive.html

Courtesy Ravi Mahajan

transistor

CNT-silicon interface
Applications of Nanoscale Energy Transport

- Energy conversion


http://www.thermoelectric.com/2005/pr/tem/


photovoltaics

thermoelectrics

laser manufacturing
Parameters obtained in a smaller scale simulation can inform larger scale simulations.
The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel "for the development of multiscale models for complex chemical systems".

http://www.nobelprize.org
THE U.S. MATERIALS GENOME INITIATIVE

Meeting Societal Needs
Advanced materials are at the heart of innovation, economic opportunities, and global competitiveness. They are the foundation for new capabilities, tools, and technologies that meet urgent societal needs including clean energy, human welfare, and national security.

Accelerating Our Pace
The U.S. Materials Genome Initiative (MGI) challenges researchers, policymakers, and business leaders to reduce the time and resources needed to bring new materials to market—a process that today can take 20 years or more.

Building Infrastructure for Success
The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.

Clean Energy  Human Welfare  National Security

Before MGI
After MGI
Discovery  Development  Deployment
Example Multiscale Multiphysics Approaches

Ab initio Calculations

Atomic Structure

Electronic Structure

Fermi’s Golden Rule

Time-domain Electronic Structure

Atomic Trajectory

Ab initio Molecular Dynamics

Energy Surface

Multi-variable Fitting

Empirical Interatomic Potentials

Non-equilibrium Molecular Dynamics

Equilibrium Molecular Dynamics

Lattice Dynamics

Green-Kubo Method

Phonon Dispersion Relation

Spectral Phonon Relaxation Time

Phonon BTE

Lattice Thermal Conductivity

Interface Thermal Resistance

Oscillator Model

Refractive Index in the Infrared Band

Refractive Index in the Visible Band

Electron-Phonon Coupling Factor, Electron Relaxation Time

Electron BTE

Absorptivity, Emissivity, Reflectivity

Maxwell’s Equations

Electrical Conductivity, Seebeck Coefficient

Heat Generation Rate
Laser material: Ti doped Al$_2$O$_3$

lubricant additives
First Principles Calculations: Band Structure

- Band structure of CdTe bulk and nanocrystals

(a)

(b)
First Principles Calculations: Interatomic Potentials

\[ V(r) = D_e (1 - e^{-\alpha (r-r_e)})^2 \]

\[ D_e = ?, \alpha = ?, r_e = ? \]

First Principles Calculations: Electron-Phonon Coupling

Bandstructure

Phonon dispersion

Conservation of energy & momentum

Coupling between electron states through phonon

Search phase space of both electron & phonon

Response of charge density to phonon perturbation

\[ \varepsilon' = \varepsilon \pm \hbar \omega \]

\[ k' = k \pm q \]
Molecular Dynamics Simulations: Trajectory

Trajectory of a BCC crystal,
Courtesy of Dr. Sylke Boyd at UMN

Laser ablation of metals,
Courtesy of Dr. L. V. Zhigilei at University of Virginia.

Laser ablation in the regime of thermal confinement
Fluence is 1.75 times the threshold for the onset of ablation
Laser pulse duration is 150 ps, penetration depth is 50 nm
Molecular Dynamics: Geometry Optimization


Phonon density of states
Molecular Dynamics: Thermal Conductivity

Thermal conductivity of graphene nanoribbon


Thermal rectification

Boltzmann transport equation: $k$

$$k_x = \frac{1}{V} \sum_\lambda c_\lambda v_{\lambda,x}^2 \tau_\lambda$$

$\tau$ can be from MD or first principles

Boltzmann transport equation: T distribution