ECE606: Solid State Devices
Lecture 1

Your Instructor and Teaching Assistants

- Gerhard Klimeck
  - Prof. at Purdue for 8 years
  - Principal at NASA/JPL, 6 years
  - Texas Instruments, 4 years
  - Over 340 papers on devices/physics
- Parijat Sengupta
  - 5th year graduate student
- Yaohua Tan
  - 5th year graduate student
- Matthias Yui-Hong Tan
  - 3rd year graduate student
- Yuling Hsueh
  - 2nd year graduate student
ECE606: Solid State Devices
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Gerhard Klimeck
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Course Information

Books
• Advanced Semiconductor Fundamentals (QM, SM, Transport) first 5 weeks
• Semiconductor Device Fundamentals (Diode, Bipolar, MOSFET) Weeks 6-15

HW/Exams
• HW (9 HW, all will be graded; solutions will be provided; distributed every Tuesday, due at the beginning of the lecture)
• 3 exams (~5 weeks apart)

Website
• http://cobweb.ecn.purdue.edu/~ee606/
• https://blackboard.purdue.edu (grades and optional notes)
• https://nanohub.org/resources/5749 (full course on-line from Spring 2009)

Office hours
• Klimeck: 1:30-2:30 Tue@EE 323, Thu 4:30pm-5:30pm@EE323
Your Purdue Resources

Klimeck
- Leads the Network for Computational Nanotechnology (NCN)
- NCN hosts nanoHUB.org
  - >230,000 users
  - 172 countries
  - ~15 professional staff
  - 5 other universities

>3,000 resources on line
Also THIS WHOLE course
nanohub.org/resources/5749
Or search for “nanohub 606”

Outline

- Course information
- Motivation for the course
- Current flow in semiconductors
- Types of material systems
- Classification of crystals
  - Bravais Lattices
  - Packing Densities
  - Common crystals - Non-primitive cells
    - NaCl, GaAs, CdS
  - Surfaces

- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org
Moore’s Law
a Self-Fulfilling Prophesy


Klimeck – ECE606 Fall 2012 - notes adopted from Alam
Technical Developments to enable Moore's Law

Robert Chau (Intel), 2004

- Industry plans have a 5-10 year horizon
- Industry has been on time:
  - 32nm node predicted in 2004 and announced 2009
- There are NO technically viable solutions beyond 2015

Device Sizes and Transport Concepts

Macroscopic dimensions

Non-Equilibrium Quantum Statistical Mechanics

Atomic dimensions

Diffusive

Ballistic

Quantum

Unified model

Non-Equilibrium Green Functions
Today's CPU Architecture
Heat becoming an unmanageable problem

Grand Challenges in Electronics

Vacuum Tubes  Bipolar  MOSFET  Now ??
1906-1950s  1947-1980s  1960-until now  Spintronics
Bio Sensors
Displays ....
Outline of the Course

- Device-specific system design
  - TFT for Displays
  - CMOS-based Circuits for µP
  - LASERS for Disk Drives
  - MEMS for Read heads

- Physical Principle of device operation
  - Resistors (5 wk)
  - Diodes (3 wk)
  - Bipolar (3 wk)
  - MOSFETs (3 wks)

- Foundation in Physics
  - Quantum Mechanics
  - Statistical Mechanics
  - Transport Equations

Relation to Other MN-Area Courses

- Device-specific system design
  - EE 695F: RF Design
  - EE 695E: Opto-system
  - BME 695A: Bio-system Design

- Application specific device operation
  - EE 654: Advanced Semi Dev.
  - EE 612: VLSI Devices
  - EE 520: Bio-Systems

- Physical Principle of device Operation
  - EE 606: Basic Semi Dev.
  - EE 604: EM, Magnetics

- Foundation
  - EE 656: Semi-Transport
  - EE 659: Quantum Transport
  - PHYS 570B: Bio-physics
  - Finite Element, Molecular Dynamics, Monte Carlo
  - Characterization
  - ECE 557: Fabrication
Motivation and Importance of 606

- Define “the language”
  - Specialty area in ECE: MN - Micro – Nano – Electronics
  - Bridge different communities, Electrical Engineering, Physics

- Fundamentals of Semiconductor Devices
  - How to “think” about electrons in a semiconductor
    - Foundation of typical job interviews –
      - technical interviews will typically not go into more detail
      - Probe the fundamental understanding of electronic behavior in Semiconductor
    => Your entry into a technical job in Semiconductor Industry

  - Required knowledge in the MN area Qualifying Exam
    => Your entry into the PhD program in the MN area

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Current Flow Through Semiconductors (5 weeks)

\[ I = G \times V = q \times n \times v \times A \]

- Depends on chemical composition, crystal structure, temperature, doping, etc.
- Could be tabulated for “known” materials
- Need a theory for engineering of new devices/materials

Quantum Mechanics + Equilibrium Statistical Mechanics
  - Encapsulated into concepts of effective masses and occupation factors (Ch. 1-4)

Transport with scattering, non-equilibrium Statistical Mechanics
  - Encapsulated into drift-diffusion equation with recombination-generation (Ch. 5 & 6)

Computing Carrier-Density and Velocity

**Atomic composition**
- *number of electrons per atom*

**Arrangement of atoms**
- *not all electrons are available for conduction*

**For Periodic Arrays**
- *simplification for computation*
  - Concept of Unit Cells
  - Simple 3-D Unit Cells
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Elemental and Compound Semiconductors
Not all combinations possible: lattice mismatch, room temp. instability, etc. are concerns

Elemental (e.g., Si, Ge, C)

Si: $260 billion industry

Compound

IV-IV: Si-Ge, Si-C
SiGe: stressors
SiC: radiation

III-V: InP, GaAs,
(\(\text{In}_x\text{Ga}_{1-x})\text{(As}_y\text{P}_{1-y})\)
Lasers/detectors expensive

II-VI: CdTe
Far IR detectors
Soft and difficult

IV-VI: PbS
First semiconductor diodes
Very soft and difficult
Arrangement of Atoms:

- **solid crystals**
  - Specific position
  - Specific orientation

- **plastic crystals**
  - Specific position
  - Random orientation

- **liquid crystals**
  - Random position
  - Specific orientation

- **liquid**
  - Random position
  - Random orientation

**Arrangement of Atoms**

- Cross section of a MOSFET
  - Poly-crystalline Thin Film Transistors
  - Amorphous Oxides
  - Crystalline

- Perfectly arranged Si Crystal

- Quantitative definition: Correlation spectrum and diffraction pattern
- Modern solid state devices use all forms these forms of materials
- Focus on Crystals first - relatively simple
- Transfer knowledge of electronic behavior in crystals to other materials
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Unit cell of a Periodic Lattice

"Infinitely" extended
2D shown
3D same concepts

\[ N_A = 6 \times 10^{23}/\text{mol} \]
\[ \Rightarrow \text{Can NEVER solve this, even on the largest computer} \]
\[ \Rightarrow \text{Simplify to a repeated (small) cell} \]

- Unit cells are not unique
- Unit cells can be Primitive or Non-primitive
- Property of ONE CELL defines the property of the solid
How to define ONE primitive cell?

- Choose a reference atom
- Connect to all its neighbors by straight lines
- Draw lines (in 2D) or planes (in 3D) normal to and at the midpoints of lines drawn in step 2
- Smallest volume enclosed is the Wigner-Seitz primitive cell

Wigner-Seitz cell is ONE definition of a Unit Cell that always works
There are other ways of construction!

Geometry of Lattice Points

In a Bravais lattice,
- every point in the lattice can be “reached” by integer translation of unit vectors
- every point has the same environment as every other point (same number of neighbors, next neighbors, …)

R' = h\vec{a} + k\vec{b}
Unit Cells in One-dimensional Crystals

There is exactly ONE primitive unit cell in a 1D system

No system truly 1-D, but ....

• 1D properties dominate behavior in some material
  • e.g.: polymers, DNA, 1D heterostructures (lasers, RTDs)
• Can often be solved analytically, many properties have 2D/3D analogs

Polyacetylene

PPP

Periodic Lattice in 2D (5-types)

Original image from: http://upload.wikimedia.org/wikipedia/commons/e/ee/2d-bravais.svg

1. Parallelogrammic or oblique
2. Square
3. Centered rectangular or rhombic or triangular
4. Hexagonal
5. Rectangular
A and B do not have identical environments

This is a Graphene sheet which has recently been isolated from Graphite by adhesive tape stamping.

Ref. Novoselov, Geim, et al.

Conversion into a Bravais lattice:
- Combine A and B into a single basis
- Obtain a rhombic Bravais lattice


Not a Bravais Lattice, but ...

Escher Tiling  Kepler Tiling

....but these can be converted into Bravais lattice
Not a Bravais Lattice and ...

Penrose Tiles

Ancient Tiles

Two different unit cells in **random order**

... these **CANNOT** be transformed to Bravais lattice

ex. Aluminum-Manganese compounds, non-sticky coats

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Bravais lattice in 3D (14-types)

<table>
<thead>
<tr>
<th>Triclinic</th>
<th>Cubic</th>
<th>Tetragonal</th>
<th>Orthorhombic</th>
<th>Rhombohedral</th>
<th>Hexagonal</th>
<th>Monoclinic</th>
</tr>
</thead>
<tbody>
<tr>
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</table>
Duplicated Bravais Lattice

Unlucky Frankenheim (1842) counted 15 unit cells! Bravais pointed out that 2 cells were duplicated.

Tetragonal face centered

Tetragonal body centered

Tetragonal FC = Tetragonal BC

3 Dominant Bravais Lattices

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Cubic conceptionally simple, but experimentally very unusual. Polonium84

70-75% of all natural crystalline materials.
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Simple Cubic Cubic Lattice: Number of atoms

Points per cell
= \frac{1}{8} \text{ points/corner} \times 8 \text{ corners}
= 1 \text{ Point/cell}
\text{(depends on definition of cell)}

Number density
= \frac{1}{a^3} \text{ points/cm}^3
\text{(does not depend on cell definition)}
Surfaces are critical in semiconductors:
- Vertical stacking of materials
  => misalignment
  => dangling bonds
  => loose electrons
  => Different surface chemistry

Areal Density

\[ \text{Areal Density} = \frac{1}{4 \text{ per corner}} \times \frac{4 \text{ corners}}{a^2} = \frac{1}{a^2} \text{ cm}^{-2} \]

Areal density (face diagonal)

\[ \text{Areal density (face diagonal)} = \frac{1}{4 \text{ points/corner}} \times \frac{4 \text{ corners}}{\sqrt{2}a^2} \approx 0.7/a^2 \text{ cm}^{-2} \]

Packing density

\[ \text{Packing density} = \frac{\text{volume filled}}{\text{total volume}} \]

\[ R = \frac{a}{2} \text{ maximum radius} \]

\[ V = \frac{4}{3} \pi R^3 \text{ Volume of a sphere} \]

\[ P = \frac{1}{8} \times \frac{4}{3} \pi R^3 \times (8 \text{ corners}) / a^3 \]

\[ = \frac{\pi}{6} \]

\[ \approx 52\% \]

(about HALF of the volume is EMPTY)

Typical for crystals and amorphous materials

(does not depend on cell definition)
BCC and FCC lattices

Points per cell
= \frac{1}{8} \times 8 \text{ @corners}
+ 1 \text{ @inside}
= 2

Points per cell
= \frac{1}{8} \times 8 \text{ @corners}
+ \frac{1}{2} \times 6 \text{ @faces}
= 4

Hexagonal Closed-Packed

Points per cell
1/2 \times 2 \text{ @faces} = 1

1/2 \times 1/3 \times 12 \text{ @corners} = 2

3 points/cell
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In a Bravais lattice, every point has the same environment as every other point (same number of neighbors, next neighbors, …)

$$R = h \mathbf{a} + k \mathbf{b}$$
NaCl is normal household cooking salt
We see the crystals every day – what is the crystal structure?
At first glance it looks like a simple cubic cell
⇒ one atom on each corner
⇒ But they are different ⇒ not a Bravais lattice

= 

a basis
of 2 atoms
arranged in
FCC

For more discussion, see Kittel and Ashcroft/Mermin
Zinc-Blende Lattice for GaAs

Atoms/cell=(1/8)x8 + (1/2)x6 + 4=8

Tetrahedral structure

GaAs Crystal Plotted in Crystal Viewer
GaAs Crystal Just One Species
Focus on Few

GaAs Crystal Just One Species
Focus on Few - Take out a Few
GaAs Crystal Just One Species
A FCC Cell!

- FCC cell – 4 atoms per unit cell
GaAs Crystal Both Species

- FCC cell – 4 atoms per unit cell – brown species

GaAs Crystal Both Species

- FCC cell – 4 atoms per unit cell – brown species
  - Focus on a few of the “blue species”
GaAs Crystal Both Species

- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species
GaAs Crystal Both Species

- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

GaAs Crystal - 2 FCC

- Zincblende – 2 FCC bases – separated by \([\frac{1}{4} \ \frac{1}{4} \ \frac{1}{4}]\)
• Zincblende – GaAs - 2 FCC bases – separated by $[\frac{1}{4} \frac{1}{4} \frac{1}{4}]$  
• Diamond – Si - 2 FCC bases – separated by $[\frac{1}{4} \frac{1}{4} \frac{1}{4}]$

(Cd) atoms/cell = $(1/6)x12 + (1/2)x2 + 3 = 6$
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