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 10: September 14th, 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 Reciprocal Lattice Vector
- Diffraction Condition
- The Brillouin Zone
- The Bragg Condition
## Tentative Schedule [1]

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<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>
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<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>
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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**
Reciprocal Lattice

Continued
Reciprocal Lattice Vector Properties

- How is $\mathbf{G}$ related to direct lattice?
  $a/h$, $b/k$, $c/l$ are position vectors at $P$, $Q$, $N$, respectively. Three vectors defined by intersections of the $(hkl)$ plane with three coordinates are

$$
\begin{align*}
NQ &= \frac{b}{k} - \frac{c}{l} \quad \text{......}(1) \\
QP &= \frac{a}{h} - \frac{b}{k} \quad \text{......}(2) \\
PN &= \frac{c}{l} - \frac{a}{h} \quad \text{......}(3)
\end{align*}
$$

A vector $\mathbf{R}$ in the $(hkl)$ plane can be written as a linear combination of $QP$, $PN$, and $NQ$. Assume $(1) \times F + (2) \times D + (3) \times E = \mathbf{R}$ and $D$, $E$, $F$ are integers.

$$
\mathbf{R} = \frac{a}{h} (D - E) + \frac{b}{k} (F - D) + \frac{c}{l} (E - F) = \left( \frac{A}{h} \right) a + \left( \frac{B}{k} \right) b + \left( \frac{C}{l} \right) c
$$

Note, $A + B + C = 0$. \( (D - E) + (F - D) + (E - F) = 0 \)

$$
\mathbf{R} \cdot \mathbf{G}_{hkl} = \left[ \left( \frac{A}{h} \right) a + \left( \frac{B}{k} \right) b + \left( \frac{C}{l} \right) c \right] \cdot (ha^* + kb^* + lc^*) = 2\pi (A + B + C) = 0
$$
$G_{hkl}$ is the reciprocal lattice vector associated with the \((hkl)\) plane. 
$R \cdot G = 0$ indicates \(R \perp G\), or \(G_{hkl}\) is perpendicular to \((hkl)\) plane.

- **Direct Lattice Spacing** - \(d_{hkl}\)

\[
d_{hkl} = r \cdot n = r \cdot \frac{G}{|G|} = \frac{a}{h} \cdot \frac{ha^* + kb^* + lc^*}{|G|} = \frac{2\pi}{|G|}
\]

\[
G_{hkl} = \frac{2\pi}{|G_{hkl}|} \quad \text{or} \quad G_{hkl} = \frac{2\pi}{d_{hkl}}
\]

The reciprocal lattice vector indeed has a magnitude inversely proportional to the direct lattice constant (or wave vector)!
Lattice Plane Spacings (General)

Cubic: \[ \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \]

Tetragonal: \[ \frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2} \]

Hexagonal: \[ \frac{1}{d^2} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2} \]

Rhombohedral: \[ \frac{1}{d^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{\alpha^2 \left( 1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha \right)} \]

Orthorhombic: \[ \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \]

Monoclinic: \[ \frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right) \]

Triclinic: \[ \frac{1}{d^2} = \frac{1}{V^2} \left( S_{11} h^2 + S_{22} k^2 + S_{33} l^2 + S_{12} kh + S_{23} kl + S_{13} hl \right) \]

Where:
\[ S_{11} = b^2 c^2 \sin^2 \alpha \quad S_{12} = abc^2 \left( \cos \alpha \cos \beta - \cos \gamma \right) \]
\[ S_{22} = a^2 c^2 \sin^2 \beta \quad S_{23} = a^2 bc \left( \cos \beta \cos \gamma - \cos \alpha \right) \]
\[ S_{33} = a^2 b^2 \sin^2 \gamma \quad S_{13} = ab^2 c \left( \cos \gamma \cos \alpha - \cos \beta \right) \]
Diffraction Condition
Diffraction Condition

- Bragg law of diffraction requires $n\lambda = 2d_{hkl}\sin\theta$, where $n$ is an integer.
- Reciprocal lattice condition:
  Assume the incident wave vector, $|k|=2\pi/\lambda$, is incident on $(hkl)$ plane and encounters an elastic scattering (no change in wavelength). The diffracted wave has a wave vector of $|k'| = |k|$. Although no loss in energy (thus same wavelength), the wave traveling direction has been changed.

$$\Delta k = k' - k = 2|k|\sin\theta n = \left(\frac{4\pi}{\lambda}\sin\theta\right)n = \left(\frac{4\pi}{\lambda}\sin\theta\right)\frac{G}{|G|}$$

Since $d_{hkl} = 2\pi/|G_{hkl}|$ and $n\lambda = 2d\sin\theta$

$\therefore \Delta k = G_{hkl}$ or $k' = k + G_{hkl}$
Diffraction Condition (2)

\[ \Delta k = G_{hkl} \quad \text{or} \quad k' = k + G_{hkl} \]

Furthermore,

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

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

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

This is the new diffraction condition in vector form.

- Conclusions:
  - \( G_{hkl} \perp (hkl) \) plane and has a magnitude \( \propto 1/d_{hkl} \).
  - \( G_{hkl} \) satisfies the diffraction condition both in magnitude and direction.
Circle Properties

Central Angle Theorem: Proof of $\theta$, $2\theta$ Relationship
A Geometrical Observation

Central Angle Theorem: To show \( \theta, 2\theta \) relationship

\[
\sin \theta = \frac{|OB|}{2r}
\]

Assuming \( r = k = \frac{2\pi}{\lambda} \):

\[
\sin \theta = \frac{|OB|}{2 \left( \frac{2\pi}{\lambda} \right)}
\]

If O is the origin and B is a reciprocal lattice point:

\( OB = G_{hkl} \) and \( |OB| = |G_{hkl}| = \frac{2\pi}{d_{hkl}} \)

so

\[
\sin \theta = \frac{2\pi}{2 \left( \frac{2\pi}{\lambda} \right)} = \frac{\lambda}{2d_{hkl}} \quad \Rightarrow \quad d_{hkl} \sin \theta = \frac{\lambda}{2}
Moving Vectors in the Circle

$|r|$ is the magnitude of the k vector (electron energy)

$\theta$ is the angle formed by the k vector with the hkl plane

$OB$ is the reciprocal lattice vector G for the hkl plane

Recall:
Ewald Sphere

• Laue diffraction uses a broadband x-ray source.
• One of the incident x-ray on the reciprocal lattice point O has a wavelength OA = 2π/λ.
• Point A as the center, make a sphere with radius |k| = 2π/λ.
• Diffraction condition is satisfied when the sphere intersects with a reciprocal lattice point (B).
• \( OB = G_{hkl} \) and perpendicular to the direct lattice plane \((hkl)\).
• To prove this satisfies the Bragg diffraction condition we use \( G_{hkl} = 2n\pi/d_{hkl} \) and from the diagram \( |OB| = 2(2\pi/\lambda)\sin\theta \). Equating \( |OB| \) and \( G_{hkl} \) gives the Bragg condition.

\[ \Delta k = G_{hkl} \quad \text{or} \quad k' = k + G_{hkl} \]

Peak intensity depends upon a number of factors (scattering, structure, etc.)
The Brillouin Zone
The Brillouin Zone

\[(k')^2 = (k + G_{hkl})^2\]
\[k'^2 = k^2 + G_{hkl}^2 + 2k \cdot G_{hkl}\]
\[2k \cdot G_{hkl} + G_{hkl}^2 = 0\]
\[k \cdot \left(\frac{G_{hkl}}{G_{hkl}}\right) = k \cdot n = \left|G_{hkl}\right|/2\]

- **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.

- 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 $\mathbf{G}$ at $(u,v)$ in $k$-space is expressed as

$$\mathbf{G} = \frac{2\pi}{a} (ua_x + va_y)$$

(a_x and a_y are unit vectors in $k$-space)

According to the Bragg condition,

$$2k \cdot G + G^2 = 0 \quad \text{and} \quad k = k_x a_x + k_y a_y$$

$$\rightarrow \frac{4\pi}{a} (uk_x + vk_y) + \frac{4\pi^2}{a^2} (u^2 + v^2) = 0$$

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 $k_y$. 

\[\begin{array}{c}
\mathbf{Direct \ lattice} \\
\text{(square)} \\
\end{array} \quad \longleftrightarrow \quad \begin{array}{c}
\mathbf{Reciprocal \ lattice} \\
\text{(square)} \\
\end{array} \quad 2\pi/a
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:
  \[
  \begin{aligned}
  &u = 0, v = \pm 1 \quad \Rightarrow \quad k_y = \pm \frac{\pi}{a} \\
  &u = \pm 1, v = 0 \quad \Rightarrow \quad k_x = \pm \frac{\pi}{a}
  \end{aligned}
  \]

- 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 (6)
Agenda for Next Class

- Brillouin Zone
- Band Structure of Solids
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
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, Schrödinger 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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<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>
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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>
</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>
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**Guideline Only: Subject to Change**
## Tentative Schedule [3]

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<th>OCT 31: Optical Properties of Dielectric Media</th>
<th>NOV 2: Absorption in Semiconductors</th>
<th>NOV 4: Transitions Between Discrete States</th>
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<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>
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<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>
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<tr>
<td>NOV 28: Heterojunction Bipolar Transistors (HBTs)</td>
<td>NOV 30: Heterojunction Bipolar Transistors</td>
<td>DEC 2: Heterostructure Lasers</td>
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<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>
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**Guideline Only: Subject to Change**
Grading and Policies
Grading

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<tr>
<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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</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:
  C. Kittel, *Introduction to solid state physics* (any edition), John Wiley
Semiconductor physics and devices:
  S.L. Chuang, *Physics of Semiconductor Devices*
Quantum wells and heterostructures:
Compound semiconductor materials: