ECE 488: Compound Semiconductors

M,W,F 11:00 – 11:50, 3013 ECEB
Professor John Dallesasse
2114 Micro and Nanotechnology Laboratory
Tel: (217) 333-8416
E-mail: jdallesa@illinois.edu
Office Hours: Tuesday 13:00 – 14:00
Lecture 19: October 5th, 2016
Assignments

• Reading from “Compound Semiconductors and Devices – An Introduction”
  – Wed 9/28: §’s 4.4, 4.4.1, 4.4.2, 4.4.3, 4.5
  – Fri 9/30: §’s 4.6, 4.6.1, 4.6.2
  – Mon 10/3: §’s 4.7, 4.7.1, 4.7.2, 4.8
  – Wed 10/5: §’s Chapter 5
  – Fri 9/30: None

• Midterm Exam, Friday 10/7
  – TA Office Hours: Time extended if students present

• Homework: To be posted 10/7, due 10/14
Midterm Exam

- Chapters 1-3
  - Concepts
  - Detailed Calculations
- Chapter 4
  - Concepts
  - Simple Calculations
- Formula Sheet
  - One formula sheet is allowed
  - 8.5” X 11”, double sided, hand written
- Calculator Allowed
  - Cell phone cannot be used as a calculator
  - No formulae can be stored in calculator
  - Calculator must not have any type of networking capability
Today’s Agenda

• Finish Phonons
• Density of States Effective Mass
• Conductivity Effective Mass
• Mobility
• Intentional Impurities
# Tentative Schedule [1]

<table>
<thead>
<tr>
<th>AUG 22: Introductions, Objectives, Class Outline, Policies</th>
<th>AUG 24: Motivation, Intro to Quantum Theory</th>
<th>AUG 26: Infinite Square &amp; Triangle Wells</th>
</tr>
</thead>
<tbody>
<tr>
<td>AUG 29: Potential Steps, Coulomb Well (Hydrogen Atom), Atomic Bonding</td>
<td>AUG 31: Crystal Structures, Diffraction</td>
<td>SEP 2: Reciprocal Space, Diffraction Condition</td>
</tr>
<tr>
<td>SEP 5: LABOR DAY NO CLASS</td>
<td>SEP 7: The Brillouin Zone, Band Structures, Density of States</td>
<td>SEP 9: Bloch Theorem, Empty Lattice Model</td>
</tr>
<tr>
<td>SEP 12: Band Gaps</td>
<td>SEP 14: Kronig-Penny Model</td>
<td>SEP 16: Effective Mass, Bloch Oscillations, Band Structure</td>
</tr>
</tbody>
</table>

**Guideline Only: Subject to Change**
<table>
<thead>
<tr>
<th>SEP 26: Doping and Deep Levels</th>
<th>SEP 28: The Fermi Integral, Free Carrier Concentration, Surface States</th>
<th>SEP 30: III-V Semiconductor Lattice Constant and Bandgap</th>
</tr>
</thead>
<tbody>
<tr>
<td>OCT 3: III-N and Group IV Semiconductors</td>
<td>OCT 5: Crystal Growth, Phase Diagrams</td>
<td>OCT 7: Midterm Exam (Tentative)</td>
</tr>
<tr>
<td>OCT 10: Energy Band Alignment, Model-Solid Theory</td>
<td>OCT 12: Strained Layer Structures</td>
<td>OCT 14: Strain Effects on Band Edges</td>
</tr>
<tr>
<td>OCT 24: Realistic Finite Quantum Wells</td>
<td>OCT 26: Superlattices and Minibands</td>
<td>OCT 28: Heterostructures in Electric Fields and the Franz-Keldysh Effect</td>
</tr>
</tbody>
</table>

**Guideline Only: Subject to Change**
Phonons
Lattice Vibrations - Phonons

- The tetrahedron crystal lattice can be seen as an array of masses (core ions) connected by four springs (with a length of the bond length, $a_0$).
- At a finite temperature, the quantization of the lattice vibration is called “phonon”.
- The generation (emission) of phonons is the main relaxation mechanism of high energy electrons toward equilibrium in semiconductors.
- In such a spring-mass network, the springs try to keep masses remaining on their equilibrium positions, i.e., $a_0 = $ constant. The force between the neighboring atoms is governed by Hook’s law:
  \[ F = \beta x \]
  where $\beta$ is the Hook’s law constant and $x$ is the displacement.
The one-dimensional chain of diatomic crystal with different masses $m$ and $M$ ($M > m$) has a periodicity of $2a$. The atoms are connected by springs of elastic constant $\beta$. Vibration is restricted to the longitudinal direction first. Consider the nearest-neighbor interactions only. A force induced movement of mass $2n$ will also move masses $2n+1$ and $2n-1$. The force on mass $2n$ is expressed as

$$F_{2n} = F_{2n+1} + F_{2n-1}$$

$$= \beta(u_{2n+1} - u_{2n}) + \beta(u_{2n-1} - u_{2n})$$

$$= \beta(u_{2n+1} + u_{2n-1} - 2u_{2n})$$

Here $u_n$ is the displacement of the atom.

**In Equilibrium:**

$$F_{2n} = F_{2n+1} + F_{2n-1} = 0$$
All springs under tension in linear region, $F = \beta x$

Total Force on mass “m” at $x=x_{2n}$:

$$F_{2n,\text{Total}} = \beta\left(x_{2n+1} - x_{2n}\right) + \beta\left(x_{2n-1} - x_{2n}\right)$$

$$= \beta\left(\left(x_{0,2n+1} + u_{2n+1}\right) - \left(x_{0,2n} + u_{2n}\right)\right) + \beta\left(\left(x_{0,2n-1} + u_{2n-1}\right) - \left(x_{0,2n} + u_{2n}\right)\right)$$

$$= \beta\left(\left(x_{0,2n+1} - x_{0,2n}\right) + \left(u_{2n+1} - u_{2n}\right)\right) + \beta\left(\left(x_{0,2n-1} - x_{0,2n}\right) + \left(u_{2n-1} - u_{2n}\right)\right)$$

$$= \beta\left(u_{2n+1} - u_{2n}\right) + \beta\left(u_{2n-1} - u_{2n}\right)$$

Where:

$x_{2n}$ is the location of mass “m” and

$x_{0,2n}$ is the equilibrium position of mass “m”

Similar notation is used for masses at other locations
Newton’s law also tells us that the forces on mass $2n$ and $2n+1$ are

$$
\begin{align*}
F_{2n} &= m \frac{d^2u_{2n}}{dt^2} = \beta(u_{2n+1} + u_{2n-1} - 2u_{2n}) \\
F_{2n+1} &= M \frac{d^2u_{2n+1}}{dt^2} = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1})
\end{align*}
$$

Since we assumed the masses are linked by springs, we expect the solutions to be oscillating waves.

Assume the “periodic” solutions have the form $u_n \sim \exp[i(\omega t - nk\alpha)]$,

\begin{align*}
\text{Index} & & \text{Solution} \\
2n & & u_{2n} = A \exp[i(\omega t - 2nk\alpha)] \\
2n+1 & & u_{2n+1} = B \exp[i(\omega t - (2n+1)k\alpha)]
\end{align*}

where a wave number $k$ is assumed and $\omega$ is the oscillation frequency of both type of atoms. $A$ and $B$ are the amplitude of oscillation.

By the same method, we can also write

\begin{align*}
\text{Index} & & \text{Solution} \\
2n+2 & & u_{2n+2} = A \exp[i(\omega t - (2n+2)k\alpha)] = u_{2n} \exp(-2ika) \\
2n-1 & & u_{2n-1} = B \exp[i(\omega t - (2n-1)k\alpha)] = u_{2n+1} \exp(2ika)
\end{align*}
1D Dispersion Relation

- Dispersion ($\omega$-$k$) relation:

Replacing all $u$'s in $F_{2n+1} = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1}) = M[d^2u_{2n+1}/dt^2]$:

$$-M\omega^2u_{2n+1} = \beta\{[1 + \exp(-2ika)]u_{2n} - 2u_{2n+1}\}$$

$$\therefore u_{2n+1} = \frac{\beta[1 + \exp(-2ika)]}{2\beta - M\omega^2}u_{2n}$$

Similarly, by replacing all $u$'s in $F_{2n}$, we have

$$-m\omega^2u_{2n} = \beta\{[1 + \exp(2ika)]u_{2n+1} - 2u_{2n}\}$$

Combining the last two equations to remove all $u$'s.

$$(2\beta - m\omega^2)(2\beta - M\omega^2) - 4\beta^2 \cos^2(ka) = 0$$

$$\Rightarrow \omega^4 - \frac{2\beta(m + M)}{mM} \omega^2 + \frac{4\beta^2 \sin^2(ka)}{mM} = 0$$

The solutions of the $\omega$-$k$ dispersion relation is

$$\omega^2_{\pm} = \frac{\beta(m + M)}{mM}\left[1 \pm \sqrt{1 - \frac{4mM \sin^2(ka)}{(m + M)^2}}\right]$$

The two solutions, $\omega_+$ and $\omega_-$ represent the optical branch and acoustical branch of the oscillation frequencies, respectively.
Phonon Energy Gaps

Analysis:

- Near the zone center, \( k \approx 0 \) and \( \sin(ka) \approx 0 \):
  \[
  \omega_+(0) = \sqrt{\frac{2\beta(m+M)}{mM}} \quad \text{and} \quad \omega_-(0) = 0
  \]

- For small \( k \), \( \sin(ka) \approx ka \). An infinite series of \( (1+x)^{\frac{1}{2}} = 1 + x/2 + \ldots \) can be used.
  \[
  \omega_-(0) \approx ka \sqrt{\frac{2\beta}{m+M}} \propto k
  \]
  \( \omega_- \) is a linear function of \( k \) near the zone center.

- Near the zone boundary:
  First we have to determine where the boundaries are located. Consider the smallest allowed wavelength of lattice vibrations in the diatomic system. The minimum half wavelength should be the lattice constant \( 2a \) or \( \lambda = 4a \). Therefore, the zone boundaries are located at
  \[
  k = \pm \frac{2\pi}{\lambda} = \pm \frac{\pi}{2a}; \quad \sin(ka) = 1.
  \]

  \[
  \Rightarrow \omega_+ = \sqrt{\frac{2\beta}{m}} \quad \text{and} \quad \omega_- = \sqrt{\frac{2\beta}{M}}
  \]
  Since \( m \neq M \) in a diatomic system, a forbidden gap is forming between \( \omega_+ \) and \( \omega_- \).
Phonon Energy Gaps

\[ \sqrt{\frac{2\beta(m + M)}{mM}} \]

\[ \omega(k) \]

\[ \omega \text{ always positive: } \]
\[ k \text{ dependence is in a } \sin^2 \text{ function} \]

Optical Branch \( (\omega_+) \)

Acoustical Branch \( (\omega_-) \)

\[ \omega_+ = \sqrt{\frac{2\beta}{m}} \]

\[ \omega_- = \sqrt{\frac{2\beta}{M}} \]
Acoustic and Optical Phonons

Relative movement of \( m \) and \( M \), i.e., \( B/A=\)?:

\[
\frac{u_{2n+1}}{u_{2n}} = \frac{\beta\left[1 + \exp(-2ika)\right]}{2\beta - M\omega^2} = \frac{B}{A} \exp(-ika) = \left(\frac{u_{2n+1}}{u_{2n}} = \frac{\beta\left[1 + \exp(-2ika)\right]}{2\beta - M\omega^2} \right) u_{2n}
\]

Amplitude Ratio

\[
\frac{B}{A} = \frac{\beta\left[\exp(-ika) + \exp(ika)\right]}{2\beta - M\omega^2} = \frac{2\beta}{2\beta - M\omega^2} \cos(ka)
\]

- **Acoustical branch** at the zone center (\( k=0 \) and \( \cos(ka)=1 \)):
  \[
  \omega = 0 \quad \text{and} \quad \frac{B}{A} = 1
  \]

The two different atoms in each unit cell move in the **same direction** with the **same amplitude**. It is called the longitudinal acoustical (LA) mode.

(LA)

The LA mode is like a sound wave in air where atoms vibrate back and forth in the direction of the wave travels. This gives alternating zones of compression and dilation. In a 3D crystal, the vibration in the plane normal to the direction of travel is called the transverse acoustical (TA) modes. For TA mode, the two different atoms in each unit cell move in the same direction but slightly different amplitudes.
Acoustic and Optical Phonons (2)

- Optical branch at the zone center:

\[ \omega = \omega_+(0) = \sqrt{\frac{2 \beta (m + M)}{mM}} \quad \text{and} \quad \frac{B}{A} = -\frac{m}{M} \]

Now the light and heavy atoms move in the opposite directions along the wave traveling direction and the displacement is inversely proportion to the mass of the atom. This branch of lattice vibration is called the longitudinal optical (LO) mode. In 3D crystals, two additional branches of lattice vibration perpendicular to the wave front is the transverse optical (TO) modes, where the neighboring atoms also move in opposite directions.
• **Phonons in semiconductors:**
  The dispersion relation ($\omega-k$) of phonons can be plotted in the exact same way as the band structure for electrons in a crystal. The $E-k$ curves of phonons in semiconductors are more complicated due to polarization effect.

  For compound semiconductors, in optical modes, the relative displacement of two different atoms in the opposite directions sets up an electric field or a net polarization ($P$). The induced polarization ($D=\varepsilon E+P$) causes splitting of TO/LO phonons at the zone center.

