ECE 488: Compound Semiconductors

M,W,F 11:00 – 11:50, 3013 ECEB
Professor John Dallesasse
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E-mail: jdallesa@illinois.edu
Office Hours: Tuesday 13:00 – 14:00
Lecture 27: October 26th, 2016
Assignments

• Reading from “Compound Semiconductors and Devices – An Introduction”
  – Mon 10/24: §’s 7.3, 7.3.1, 7.3.2, 7.3.3, 7.3.4
  – Wed 10/26: §’s 7.4, 7.4.1, 7.4.2, 7.4.3, 7.4.4
  – Fri 10/28: §’s 7.5, 7.5.1, 7.5.2

• Homework: Assigned Friday October 21st, due Friday October 28th
Today’s Agenda

• Brief Comment: In-Situ Diagnostics for MBE
• Heterostructures: Band Alignment
• Band Alignment in Strained Structures
# Tentative Schedule [2]

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<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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<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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<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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<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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</tbody>
</table>

**Guideline Only: Subject to Change**

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MBE In-Situ Diagnostics
In-Situ Surface Diagnostic Techniques

- Auger electron spectroscopy (AES) - For chemical analysis of the substrate surface. AES was used during the development of MBE growth process to determine the surface oxide desorption conditions.
- Reflection high-energy electron diffraction (RHEED) - A collimated beam of high-energy (3-40KeV) electrons is directed at an angle of 1-2° toward the sample surface orthogonal to the molecular beam paths. The electron wave has a wavelength on the order of the lattice constant and the diffraction pattern due to surface atoms is formed on the fluorescent screen.
RHEED Patterns
RHEED and Surface Morphology

Evolution of surface morphology and RHEED pattern on GaAs

3D RHEED pattern

Elongated spots without 1/2 orders

Streaky (2x4) pattern with 1/2 order

Etched GaAs surface

After deposit 150Å GaAs at 580°C

After depositing 1μm GaAs.
MBE Flux Control

- For an ideal Knudson-type effusion cell, the molecular beam flux arriving at the substrate surface is

\[
J = 1.118 \times 10^{22} \frac{PA \cos \theta}{d^2 \sqrt{MT}} \quad \text{(}\text{# molecules/cm}^2\text{s})
\]

- P = vapor pressure in the cell (torr)
- A = area of the aperture (cm\(^2\))
- d = distance between the substrate surface and aperture (cm)
- M = molecular weight (Kg)
- T = cell temperature (K)
- \(\theta\) = angle between beam and surface normal

- Composition control in A\(^{III}\)B\(^{III}\)C\(^V\) alloys:
  To determine the Al composition in Al\(_x\)Ga\(_{1-x}\)As, one can use the growth rates (R) of Al\(_x\)Ga\(_{1-x}\)As and GaAs to calculate x:

\[
x = \frac{R(Al_{x}Ga_{1-x}As) - R(GaAs)}{R(Al_{x}Ga_{1-x}As)}
\]
Flux Control Using RHEED

In-situ flux control using RHEED intensity oscillations

- A smooth surface corresponds to a high RHEED intensity.
- As growth commences, nucleation islands form at random sites leading to a decrease in reflectivity.
- At a 50% surface coverage of deposit island (\(\Theta=0.5\)), the reflectivity reaches a minimum.
- The islands grow in size until they coalesce into a smooth surface and the reflectivity recovers to its maximum value.
MBE History

- 1968  J. Arthur @ Bell Labs - Establishment of condensation coefficient of III-V alloys with mass spectrometric studies
- 1969  A.Y. Cho @ Bell Labs - Establishment of epitaxial growth conditions with RHEED studies.
- 1971  A.Y. Cho @ Bell Labs - Demonstrated the first GaAs/AlGaAs periodic structure
- 1974  A.Y. Cho @ Bell Labs - First active device (GaAs varactor) Cho and Casey @ Bell Labs - First MBE grown DH laser R. Dingle et al @ Bell Labs - First optical measurement of superlattice/quantum wells.
- 1976  van der Ziel et al @ Bell Labs - First observation of laser oscillation from quantum state in a SL Cho et al @ Bell Labs - First MBE grown DH laser operation cw at room temperature
- 1978  Dingle et al @ Bell Labs - Observation of mobility enhancement in modulation doped GaAs/AlGaAs heterostructure
- 1979  W.T. Tsang @ Bell Labs - Current injection QW laser demonstrated
- 1980  M. Panish et al @ Bell Labs - gas source MBE demonstrated T. Mimura et al @ Fujitsu, Japan - HEMT
Production-Scale MBE
Heterostructure Fundamentals: Energy Band Alignment
6.1.1. Anderson’s electron affinity model:

It is based on the ideal Schottky barrier structure. The model uses the ‘vacuum level’ as the ‘reference energy level’ to estimate the band alignment.

- It replaces the ‘metal’ by a ‘semiconductor’.
- The ‘electron affinity difference’ between two semiconductors determines the ‘band discontinuity’ at the heterojunction.

Note: All terms should be multiplied by $q$ to give energy in eV.
Anderson’s Model

\[
\begin{align*}
\Delta E_C &= \chi_1 - \chi_2 \\
\Delta E_V &= (E_{g2} - E_{g1}) - \Delta E_C \\
\Delta E_C + \Delta E_V &= E_{g2} - E_{g1} = \Delta E_g
\end{align*}
\]

Advantages:
- Simple and intuitive model
- All parameters are experimentally determined and available

The Anderson’s model provided early understanding of heterostructures. However, the match between the Anderson’s model and experiments was poor.
Anderson Model Deficiencies

Problems with Anderson’s Model:

• Ideal Schottky barrier case:
  ▪ Vacuum level has been used as the reference.
  ▪ Vacuum level kept constant on the metal side.
    → There is a well defined level at the M-S interface for barrier height determination.

• Anderson’s Model:
  ▪ The HJ is located inside semiconductor where there is no well-defined energy level like the vacuum level as in the case of metal. Unlike in metal, the vacuum level is bended inside the semiconductor near the junction.
  ▪ Besides the vacuum level, there is no other fixed level for referencing in Anderson’s model.
    → Poor match between the model and experiments.
Other Band Alignment Methods

Theoretical models:

- **Self-consistent interface calculations (SCIC)**
  - Complicate heavy calculations involved
  
  \[(Phys. Rev. B34, p.5621, 1986)\]

- **Linear combination atomic orbit (LCAO) model by W. Harrison**
  - Cannot incorporate strain effects
  
  \[(Electronic structure and the properties of solids; Freeman)\]

- **Mid-gap energy level model by J. Tersoff**
  - Cannot incorporate strain effects
  

- **Linear muffin-tin orbital (LMTO) model**
  - Strain effect calculation inaccurate
  

- **Model solid theory by C. Van de Walle and R. Martin**
  
Comparison of Methods


<table>
<thead>
<tr>
<th>Heterojunction</th>
<th>SCIC</th>
<th>Model solid</th>
<th>Empirical pseudopotential</th>
<th>( \Delta E_v ) (eV)</th>
<th>Harrison(^b)</th>
<th>LMTO(^c)</th>
<th>Tersoff theory(^d)</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlAs/Ge</td>
<td>1.05</td>
<td>1.19</td>
<td></td>
<td>0.70</td>
<td>0.78</td>
<td>0.73</td>
<td>0.87</td>
<td>0.95(^e)</td>
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<td>GaAs/Ge</td>
<td>0.63</td>
<td>0.59</td>
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<td>0.32</td>
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<td>0.55(^g)</td>
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<td>0.80(^h)</td>
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<td>ZnSe/GaAs</td>
<td>1.59</td>
<td>1.48</td>
<td>2.0±0.3</td>
<td>1.42</td>
<td>1.35</td>
<td>1.75</td>
<td>1.20</td>
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<tr>
<td>ZnSe/Ge</td>
<td>2.17</td>
<td>2.07</td>
<td>2.0±0.3</td>
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<td>2.01</td>
<td>1.99</td>
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<td>0.51(^j)</td>
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<tr>
<td>InAs/GaSb</td>
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<td>0.58</td>
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<td>0.72</td>
<td>0.42</td>
<td>0.36</td>
<td>0.43</td>
<td>0.45(^k)</td>
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<tr>
<td>AlSb/GaSb</td>
<td>0.38</td>
<td>0.49</td>
<td></td>
<td>0.09</td>
<td>0.18</td>
<td>0.17</td>
<td>0.38</td>
<td></td>
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</tbody>
</table>

Heavy calculations

Cannot incorporate strain effect

Ideal Heterojunction Model:

- Includes the interface effects such as redistribution of electron charges induced dipole moments.
- Can include strain effects.
- Easy of calculation.
- Apply to a wide variety of heterojunctions.
(a) Model-Solid Theory

- The model-solid theory is currently the most successful model for heterojunction calculation. It considers the ‘absolute reference energy level’ for each bulk semiconductor in a heterojunction with corrections due to detailed electron charge density at the interface. The band alignment can be easily calculated even when strain is presented. It has been extended to ternary and quaternary heterojunctions.

- Accurate band structures are accomplished by performing density-function calculations. However, it has problems in predicting an accurate bandgap. Thus, the conduction band edge value is determined by adding calculated $E_V$ values to experimentally determined $E_g$.

- Absolute energy scale establishment:
  The absolute reference is presented when the energy in the bulk can be referred to a ‘vacuum level’.
  - By modeling the solid as a superposition of neutral atoms.
  - In each atom, the electrostatic potential is defined with respect to the vacuum level.
  - The combination of the above elements will give the band positions on an absolute energy scale.
  - The critical parameter is $E_{V,av}$, which is the average of valence bandedge of the three uppermost bands at $\Gamma$ in ‘absolute energy scale’.
Model Solid Band Alignment Calculation

\[ E_v = E_{v,av} + \frac{\Delta_o}{3}; \quad E_c = E_v + E_g \]

\( E_{v,av} \) is calculated value, and \( E_g \) and \( \Delta_o \) are experimentally determined.

Lattice constant \( a_o \), spin-orbit splitting \( \Delta_o \), average valence band energy \( E_{v,av} \), conduction band hydrostatic deformation potential \( a_c \), valence band hydrostatic deformation potential \( a_v \), shear deformation potential \( b \), 300K bandgap energy \( E_g \), and elastic constants \( C_{11} \) and \( C_{12} \) for cubic semiconductors.

<table>
<thead>
<tr>
<th></th>
<th>( a_o ) (Å)</th>
<th>( \Delta_o ) (eV)</th>
<th>( E_{v,av} ) (eV)</th>
<th>( a_c ) (dir) (eV)</th>
<th>( a_c ) (ind) (eV)</th>
<th>( a_v ) (eV)</th>
<th>( b ) (eV)</th>
<th>( E_g ) (eV)</th>
<th>( C_{11} ) (10^{11} dyn/cm²)</th>
<th>( C_{12} ) (10^{11} dyn/cm²)</th>
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<tbody>
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<td>0.044</td>
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<td>1.98</td>
<td>4.18</td>
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<td>-1.54</td>
<td>1.24</td>
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<td>12.40</td>
<td>4.13</td>
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<td>-6.92</td>
<td>-7.17</td>
<td>-</td>
<td>1.16</td>
<td>-1.7</td>
<td>1.424</td>
<td>11.88</td>
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<td>AlAs</td>
<td>5.660</td>
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<td>-7.49</td>
<td>-5.64</td>
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<td>2.47</td>
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<td>-</td>
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<td>-</td>
<td>2.405</td>
<td>13.82 ?</td>
<td>6.71 ?</td>
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<td>-5.04</td>
<td>-</td>
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<td>0.36</td>
<td>-2.0</td>
<td>0.169</td>
<td>6.669</td>
<td>3.645</td>
</tr>
</tbody>
</table>
Unstrained Heterostructures

Band Discontinuity for Unstrained Heterojunctions

\[ \Delta E_v = E_v^B - E_v^A \]
\[ \Delta E_c = E_c^B - E_c^A = (E_v^B + E_g^B) - (E_v^A + E_g^A) \]

**Example:** Calculate the band alignment of an AlAs/GaAs heterojunction.

- \( E_v \) calculation:
  \[ E_v(GaAs) = E_{v,av} + \Delta_\sigma/3 = -6.92 + 0.34/3 = -6.807 \text{ (eV)} \]
  \[ E_v(AlAs) = -7.47 + 0.28/3 = -7.397 \text{ (eV)} \]

- \( \Delta E_v \) calculation:
  \[ \Delta E_v = -6.807 - (-7.397) = 0.59 \text{ (eV)} \]
  → \( E_v(GaAs) \) is above \( E_v(AlAs) \).

- \( E_c \) calculation:
  \[ E_c(GaAs) = E_v(GaAs) + E_g^D(GaAs) = -6.807 + 1.424 = -5.383 \text{ (eV)} \]
  \[ E_c(AlAs) = E_v(AlAs) + E_g^I(AlAs) = -7.397 + 2.168 = -5.229 \text{ (eV)} \]

- \( \Delta E_c \) calculation:
  \[ \Delta E_c = -5.383 - (-5.229) = -0.154 \text{ (eV)} \]
  → \( E_c(GaAs) \) is below \( E_c(AlAs) \).
Example: GaAs-AlAs

- Band alignment:
  The bandgap of GaAs is completely inside the bandgap of AlAs. The GaAs/AlAs heterojunction has a ‘type-I’ band alignment.

- Partition ratio:

  \[
  Q_c = \frac{\Delta E_c}{\Delta E_g} = \frac{0.154}{2.168 - 1.424} = 0.207; \quad Q_v = \frac{\Delta E_v}{\Delta E_g} = \frac{0.59}{0.744} = 0.793
  \]

  experimental values: \( Q_c = 0.26, Q_v = 0.74 \).
Summary and Comments

• The model-solid theory relies on calculated $E_{v,av}$ and experimental $E_g$ values to determine the band alignment.
• It still contains uncertainties that depend upon the accuracy of experiments.
• The uncertainty could be as large as 200 meV, in some cases. This offers opportunities to develop other empirical methods.
• It provides a much closer to reality and accurate picture of band alignment for common heterojunctions.
• The calculation procedures are simple and easy to use.
• It allows strain effects to be incorporated.
• The method can be extended to ternary and quaternary alloys.
Empirical Band Alignment
Empirical Band Discontinuities

(a) Basic properties:

- Transitivity: $\Delta E$ at A-B interface plus $\Delta E$ at B-C interface yields $\Delta E$ at A-C interface.
- Commutativity: $\Delta E_{AB}$ has the same value independent of the order of A and B.
- Strong correlation between the Schottky barrier height difference of p-type semiconductor and valence band discontinuity, $\Delta E_v$.

(b) Calculation procedures:

- Determine the value of $E_v$ using the p-type Schottky barrier height. Example: $\phi_{BV}(GaAs) = 0.562$ eV below the zero energy level.
- Calculate $E_c$ from experimental $E_g$ data. Example: $E_c(GaAs) = 1.424 - 0.562 = 0.862$ eV above the zero energy level.
- Ternary alloys:
  - Conduction band - Incorporating the bowing parameter, $c$.
  - Valence band - Using straight-line approximation.

Agenda for Next Class

- Empirical Band Alignments
- Strained Structures
Thank You!
## Final Exam

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<th>CRN</th>
<th>Date</th>
<th>Day</th>
<th>Start Time</th>
<th>End Time</th>
<th>Room</th>
<th>Exam Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>ECE 488</td>
<td>C</td>
<td>66375</td>
<td>12/12/2016</td>
<td>M</td>
<td>7:00 PM</td>
<td>10:00 PM</td>
<td>3017 Electrical &amp; Computer Eng Bldg</td>
<td>Extra Space</td>
</tr>
</tbody>
</table>
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.Light Emitting Diodes.org
Contact Information & Website

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