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 11: September 16th, 2016
Assignments

• Reading from “Compound Semiconductors and Devices – An Introduction”
  – Mon 9/12: §’s 3.3, 3.3.1, 3.3.2
  – Wed 9/14: §’s 3.4, 3.4.1, 3.4.2
  – Fri 9/16: §’s 3.5, 3.6, 3.6.1, 3.6.2, 3.6.3, 3.6.4

• HW2 (Chapter 2): Posted Monday 9/12, due Monday 9/19
Today’s Agenda

• Finish The Brillouin Zone
• The Bragg Condition
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<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>
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<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>
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<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>
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<td>SEP 12: Band Gaps</td>
<td>SEP 14: Kronig-Penny Model</td>
<td>SEP 16: Effective Mass, Bloch Oscillations, Band Structure</td>
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**Guideline Only: Subject to Change**
FCC Versus HCP

**FCC Structure**

- A-B-C-A-B-C

**HCP Structure**

- A-B-A-B

**Zinc Blende:** 2 interlaced FCC structures separated by $\frac{1}{4}a$, $\frac{1}{4}a$, $\frac{1}{4}a$

**Wurtzite:** 2 interlaced HCP structures separated by $\frac{2}{3}c$
• “The wurtzite structure is formed by two HCP structures having different atoms A (e.g., Ga) and B (e.g. N), along the c-axis.”

Should Be:

• “The wurtzite structure is formed by two HCP structures having different atoms (e.g., Ga and N), along the c-axis.”

• Remove references to “A” and “B” when discussing Ga and N

Why?

• The atoms are not the same “A” and “B” discussed in the previous paragraph where differences between FCC and HCP structures are covered
The Brillouin Zone
The Brillouin Zone

\[(k')^2 = (k + G_{hkl})^2\]

\[k'^2 = k^2 + G_{hkl}^2 + 2k \cdot G_{hkl}\]

\[2k \cdot G_{hkl} + G_{hkl}^2 = 0\]

\[k \cdot (G_{hkl}/G_{hkl}) = k \cdot n = |G_{hkl}|/2\]

• **Bragg plane**: a perpendicular bisector of the reciprocal lattice vector $OG$.
• Every wave with $k$ extending from the origin to the Bragg plane in reciprocal lattice space gives rise to Bragg reflected wave. Therefore, only certain waves fulfill the Bragg condition requirement.
• Since reciprocal lattice is also periodic, we can use limited volume of reciprocal lattice, or $k$-space.
The Brillouin Zone (2)

- The Brillouin zone is the smallest polyhedron centered at the origin and enclosed by perpendicular bisectors of reciprocal lattice vectors.

![Diagram of the Brillouin zone with labeled points and vectors]

- Analysis: Every wave with $k$ extending from the origin to the zone boundary gives rise to Bragg reflected wave. (See illustration above). Therefore, only certain waves fulfill the Bragg condition requirement.
- For 3D periodic lattice structures, the interference of the incident ‘primary’ waves and the Bragg ‘reflected’ waves produces a “standing wave”.
  - X-ray diffraction patterns
  - Band gap formation in semiconductors

Brillouin Zone:
Wigner-Seitz primitive cell of the reciprocal lattice.
The Brillouin Zone (3)

(a) Brillouin Zone of 2D Lattices

- A reciprocal lattice vector $G$ at $(u,v)$ in $k$-space is expressed as
  \[ G = \frac{2\pi}{a} (u a_x + v a_y) \]
  \[ (a_x \text{ and } a_y \text{ are unit vectors in } k\text{-space}) \]

According to the Bragg condition,
\[ 2k \cdot G + G^2 = 0 \quad \text{and} \quad k = k_x a_x + k_y a_y \]

\[ \Rightarrow \quad \frac{4\pi}{a} (uk_x + vk_y) + \frac{4\pi^2}{a^2} (u^2 + v^2) = 0 \]

or
\[ f(k_x, k_y) = uk_x + vk_y + \frac{\pi}{a} (u^2 + v^2) = 0 \]

This is a line equation of $k_x$ and $k_y$. 
\[ k_y = -\frac{u}{v} k_x - \frac{\pi}{av} (u^2 + v^2) \]
The Brillouin Zone (4)

Since the wave vector \( k \) of the direct lattice is defined as \( k = 2\pi/a \), the \( k \)-space \((k_x, k_y)\) is equivalent to the reciprocal lattice space \([|G| = 2\pi/a]\). Therefore, the Brillouin zone in the reciprocal lattice can be seen as the area bounded by various \( f(k_x, k_y) \) which are defined by reciprocal lattice points \((u,v)\).

\[
f(k_x, k_y) = uk_x + vk_y + \frac{\pi}{a}(u^2 + v^2) = 0
\]

- First Brillouin zone:
  \[
  \begin{cases}
  u = 0, v = \pm 1 & \Rightarrow k_y = \pm \frac{\pi}{a} \\
  u = \pm 1, v = 0 & \Rightarrow k_x = \pm \frac{\pi}{a}
  \end{cases}
\]

- Second Brillouin zone:
  \[
  u = \pm 1, v = \pm 1 \quad \Rightarrow \quad k_x \pm k_y = \pm \frac{2\pi}{a}
  \]
The Brillouin Zone (5)

- Higher order Brillouin zones can be derived through the same procedure. For example, using $u=0, v=\pm 2$ and $v=0, u=\pm 2$, one can get the third Brillouin zone.
- Note, there are rules in determining the higher order Brillouin zones.
  - All zones encompass the same area in $k$-space.
  - In traveling along a general radial line which does not go through any intersection of Bragg reflection lines, starting from the origin, one must pass through the 1st, 2nd, 3rd, 4th... etc, zones successfully.
  - Each successive Bragg reflection line which is crossed forms the boundary along the radial path between a zone and the next highest neighboring zone.
The Brillouin Zone: Higher Order Zones
The Bragg Condition
Bragg Condition in the Brillouin Zone

On the boundary of the Brillouin zone, any wave should follow the Bragg condition. Assume, for the first zone, \( n=1 \),

\[ 2\alpha \sin \theta = \lambda. \]

For an incident wave of wavelength \( \lambda \), the corresponding wave vector lies from the zone center to the zone boundary is

\[
|k| = \frac{2\pi}{\lambda} = \sqrt{k_o^2 + \left(\frac{\pi}{a}\right)^2}
\]

\[
\sin \theta = \frac{k_y}{\sqrt{k_x^2 + k_y^2}} = \frac{\pi/a}{\sqrt{k_o^2 + (\pi/a)^2}}
\]

Since

\[
\lambda = \frac{2\pi}{|k|} = \frac{2\pi}{\sqrt{k_o^2 + (\pi/a)^2}}
\]

\[ \therefore \sin \theta = \frac{2\pi}{\sqrt{k_o^2 + (\pi/a)^2}} \cdot \frac{1}{2a} = \frac{\lambda}{2a} \]

It fulfills the Bragg condition.

All wave vectors fit the Brillouin zone construction will have constructive diffraction. All other waves get weakened and non-existing eventually.
3D Brillouin Zone: FCC Crystals

To investigate the Brillouin zone in FCC structure, we need to define the reciprocal lattice structure first. This requires the knowledge of translational vectors $a'$, $b'$, and $c'$ defining the primitive unit cell of the FCC structure.

$$
\begin{align*}
  a' &= \frac{a}{2}(b + c) \\
  b' &= \frac{a}{2}(c + a) \\
  c' &= \frac{a}{2}(a + b)
\end{align*}
$$

$a$, $b$, $c$ are the unit vectors of the FCC structure along $x$, $y$, and $z$, respectively. The unit cell is a cube with $a/2$ on each side and has a volume of $a' \cdot b' \cdot c' = a^3/4$.