The bonding in III-V compound semiconductors is not purely covalent but with some ionic properties. The group-III and group-V atoms carry negative and positive charge, respectively.
Under equilibrium, the polarization components compensate each other and the net polarization equals zero.

When the neighboring atoms in a tetrahedron structure is stretched or compressed, a net polarization is created.

The created piezoelectric field adds to additional carrier scattering and lowers the carrier mobility.
Phonons in GaAs and Si

- Si has a higher optical phonon frequency due to its lighter mass.
- Si crystal is a monoatomic system. However, the springs on either side of a silicon atom are arranged different. This causes the generation of the optical branch modes.
- At zone center, the piezoelectric effect in GaAs causes LO/TO mode splitting.
- GaAs has a LO phonon energy of 36 meV.
Phonon Momentum

A phonon of wave vector $\mathbf{K}$ will interact with particles such as photons and electrons as if it had a momentum $\hbar \mathbf{K}$. However, a phonon does not carry physical momentum, since the only true mechanical momentum that can arise is a rigid motion of the whole crystal. The vibration modes transport energy, but they are completely described by the relative motion of the individual atoms, whose average displacement is zero. Therefore, they cannot contain a net linear momentum, i.e.,

$$p = M(d/dt)\sum u_n = 0.$$  

For most practical purposes a phonon acts as if its momentum were $\hbar \mathbf{K}$, sometimes called the crystal momentum. When vibration modes interact, they not only demand that energy be conserved but also the quantity $\hbar \mathbf{K}$. In the process of interacting with photons and electrons in a crystal, the inelastic diffraction condition becomes

$$k' \pm \mathbf{K} = k + \mathbf{G}$$

This is the wave vector selection rule for the allowed transitions between quantum states. The $\pm$ sign represents the creation (emission) or annihilation (absorption) of a phonon, respectively.
Electrical Properties
Direct and Indirect Bandgaps

Note:
E\textsubscript{i} is the initial energy
E\textsubscript{f} is the final energy

![Diagram of Direct Bandgap](image)

- For efficient optical transition between E\textsubscript{c,min} and E\textsubscript{v,max}, the energy and momentum have to be conserved.

\[
\begin{align*}
  k_i &= k_f \quad \text{momentum conservation} \\
  E_i - E_f &= h\nu \quad \text{energy conservation}
\end{align*}
\]

The subscripts \( i \) and \( f \) indicate the initial and final states, respectively.
Conservation of Momentum

- For direct bandgap materials, the momentum of photons is essentially zero due to its near zero mass. Therefore,

\[ k_i = k_{\text{photon}} + k_f \approx k_f \]

\[ E_i - E_f = h\nu \]

The direct band gap semiconductor is, therefore, an efficient light emitting material. The emission wavelength relates to the energy difference is

\[ \lambda = \frac{1.24}{E_i - E_f} = \frac{1.24}{E_g(eV)}(\mu m) \]

- For indirect bandgap materials, the momentum of photon emission is too small (zero mass) to conserve the momentum difference between the initial and the final states. Phonon emissions are required to conserve the momentum.

\[ k_f = k_i \pm k_{\text{phonon}} \]

\[ \therefore k_i \neq k_f \]

The non-radiative process dominate the carrier recombination in indirect semiconductors.
Agenda for Next Class

• Electrical Properties
Thank You!
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.
Common Semiconductors

Fig. 21.4. Room-temperature bandgap energy versus lattice constant of common elemental and binary compound semiconductors.

“Italic” = indirect gap
“Roman” = direct gap
• hexagonal structure
□ cubic structure

E. F. Schubert
Light-Emitting Diodes (Cambridge Univ. Press)
www.LightEmittingDiodes.org

27
Contact Information & Website

Professor John M. Dallesasse
2114 Micro and Nanotechnology Laboratory
Office Hours: Tuesdays, 1-2 pm, 2114 MNTL
Office: (217) 333-8416
jdallesa@illinois.edu

John Carlson (TA)
3034 Micro and Nanotechnology Laboratory
Office Hours: Thursdays, 10-11 am, 3034 ECEB
jcarls21@illinois.edu

Website:
https://courses.engr.illinois.edu/ece488/
Course Objectives
Course Objectives

• Develop a working knowledge of compound semiconductor materials and devices
• Provide a foundation for future advanced physical electronics courses
• Provide basic device knowledge to support a career in wireless communications or photonics
• Provide sufficient background such that you can begin to read and understand the literature on compound semiconductor materials and devices
Course Outline
Course Outline

