NanoEnergy

ECE 597/697 Special Topics: Energy Transport and Conversion at the Nanoscale
http://blogs.umass.edu/eceng597en-zlatana/
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Meeting time and place: MWF 12:20 in Elab 306
*Office Hours*: Tue 10:30am, Wed/Fri after class?
Let’s start with a thought experiment

• There are 3 switches connected to 3 light bulbs separated by a door

• **Challenge**: determine which switch (1-3) controls which bulb (a-c) while passing through the door only once (no peeking)!
Answer: use the “thermal signature”!

- Flip switch #1, wait 5 mins. Then flip switch #2 and go through
- **Solution:** hot bulb is connected to #1, the lit bulb is connected to #2

- **Moral:** heat is not just a waste by-product of all processes
- Heat stores and transmits useful information, a “thermal signature”, of a process and is the ultimate destination of all the energy we use!
Some examples of energy processes

- **Coal fired power plant:**
  - Chemical $\rightarrow$ thermal $\rightarrow$ mechanical $\rightarrow$ electrical

- **Solar power plant:**
  - Optical $\rightarrow$ electrical
  - Optical $\rightarrow$ thermal $\rightarrow$ mechanical $\rightarrow$ electrical

- **Internal combustion engine:**
  - Chemical $\rightarrow$ thermal $\rightarrow$ mechanical
Course Themes

- “Phonons are bosons and electrons fermions” (say it fast 10 times)
- What are all these “-ons”?
- Which “-ons” do we care about and why?
- How is energy stored in crystalline solids (energy storage)?
- How is energy converted between different forms (energy conversion)?
- How is energy moved from one place to another (energy transport)?
- Why does size matter at the nanoscale?

M. E. Siemens et al., Nature Materials 9, 26-30 (2009)
In a nutshell

• We care about electrical, optical, thermal, and chemical forms of energy:
  – Electrical energy in the form of charge (electrons)
  – Thermal energy in the form of heat (phonons)
  – Optical energy in the form of light (photons)
  – Chemical energy in the form of molecules or ions

• We care about coupling between different forms of energy:
  – Photons and electrons (optical absorption ex. Solar cells)
  – Electrons and phonons (Joule Heating ex. Hot-spot in microelectronic chip)
  – Phonons and photons (radiative heat transfer, ex. Black body radiation)
  – Phonons and molecules (Vibrational and kinetic)

• We care about 3 types of transport:
  – classical (continuum) given by F=m*a, current continuity, drift-diffusion, Navier-Stokes
  – quantum (wave) given by the Schrodinger equation
  – semiclassical (particle) expressed by the Boltzmann Transport equation
Course Description:

- As electronic, optoelectronic, photonic, and fluidic devices shrink from the microscale down to the nanoscale, the mechanisms for transmitting heat, light, and energy become dramatically different.

- This course aims to provide a detailed look at thermal, electrical, optical, and molecular energy transport and conversion mechanisms at the nanoscale through a parallel treatments of phonons, electrons, photons, and molecules as energy carriers.

- This course aims to develop both fundamental understanding and descriptive tools for energy and heat transport processes from nanoscale continuously to macroscale.
Connecting nanoscale to macroscale

• How is NanoEnergy different from other sub-fields of Nanotechnology and Nanoscience?
  – Unlike nanoscale devices, for energy applications it does not suffice to study just one nanoscale object
  – Instead we must continuously connect the nanoscale to the macroscale
  – Understand how energy processes change fundamentally when we go from the macroscale (ex. engine, electric motor, solar panel) to the nanoscale (ex. Silicon nanowire, 22 nm gate MOSFET, graphene nanoribbon)
  – Focus not only on properties of nanoscale devices, but also on how they differ from their macroscale counterparts

• Example:
  – Macroscale heat transfer given by Fourier Law: \( \dot{q} = \kappa \nabla T \)
  – Nanoscale ballistic phonon transport: \( q = \sigma (T_H^4 - T_C^4) \)
Course Topics:

Topics covered each week:

0. Review of basic Classical and Quantum Mechanics
1. Intro to Nanotechnology and Nanoscale Transport Phenomena
2. Material Waves and Energy Quantization
3. Energy States in Solids
4. Statistical Thermodynamics and Thermal Energy Storage

~Oct. 1 Reading Assignment Begins

5. Energy Transfer by Waves
6. Particle Description of Transport Processes
7. Nanoscale Size Effects

~Oct. 27 Exam practice in class, Mid-term paper due

~Oct. 29 Mid-term Exam to be given in class

~Oct. 31 Discuss Final project and select topics

8. Energy Conversion and Coupled Transport Processes
9. Special Topic I: Thermoelectric energy conversion
10. Special Topic II: Computational Methods for Nanoscale Simulation

~Dec. 8 Final Projects presented, final reports due
Course Assignments

• Your grade is composed of 4 parts:
  1. Homework completion and homework quizzes
  2. reading assignment/term paper
  3. midterm exam and
  4. final project presentation and final report

• 6 homeworks assigned on a (roughly) bi-weekly schedule
• Homework collected each time next homework is assigned, but ultimately due at the exam practice class and last day of class
• Each homework followed by a short HW quiz
• Best 5 homework quiz scores count 20% of the grade
• Another 5% is for homework completion
• Reading assignment mainly consisting of review papers from the literature (typically Reviews of Modern Physics) followed by discussion and a mid-term paper
• Mid-term paper scores count 15% of the grade
• Mid-term exam counts 25%
Suggested Readings


6. Other reading assignments are possible to correlate with the final project or your interests
Final Project

- Project will be computational in nature
- Develop a Matlab code to simulate a physical process or implement a calculation based on a reading assignment
- Project done in teams of 2, however:
  - Undergraduate and Graduate students teamed up and graded separately
  - Undergraduate students present as teams and submit one report
  - Graduate students give conference-level talks individually and present a collaborative paper following guidelines and formatting for a research journal
  - All presentations are 15 min plus 5 min for questions
- Project can be selected to enhance your own research project
- Final presentation is worth 10% and project report is 25% of the grade
- Presentation grade will be based on class feedback
Resources

• Course textbook:
  – “Nanoscale Energy Transport and Conversion” by Gang Chen
  – Highly recommended but not strictly required in the sense that I will not assign problems directly from the book nor test on sections that were not covered in lectures

• Lots of great resources on the internet:
  – MIT Open Courseware based on Gang Chen’s book
  – Available under ocw.mit.edu/courses
  – Look for Mechanical Engineering 2.57 “Nano-to-Macro Transport Processes”
  – Lecture videos, notes, homeworks, exams, and projects
Other “sister” courses

- Eric Pop’s “Hot Chips: Atoms to Heat Sinks” course, formerly at UIUC, now at Stanford
- Slightly more focused on devices/chips
- Lecture notes have similar coverage
- Look under Poplab@Stanford: http://poplab.stanford.edu/teaching.html
  And look for ECE598EP in the Fall of 2010

How (not) to cook an egg on your CPU.
Other web resources

• The NanoHUB is an excellent resource providing an on-line community portal
• Key features:
  – Lectures (slides+video/sound) by leading researchers in the nano area
  – Tools: simulation widgets with nice GUIs on various topics, especially in electronic structure, electron and phonon transport
  – Great way to interact with topics in electronic structure, transport, and even thermal properties

• Go to http://nanohub.org and set up a free user account
• Hosted by Purdue University, network of contributors
• thermalHub was also rolled into the nanoHub recently
• Could be used for projects (some tools even have source code available, many are in Matlab)
Particles and Kinetic Theory

- “Phonons are bosons and electrons fermions” (say it fast 10 times)
- What are all these “-ons”?
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To answer these questions, we will have to begin with a single atom, then a collection of atoms (called a crystal if the collection has a regular, periodic arrangement), and finally a collection of particles in the solid.
Conductivity from Kinetic Theory

- No energy/heat flux at equilibrium: apply a temperature gradient!
- Set an imaginary boundary and calculate the net flux through it
- Only particles within a distance $\Lambda_x = v_x \tau$ contribute to flux through the boundary
- The rest of the particles scatter in a completely random direction and do not contribute
- Number of particles lost due to motion through the barrier (assuming half goes in the $+x$ and half in the $-x$ direction):
  \[
  \frac{dn^+}{dt} = \frac{1}{2} n v_x \\
  \frac{dn^-}{dt} = \frac{1}{2} n v_x
  \]
- They take with them a total energy of:
  \[
  U^+ = n c_v \left( T - v_x \tau \frac{dT}{dx} \right) \\
  U^- = n c_v \left( T + v_x \tau \frac{dT}{dx} \right)
  \]
Conductivity from Kinetic Theory

- The total flux is then the rate of change of energy per unit time:

\[
Q^+ = \frac{dU^+}{dt} = \frac{dU^+}{dn} \frac{dn}{dt} = C_v \left( T - v_x \tau \frac{dT}{dx} \right) \frac{1}{2} n v_x \\
Q^- = \frac{dU^-}{dt} = \frac{dU^-}{dn} \frac{dn}{dt} = C_v \left( T + v_x \tau \frac{dT}{dx} \right) \frac{1}{2} n v_x
\]

- Therefore the net flux is:

\[
Q = Q^+ - Q^- = -n c_v v_x^2 \tau \frac{dT}{dx} = -\frac{1}{3} v^2 \tau C_v \frac{dT}{dx} = -\kappa \frac{dT}{dx}
\]

- Which gives conductivity as:

\[
\kappa = -\frac{Q}{\frac{dT}{dx}} = C_v v_x^2 \tau = \frac{1}{3} v^2 \tau C_v = \frac{1}{3} v \Lambda C_v
\]

- This expression is widely used, especially to estimate MFPs!
Aside

- How did $v_x^2$ become $v^2$?
- We know that $v^2 = v_x^2 + v_y^2 + v_z^2$
- Then the averages are also $<v^2> = <v_x^2> + <v_y^2> + <v_z^2>$
- Since we assume motion is random and isotropic, then there is no preferred direction of motion so $<v_x^2> = <v_y^2> = <v_z^2>$
- Therefore $<v^2> = <v_x^2>/3$
- How else could we obtain the same conclusion (with a lot more work)?
- What would the result look like in 2D?
- Hint: motion only in plane, such as many of the new 2-dimensional materials like graphene and MoS$_2$
Example: Ultrathin SOI

- L=100 nm layer of silicon surrounded by oxide

Si lattice constant is $5.43 \times 10^{-10}$ m with ?? atoms per unit cell

Matlab!
- Boltzmann constant $k_B=1.38 \times 10^{-23}$ J/K
- Average phonon velocity $v=5000$ m/s
- Mean free path $\Lambda=$average distance a particle travels before collision
- What is $\Lambda$ in this case due to collisions with the walls?
Example continued

- $\Lambda = L/2$
- $\kappa = 1/3 C_v \nu \Lambda = 1/4 k_B N \nu L$
- $\kappa = 86.25 \text{ W/m/K}$

- NOTE: conductivity scales directly with size!
- How does this compare with actual SOI?
- What happened to the temperature dependence?

- How can we have a better theory of nanoscale energy conduction?
- We need to define states better so we can count them better!
- We need to understand interactions between particles better!
- We need to take better averages!
Bulk silicon and ultrathin SOI: comparison with experiments

- Left: bulk silicon thermal conductivity over a wide range of temperatures (Glassbrenner and Slack, Phys. Rev. 134, A1058-A1069 (1964))
- Right: measurements of thermal conductivity in 20, 30, and 100 nm SOI (Liu and Asheghi, JHT 2006) and theoretical calculations based on full phonon dispersion
Example 2: Graphene nanoribbons

• Graphene is a single atomic sheet of carbon atoms with many unique electronic, mechanical, and thermal properties
• 2010 Nobel Prize in Physics went to Geim and Novoselov for work on graphene
• Take a narrow ribbon of graphene, $W=100$ nm
• Sound velocity $v=2.1\times10^4$ m/s
• What about atomic density for a 2D material?
• Take the thickness to be the same as the spacing between atomic layers in graphite ($d=0.335$ nm)
• Atomic density $\sim36$ atoms/nm$^2$
• $\kappa=\frac{3}{8}k_B N v L=1168$ W/m/K
Thermal conductivity in graphene ribbons

- How well did we do?

\[ \theta_C = 30^\circ \]

\[ \theta_C = 0^\circ \]

\[ \Delta (\text{nm}) \]

\[ k (\text{Wm}^{-1}\text{K}^{-1}) \]

\[ T (\text{K}) \]

\[ \omega (\text{meV}) \]

\[ k_{\text{V15 \mu m}} \]

\[ k_{\text{V10 \mu m}} \]

\[ k_{\text{V0.65 \mu m}} \]

\[ k_{\text{V0.45 \mu m}} \]

\[ k_{\text{V0.26 \mu m}} \]

\[ \text{GNR W} \sim 65 \text{ nm}, L = 260 \text{ nm} \]  
\[ \Delta = 0.65 \text{ nm} \]

Answer: depends on the sample!

We are still missing too many details:
- temperature
- direction
- environment (substrate)