Next we will derive the unit vectors in the reciprocal lattice.
The unit vectors of the reciprocal lattice structure are related to the FCC unit vectors $a$, $b$, and $c$ as

\[
\begin{align*}
\mathbf{a}^* &= 2\pi \frac{\mathbf{b}' \times \mathbf{c}'}{\mathbf{a}' \cdot \mathbf{b}' \times \mathbf{c}'} = \frac{2\pi (a^2/4)(-a + b + c)}{a^3/4} = \frac{2\pi}{a} (-a + b + c) \\
\mathbf{b}^* &= 2\pi \frac{\mathbf{c}' \times \mathbf{a}'}{\mathbf{a}' \cdot \mathbf{b}' \times \mathbf{c}'} = \frac{2\pi (a^2/4)(a - b + c)}{a^3/4} = \frac{2\pi}{a} (a - b + c) \\
\mathbf{c}^* &= 2\pi \frac{\mathbf{b}' \times \mathbf{c}'}{\mathbf{a}' \cdot \mathbf{b}' \times \mathbf{c}'} = \frac{2\pi (a^2/4)(a + b - c)}{a^3/4} = \frac{2\pi}{a} (a + b - c)
\end{align*}
\]

These are vectors oriented along $[\overline{1}11]$, $[1\overline{1}1]$, and $[11\overline{1}]$ directions in a cubic, respectively. The unit vectors $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ form a volume which is the primitive cell of the BCC structure. (next page)
The volume of the primitive cell in the reciprocal lattice is $\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^* = 4(2\pi/a)^3$. 
To construct the first Brillouin zone, we set up the general form of $G_{hki}$ first.

$$G_{hki} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

$$= \frac{2\pi}{a} \left( (-h+k+l)\mathbf{a} + (h-k+l)\mathbf{b} + (h+k-l)\mathbf{c} \right)$$

In a BCC structure, there are eight nearest neighbors from the body center lattice point along $<111>$. For $h=k=l=\pm 1$, there are eight reciprocal lattice vectors pointing to each corner of the BCC structure. The boundary of the first Brillouin zone is located at $G/2$.

$$\frac{G_{(111)}}{2} = \frac{2\pi}{2d_{(111)}} = \frac{\pi}{a} (\pm a \pm b \pm c)$$
The final shape of the first Brillouin zone of FCC structure is a truncated octahedron defined by

\[ \frac{G_{(111)}}{2} = \frac{\pi}{a} (\pm a \pm b \pm c) \]

By connecting the truncated octahedrons, the whole space can be occupied completely.
Using the rhombohedral unit cell of a simple hexagonal crystal, one can derive the reciprocal lattice parameters

\[ a^* = \frac{4\pi}{\sqrt{3}a} \quad \text{and} \quad c^* = \frac{2\pi}{c} \]

Base area (unit cell) = \( \frac{(8\pi)^2}{\sqrt{3}a^2} \)

Unit cell volume = \( \frac{16\pi^3}{\sqrt{3}a^2c} \)
Agenda for Next Class

- The Free Electron Model
- Density of States in 1, 2, and 3 Dimensions
Thank You!
### Periodic Table of the Elements

![Periodic Table](https://ptable.com/pimages/ptable/ptable.png)

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

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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
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 [2]

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<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>
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<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>
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<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>
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<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>
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**Guideline Only: Subject to Change**
| Nov 7: Radiative and Non-Radiative Transitions Between Bands | Nov 9: Introduction to Heterojunction Devices, MESFETs | Nov 11: Modulation Doping |
| Nov 14: High Electron Mobility Transistors (HEMTs) | Nov 16: High Electron Mobility Transistors (HEMTs) | Nov 18: GaN High Electron Mobility Transistors; Nov 21-25: Thanksgiving |
| Dec 5: Heterostructure Lasers | Dec 7: Photodiodes and Solar Cells; Last Lecture | Final Exam: Per Registrar’s Office |

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

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<td>Homework &amp; Class Participation</td>
<td>30%</td>
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<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>
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**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: