HOW DO WE TAILOR AND CONTROL ELECTRONIC PROPERTIES?
How can we modify bandstructure?

Energy needs: new bandgaps;
Optical device needs: tailorable bandgaps
High speed devices: lower masses
High power, high temperature devices: Large bandgaps
Novel devices: Low dimensional systems, heterostructures, junctions, …
Approaches to Bandstructure Modification

**Alloys**
- By combining two or more materials, a new lattice constant and bandgap can be produced.

**Quantum Wells, Wires & Dots**
- 2-dimensional or even lower dimensional electronic systems can be produced.
- Effective bandgap and density of states can be altered.

**Strain Field**
- Degeneracies can be removed.
- Character of bandedge wavefunctions can be altered.
- Bandedge density of states can be altered.
Alloys: Mixing of two or more materials

![Graph showing lattice constant vs mole fraction for various alloys like InSb, Ga\(_x\)In\(_{1-x}\)Sb, InAs\(_x\)Sb\(_{1-x}\), GaAs\(_x\)Sb\(_{1-x}\), Ga\(_x\)In\(_{1-x}\)As, Al\(_x\)In\(_{1-x}\)P, Al\(_x\)In\(_{1-x}\)As, Al\(_x\)Ga\(_{1-x}\)As, and Al\(_x\)Ga\(_{1-x}\)P.

Latent constant, \(a\) (nm)

- InSb
- Ga\(_x\)In\(_{1-x}\)Sb
- InAs\(_x\)Sb\(_{1-x}\)
- GaAs\(_x\)Sb\(_{1-x}\)
- Ga\(_x\)In\(_{1-x}\)As
- Al\(_x\)In\(_{1-x}\)P
- Al\(_x\)Ga\(_{1-x}\)As
- Al\(_x\)Ga\(_{1-x}\)P

Mole fraction, \(x\)
Alloys: Types of Alloys

Clustered

Random

Ordered
Alloys: Models for Alloy Bandstructure

Alloys are not periodic structures so Bloch theorem is not applicable. An average potential model is used to understand alloy electronic states.
When an alloy $A_xB_{1-x}$ is produced the lattice constant of the alloy is given by Vegard’s law:

$$a_{\text{alloy}} = xa_A + (1 - x)a_B$$

Bandgap of alloys is reasonably well described by:

$$E_g^{\text{alloy}} = a + bx + cx^2$$

where $c$ is the bowing parameter.

Since

$$E_{\text{alloy}}(k) = \frac{\hbar^2 k^2}{2m_{\text{alloy}}^*}$$

$$= x\frac{\hbar^2 k^2}{2m_A^*} + (1 - x)\frac{\hbar^2 k^2}{2m_B^*}$$

Effective Mass:

$$\frac{1}{m_{\text{alloy}}^*} = \frac{x}{m_A^*} + \frac{1 - x}{m_B^*}$$
### Bandgaps of Some Alloys

<table>
<thead>
<tr>
<th>Compound</th>
<th>Direct Energy Gap $E_g$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Al}<em>x\text{In}</em>{1-x}\text{ P}$</td>
<td>$1.351 + 2.23x$</td>
</tr>
<tr>
<td>$\text{Al}<em>x\text{Ga}</em>{1-x}\text{ As}$</td>
<td>$1.424 + 1.247x$</td>
</tr>
<tr>
<td>$\text{Al}<em>x\text{In}</em>{1-x}\text{ As}$</td>
<td>$0.360 + 2.012x + 0.698x^2$</td>
</tr>
<tr>
<td>$\text{Al}<em>x\text{Ga}</em>{1-x}\text{ Sb}$</td>
<td>$0.726 + 1.129x + 0.368x^2$</td>
</tr>
<tr>
<td>$\text{Al}<em>x\text{In}</em>{1-x}\text{ Sb}$</td>
<td>$0.172 + 1.621x + 0.43x^2$</td>
</tr>
<tr>
<td>$\text{Ga}<em>x\text{In}</em>{1-x}\text{ P}$</td>
<td>$1.351 + 0.643x + 0.786x^2$</td>
</tr>
<tr>
<td>$\text{Ga}<em>x\text{In}</em>{1-x}\text{ As}$</td>
<td>$0.36 + 1.064x$</td>
</tr>
<tr>
<td>$\text{Ga}<em>x\text{In}</em>{1-x}\text{ Sb}$</td>
<td>$0.172 + 0.139x + 0.415x^2$</td>
</tr>
<tr>
<td>$\text{GaP}<em>x\text{As}</em>{1-x}$</td>
<td>$1.424 + 1.150x + 0.176x^2$</td>
</tr>
<tr>
<td>$\text{GaAs}<em>x\text{Sb}</em>{1-x}$</td>
<td>$0.726 + 0.502x + 1.2x^2$</td>
</tr>
<tr>
<td>$\text{InP}<em>x\text{As}</em>{1-x}$</td>
<td>$0.360 + 0.891x + 0.101x^2$</td>
</tr>
<tr>
<td>$\text{InAs}<em>x\text{Sb}</em>{1-x}$</td>
<td>$0.18 + 0.41x + 0.58x^2$</td>
</tr>
</tbody>
</table>
Alloys: Models for Alloy Bandstructure

Alloy $\text{Ga}_x\text{Al}_{1-x}$

Direct to indirect transition can occur with alloy composition change.
Mercury-Cadmium-Telluride

Alloy: $\text{Cd}_x\text{Hg}_{1-x}$

Very important alloy for night vision, thermal imaging
Experiments needed for band alignment information
Heterostructures: Formation of subbands

Electrons are confined in the growth direction and levels are quantized.
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Schrödinger equation for the electron states in the quantum well:

\[
-\frac{\hbar^2}{2m^*} \nabla^2 + V(z) \Psi = E \Psi
\]

where \( m^* \) is the effective mass of the electron.

Wavefunction:

\[
\Psi(x, y, z) = e^{ik_rx} \cdot e^{ikrzy} f(z)
\]

where \( f(z) \) satisfies

\[
-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} + V(z) f(z) = E_n f(z)
\]

For Infinite Barrier Model:

\[
f(z) = \cos \left( \frac{\pi n z}{W} \right), \text{ if } n \text{ is even}
\]

= \sin \left( \frac{\pi n z}{W} \right), \text{ if } n \text{ is odd}

with energies

\[
E_n = \frac{\pi^2 \hbar^2 n^2}{2m^* W^2}
\]

The energy of the electron bands are then

\[
E = E_n + \frac{\hbar^2 k^2}{2m^*}
\]

leading to subbands.
For realistic wells the problem can be solved numerically.

For finite barrier case:

$$\alpha \tan \frac{\alpha W}{2} = \beta$$
$$\alpha \cot \frac{\alpha W}{2} = -\beta$$

where

$$\alpha = \sqrt{\frac{2m^*E}{\hbar^2}}$$
$$\beta = \sqrt{\frac{2m^*(V_c - E)}{\hbar^2}}$$

These equations can be solved numerically. The solutions give the energy levels $E_1, E_2, E_3$
... and the wavefunctions.
Bandstructure of Quantum Wells

E-k is altered

Density of states is modified
Low-dimensions structures: Density of states

Density of states control scattering response and optical response.
Valence bands are non-parabolic because of degenerate hole states near the valence bandedge.
Low-dimensions structures

Low dimensional structures have become integral to device technologies.

De Broglie wavelength of electrons in most semiconductors is about 10 nm, a dimension that is easily reached in essentially all next generation technologies.