Purdue University Fall 2017

ECE 656: Electronic Transport in Semiconductors: *A Modern Approach*

M.S. Lundstrom (lundstro at purdue.edu)

Tuesday and Thursday 10:30 – 11:45 AM EE 115

Course Description: This course is about the flow of charge and heat in semiconductors with an emphasis on transport in novel materials and nanoscale devices. The objective is to develop a broad understanding of basic concepts. In 1990, the first edition of *Fundamentals of Carrier Transport* was written as a text for this course. The second edition was written in 2000, but much has changed since then. Today, in work at the nanoscale, we encounter ballistic, quasi-ballistic, and quantum transport, but just as often, problems involve traditional transport theory, such as diffusion equations, Hall effect, etc. Those who work on electronic materials and devices need to understand both traditional and modern transport theory and how to apply it in practice. Covering all this ground in one semester without assuming a long string of prerequisites, requires a new approach. Fortunately, research over the past three decades has provided us with a deep understanding of transport at the nanoscale and with simple, clear, elegant approaches that seamlessly connect transport at the nanoscale to transport at the macroscale. This course is a first draft of a third edition of the book with a new title: *Fundamentals of Carrier Transport: A Modern Approach.* This course is designed for experimentalists, device physicists, theorists, and computational experts who work on electronic materials and devices. It is accessible to students with a general, introductory background in semiconductors and addresses the fundamentals of charge and heat transport that every materials and device researcher should understand and be able to apply.

The course consists of three five-week modules:

Part 1 reviews advanced semiconductor fundamentals and addresses new topics such as electron and phonon scattering.

Part 2 examines near-equilibrium transport of electrons and phonons in the presence of small gradients in the electrochemical (quasi-Fermi) potential and/or temperature. The influence of magnetic fields is also discussed. Commonly used characterization methodologies, such as Hall effect measurements, are described. The Landauer approach is used to describe transport from the ballistic to diffusive limits and is related to the traditional Boltzmann Transport Equation approach.

Part 3 focuses on far-from-equilibrium transport. High-field transport in bulk semiconductors is discussed as are so-called "non-local" transport effects that lead to "velocity overshoot" in nanoscale devices. A gentle introduction to the Non-equilibrium Green's Function (NEGF) approach to dissipative quantum transport is also presented. Sophisticated numerical simulations are used to illustrate the effects discussed in this part. Some understanding of the numerical methods is necessary, but our goal is not to learn how to write simulation programs; it is to understand how the simulations work, so that we know when a simulation should be used and how to interpret the results.

ECE 656 Fall 2017: Course information

Instructor: M.S. Lundstrom (lundstro at purdue.edu)

Class meetings: Tues, Thurs. 10:30 – 11:45 PM EE-115

Office Hours: MWF, 11:00-12:00 noon, Wang Hall 3055
(or make an appointment for a different time by e-mail.)

In addition to office hours, students are encouraged to make use of the discussion forum.

Discussion Forum: piazza.com/purdue/fall2017/ece656/home

Prerequisites: ECE 606 or equivalent (basic introduction to semiconductor materials and devices, solid-state physics, and quantum mechanics). Or consent of instructor.

Texts:

Near-equilibrium Transport: Fundamentals and Applications (NET)
Mark Lundstrom, World Scientific (2012).
(a draft copy of this text will be distributed to 656 students)

Fundamentals of Carrier Transport, 2nd Edition (FCT)
Mark Lundstrom, Cambridge University Press (2000)
ISBN-13: 9780521637244 (paperback)

Handouts and class notes will also be distributed from time to time

The **course homepage** provides complete information about the course and will be used for posting weekly reading assignments, homework assignments and solutions, supplemental material, announcements, etc.).

http://nanohub.org/groups/ece656f17

Learning Objectives:
This course addresses the fundamentals of charge and heat transport that every semiconductor materials and device researcher should understand and be able to apply. A successful student will have demonstrated:

i. An understanding of electron and phonon scattering in semiconductors and the Boltzmann Transport Equation and how to solve it.
ii. Knowledge of near-equilibrium (i.e. low-field, small bias) semi-classical electron and phonon transport. An ability to relate transport coefficients to material parameters and to analyze and interpret common measurements.
iii. An understanding of far-from-equilibrium semi-classical transport in bulk semiconductors and devices and an acquaintance with quantum transport in small devices.

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Course Format: During a typical class session, I plan to present 2 or 3 ~20 minute lectures with time after each of these for questions and discussion. The course will make use of two different textbooks to amplify and extend the material covered in the lectures. Online lectures to supplement much of the material covered are also available.

Homework Assignments: Working homework problems is where "active learning: happens. It is essential for understanding a course like this. Homework will be assigned. It will not be graded, but solutions will be posted and discussed in class.

Exams: Three (3) exams will be given. Studying for exams cements your understanding of the material. My goal is that each of you develops an understanding of this body of knowledge that provides you with a foundation for a decades long career. To help you achieve this solid understanding, every student will have an opportunity to repeat the first two exams, and only the highest score will count. The first two exams will be conducted in class. The third exam will be conducted during finals week, but it will only cover Part 3.

Quizzes: Three short, multiple-choice quizzes will test your understanding of the material covered in each of the three parts of the course. These quizzes will be given during office hours, and you will have two opportunities to take each quiz. The goal is to be sure that you have a basic understanding of the material covered, so that you can carry on a thoughtful conversation about transport theory with colleagues or with experts.

Project: Another good way to learn the material, is to do a project; one mini-project will be assigned. I will assign one topic that each student in the class will work on. The work must be yours and yours alone. You will write a report of no more than 20 pages (space and one-half) including figures but not including references. You will be graded on technical accuracy, but also on the organization, clarity, and quality of the writing. More information on the project will be provided later in the semester.

Class participation: You can help me make this course better by identify good references for each of the 15 weeks, good papers that can illustrate the applications of methods covered in class, etc. By providing me with one, good, relevant reference for the course, you will receive 25 participation points.

Grading:

Exams: (3)	100 points each
Quizzes (3)	25 points each
Class participation	25 points
Project:	100 points
Total:	500 points

Class Attendance is important. If you must miss class, you are responsible for any material, information, handouts, announcements, etc. that you missed.

Academic Dishonesty

Every member of the Purdue community is expected to practice honorable and ethical behavior inside and outside the classroom. Any actions that might unfairly improve a student's score on the exams, quizzes, or project will be considered cheating and will not be tolerated.

Examples of cheating include (but are not limited to):

- Sharing results or other information during an examination.
- Bringing forbidden material or devices to an examination.
- Working on an exam before or after the official time allowed.
- Requesting a re-grade of answers or work that has been altered.
- **Submitting a project that is not completely your own work.**

At the instructor's discretion, cheating will result in a reduced score, a zero score, or a failing grade for the course. **All occurrences** of academic dishonesty will be reported to the Assistant Dean of Students and copied to the ECE Associate Head of Education. If there is any question as to whether a given action might be considered as cheating, please see the instructor before you engage in any such action.

Academic integrity is one of the highest values that Purdue University holds. Individuals are encouraged to alert university officials to potential breeches of this value by either emailing integrity@purdue.edu or by calling 765-494-8778. While information may be submitted anonymously, the more information that is submitted provides the greatest opportunity for the university to investigate the concern.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Here are ways to get information about changes in this course.

- Course webpage
- Instructor's email
- Instructor's phone

Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructor via email or phone. <u>You are expected to read your @purdue.edu email on a frequent basis.</u>

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Disclaimer: This information is subject to change.
Class announcements will supersede prior written information and will be posted on the course homepage.

ECE 656 Fall 2017: Course information (continued)

Some concluding comments:
Over the past several decades, theory, modeling, and simulation have developed and matured to support advancing semiconductor technology. It began in 1950 with Van Rooesbroeck's formulation of "the semiconductor equations" (the continuity and Poisson equations with the drift-diffusion equations) and continued through the development of the "full quantum" Non-Equilibrium Green's Function (NEGF) approach. Today, we have a comprehensive set of powerful approaches and simulation tools, and the use of these tools and techniques is now integral to research and development in semiconductor materials and devices. Unfortunately, there is no single tool or technique that can be guaranteed to give the correct answer to any given problem. Actually, I consider this to be fortunate because it makes the topic much more interesting. When we encounter a problem, we need to select an appropriate analysis technique, understand what it can and cannot do, and then extract the information and more importantly, insights, that are possible. We often find that a problem requires more that one analysis or simulation technique. To make use of the powerful set of techniques and tools that are available today requires a broad and deep understanding of both electron and phonon transport. The goal of this course is to help students develop such an understanding.

To adequately cover the topics addressed in the course would require several three-credit courses, but we do not need to be experts in everything. We need to understand the broad principles that tie the field together along with a few analysis techniques that are routinely used. With this broad understanding, we should be able to follow conference presentations and papers by experts and analyze the experiments commonly done while developing electronic materials and devices. I will explain how I understand transport theory, but each of us needs to develop our own understanding. This doesn't mean remembering what I say, or what other textbooks say, it means ***understanding*** transport theory. Steven Chu (the 1997 Nobel laureate in physics) has this advice:

> "Learning science and thinking about science or reading a paper in science is not about learning what a person did. You have to do that, but to really absorb it, you have to turn it around and cast it in a form as if you invented it yourself…. you try to internalize it in such a way that it really becomes intuitive."
>
> -- Steven Chu (1997 Nobel laureate in Physics)

This course provides you with an opportunity to develop a broad, intuitive understanding of transport theory and to become familiar with many of the techniques commonly used in work on semiconductor materials and devices. Good luck in ECE-656.

ECE 656 Fall 2017: Course information (continued)

Part 1 Advanced semiconductor fundamentals

Week 1: August 21, 2017: Review of Fundamantals
Reading Assignment: FCT 1.1-1.6, 1.8 / NET 1.1-1.6, 9.1-9.2

Lecture 0: Course Overview
Lecture 1: Band Structure and Phonon Dispersion
Lecture 2: Semiclassical Transport
Lecture 3: Heterostructures
Lecture 4: Quantum Confinement
Lecture 5: Density of States
Lecture 6: Sums and Integrals

Week 2: August 28, 2017: Introduction to Carrier Scattering
Reading Assignment: FCT 1.7, 2.1-2.3, 5.2 / NET 6.2

Lecture 7: Fermi's Golden Rule
Lecture 8: Characteristic Times
Lecture 9: Introduction to Carrier Scattering

Week 3: September 4, 2017: Charged Impurity Scattering
Reading Assignment: FCT 2.4

Lecture 10: Conwell-Weiskopff Approach
Lecture 11: Screening
Lecture 12: Brooks-Herring Approach

Week 4: September 11, 2017: Electron-Phonon and Phonon-Phonon Scattering
Reading Assignment: FCT 2.5-2.14 and phonon-phonon scattering handout.

Lecture 13: Electron-Acoustic Phonon Scattering
Lecture 14: Other Electron-Phonon Scattering
Lecture 15: Electron Scattering in a Nutshell
Lecture 16: Phonon-Phonon Scattering

Week 5: September 18, 2017: Introduction to the BTE
Reading Assignment: FCT 3.1-3.4 / NET 7.1-7.4

Lecture 17: The Boltzmann Transport Equation (BTE)
Lecture 18: Solving the BTE using the Relaxation Time Approximation (RTA)
Lecture 19: Review of Indicial Notation

Exam 1: September 21, 2017

Part 2 Near-equilibrium transport of electrons and phonons

Week 6: September 25, 2017: The Landauer Approach to Electron Transport
Reading Assignment: FCT 9.9 - 9.11 / NET 2.1-2.7, 3.1-3.5

Lecture 20: From the BTE to the Landauer Approach
Lecture 21: Channels and Transmission
Lecture 22: Fermi Window and the Current Expression
Lecture 23: Resistors: 1D, 2D, and 3D / Ballistic, diffusive, and in between

Week 7: October 2, 2017: Near-equilibrium Transport in the Presence of B-fields
Reading Assignment: NET 3.1-3.5, 7.5, 8.6

Lecture 24: Solving the BTE with a B-field
Lecture 25: Simpler Approach
Lecture 26: Hall Effect
Lecture 27: Quantum Effects (Shubnikov-deHaas (SdH) and Quantum Hall Effect)

Week 8: October 9, 2017: Application of Landauer Approach to Phonons
Reading Assignment: NET 9.3-9.5,9.7, 9.8

Lecture 28: Phonons
Lecture 29: Heat Transport by Phonons
Lecture 30: Conductivity Accumulation Function
Lecture 31: Phonons vs. Electrons

Week 9: October 16, 2017: Thermoelectric Transport
Reading Assignment: NET 4.1-4.7, 5.1-5.6

Lecture 32: Overview of Thermoelectricity
Lecture 33: Charge Current
Lecture 34: Heat Current
Lecture 35: Coupled Current Equations
Lecture 36: TE Materials
Lecture 37: TE Devices

Week 10: October 23, 2017: Experimental Characterization
Reading Assignment: NET 8.1-8.7 /FCT4.7-4.9

Lecture 38: Two-probe, Four-probe, and TLM measurements
Lecture 39: Hall effect characterization
Lecture 40: Seebeck Coefficient, Thermal Conductivity, and zT

Exam 2: October 26, 2017
Part 3 Far from equilibrium transport in materials and devices

Week 11: October 30, 2017: The BTE revisited
Reading Assignment: FCT 3.1-3.5, 4.1-4.6 / NET 7.1-7.7

Lecture 41: Solving the BTE: Near-equilibrium/in the bulk
Lecture 42: Near-equilibrium Transport Effects
Lecture 43: The BTE Collision Operator and Relaxation Time Approximation
Lecture 44: Solving the BTE in Devices: The challenge

Week 12: November 6, 2017: Balance Equations for Near-Equilibrium Transport
Reading Assignment: FCT 5.1-5.3.2 and 5.7

Lecture 45: Moment Equation Approach
Lecture 46: Moment Equations and the DD Equations
Lecture 47: Moment Equations for Thermoelectric Transport

Week 13: November 13, 2017: Hot Carrier Transport
Reading Assignment: FCT 5.3.3, 5.4, 5.5, 6.1-6.9, 7.1-7.7

Lecture 48: Energy Transport Equations
Lecture 49: Monte Carlo Simulation
Lecture 50: Hot Carrier Transport in Bulk Semiconductors

Week 14: November 20/ November 27, 2017: Transport in Devices
Reading Assignment: FCT 8.1-8.10

Lecture 51: Nonlocal Carrier Transport
Lecture 52: Velocity Overshoot
Lecture 53: Ensemble Effects in Non-Local Transport
Lecture 54: Diffusion Equations at the Nanoscale
Lecture 55: Solving the Ballistic BTE in Devices

Week 15: December 4, 2017: Ballistic and Quantum Transport in Devices
Reading Assignment: FCT 9.7, 9.8, 9..11

Lecture 56: The Local Density-of-States: Semi-classical
Lecture 57: Introduction to Quantum Transport in Devices

Exam 3: During finals week