• Review of semiconductor fundamentals
  – Elementary quantum mechanics
  – Atomic bonding and crystal structures
  – Electronic band structures of solids
• Compound semiconductor materials
  – Compound semiconductor crystals
  – Material technologies
• Properties of heterostructures
  – Basic heterostructure properties
  – Electrical properties of heterostructures
  – Optical properties of heterostructures
• Heterostructure devices
  – High-speed electronic devices
  – Semiconductor lasers
  – New device development
Course Description (Detailed)

- Review of quantum, mechanical basics including wave-particle duality, Schroedinger wave equation, one-dimensional free and bounded particles in quantum wells
- Introduction to compound semiconductor crystals, structural and electrical properties, free carrier concentration and Fermi-Dirac integral, III-V alloys
- Phase equilibrium, growth of bulk crystals and phase equilibrium, liquid phase epitaxy, vapor phase epitaxy, metalorganic chemical vapor deposition, molecular beam epitaxy
- Basic heterostructure properties, energy band alignment models, strain effect on the bandgap energies, abrupt p-n heterojunction in equilibrium, heterojunction under bias
- Electronic properties of real quantum wells, potential barrier and tunneling, superlattices and miniband, quantum wells in electric fields, modulation doping and two-dimensional electron gas
- Optical properties of dielectrics, absorption, radiative transitions - Einstein relations, stimulated emission, absorption and emission rates in semiconductors, transitions in degenerated semiconductors, nonradiative recombination processes
- Metal-semiconductor field-effect transistors, pseudomorphic high-electron mobility transistors, heterojunction bipolar transistors, transfer electron devices, resonant tunneling devices
- Photodetectors, solar cells, light-emitting diodes (LEDs), dielectric waveguide and heterostructure laser theories, quantum well lasers, distributed feedback lasers, vertical cavity surface emitting lasers
Prerequisites

• ECE340 or equivalent basic semiconductor course
• Physics background – Basic modern physics
• Math background – differential equations
## Tentative Schedule [3]

<table>
<thead>
<tr>
<th>OCT 31: Optical Properties of Dielectric Media</th>
<th>NOV 2: Absorption in Semiconductors</th>
<th>NOV 4: Transitions Between Discrete States</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOV 7: Radiative and Non-Radiative Transitions Between Bands</td>
<td>NOV 9: Introduction to Heterojunction Devices, MESFETs</td>
<td>NOV 11: Modulation Doping</td>
</tr>
<tr>
<td>NOV 14: High Electron Mobility Transistors (HEMTs)</td>
<td>NOV 16: High Electron Mobility Transistors (HEMTs)</td>
<td>NOV 18: GaN High Electron Mobility Transistors; NOV 21-25: Thanksgiving</td>
</tr>
<tr>
<td>NOV 28: Heterojunction Bipolar Transistors (HBTs)</td>
<td>NOV 30: Heterojunction Bipolar Transistors</td>
<td>DEC 2: Heterostructure Lasers</td>
</tr>
<tr>
<td>DEC 5: Heterostructure Lasers</td>
<td>DEC 7: Photodiodes and Solar Cells; Last Lecture</td>
<td>FINAL EXAM: Per Registrar’s Office</td>
</tr>
</tbody>
</table>

**Guideline Only: Subject to Change**
Grading and Policies
## Grading

<table>
<thead>
<tr>
<th>Grading Category</th>
<th>Percentage of Grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homework &amp; Class Participation</td>
<td>30%</td>
</tr>
<tr>
<td>Quizzes (Dates Will be Announced)</td>
<td>10%</td>
</tr>
<tr>
<td>Mid-Term Exam</td>
<td>20%</td>
</tr>
<tr>
<td>Final Exam</td>
<td>40%</td>
</tr>
</tbody>
</table>

**Homework:**
- Due 1 week after assigned, due in class, no late homework accepted

**Quizzes:**
- 2 quizzes, dates will be announced ahead of time, 20 minutes

**Exam(s):**
- Calculator allowed
- 8.5 X 11, hand-written, double-sided formula sheet

**Key Points:**
- Come to class
- Do your homework
- If you’re having problems attend office hours
Other Comments

- Ask questions if you have them
- Don’t miss quizzes, exams, or homework
- Turn off your cell phones
- No video recording or photography in class
- Include name and NetID on all documents turned in for credit
• Class notes (required) can be purchased from the ECE Supply Center
• Additional reading materials will be distributed in class or through the course website
• Reference for further reading (NOT required):
  • Solid state physics:
  • Semiconductor physics and devices:
    – S.L. Chuang, *Physics of Semiconductor Devices*
  • Quantum wells and heterostructures:
  • Compound semiconductor materials: