Heterostructures + Quantum Wells

"Bandgap engineering" with semiconductor alloys.

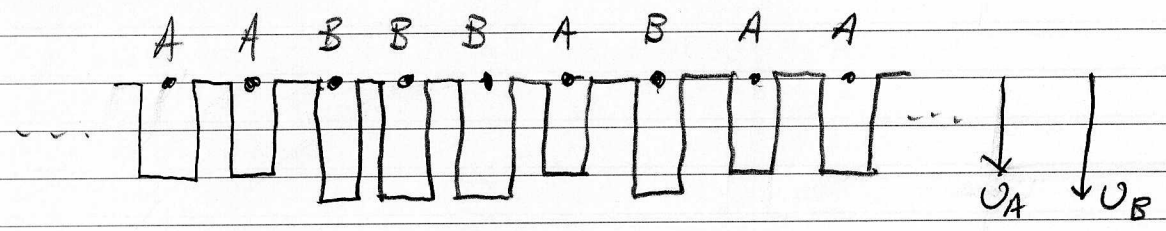
Most common alloy system: GaAs/AlAs

Alloy is $Ga_x Al_{1-x} As$ $\quad 0 \leq x \leq 1$

mixture of GaAs + AlAs. For generality denote a two-component alloy as: $A_x B_{1-x}$

lattice constant of alloy is weighted average:

Bandstructure



The alloy is a random mixture, so the lattice potential is not strictly periodic. But the difference in potential is relatively small $|U_A - U_B| \ll U_A, U_B$, so the random potential is a small perturbation about the average.

$$U_{AB}(\vec{r}) = x\, U_A(\vec{r}) + (1-x)\, U_B(\vec{r})$$

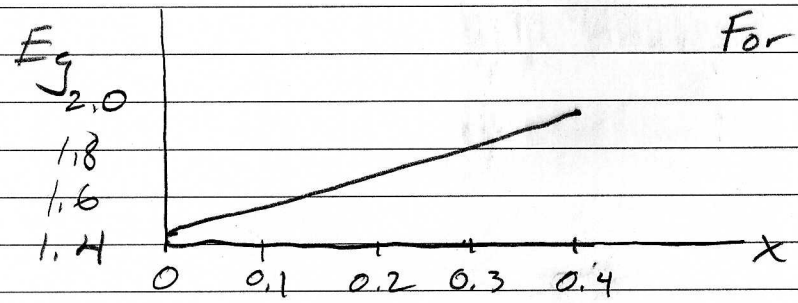
Then we can expect to 1st order

Effective masses generally also scale

$$\frac{1}{m^*_{AB}} = \frac{x}{m^*_A} + \frac{(1-x)}{m^*_B}$$

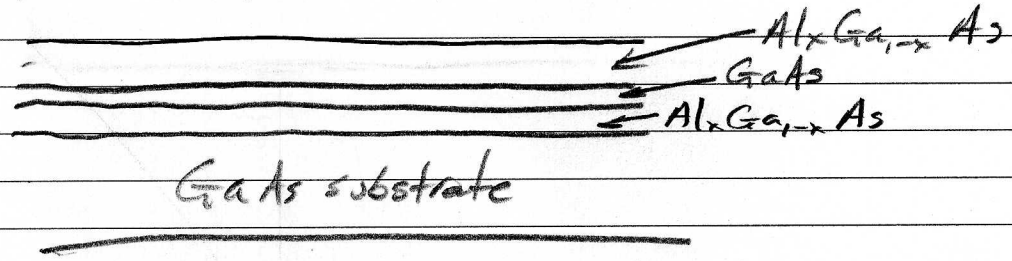
Since $\quad E^{AB} = \dfrac{\hbar^2 k^2}{2 m^*_{AB}}$

Layered structures - quantum wells

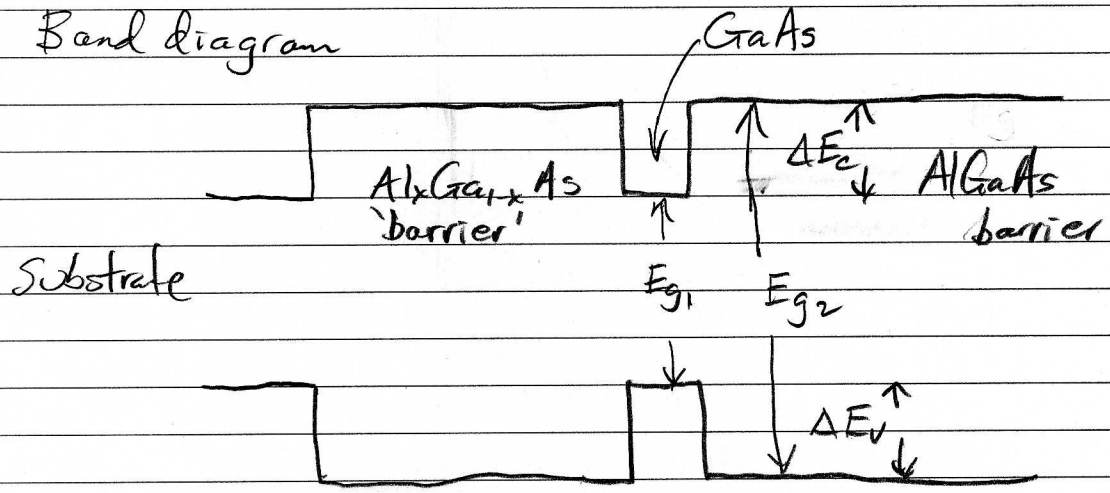


For $x \geq 0.35$, the material becomes indirect. But even within this range, the bandgap can be varied from ~1.42 to ~1.9 eV.

$Al_xGa_{1-x}As$ can be grown epitaxially on GaAs substrates, in a layer-by-layer fashion, which allows us to design very interesting structures. Perhaps the simplest is the quantum well



Band diagram



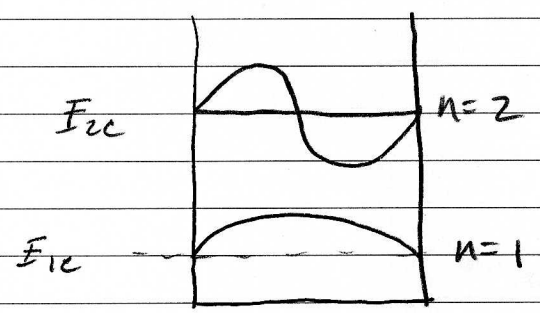
The difference in bandgap divides among CB and VB with

Electrons and holes can be confined within the GaAs "well" by the band-edge discontinuity. If the well thickness is ~ 10-20 nm, which is of the same order as the electron de Broglie wavelength, then the electronic structure is strongly modified.

For simplicity, model the quantum well with infinitely high barriers. Taking the direction normal to the water as $\hat{z}$, the wavefunction in the z direction becomes

$$\boxed{\psi_z(z) = \sin\left(\frac{n\pi z}{L_z}\right)} \qquad n = 0, 1, 2, \ldots$$

This is the classic "particle in 1D box" problem.



The energy levels are given by

But within the plane of the quantum well (x-y plane) the electrons are free to move as in the bulk semiconductor. The total wavefunction is

$$\psi_c^{tot}(\vec{r}) = U_c(\vec{r}_\perp)\, e^{j\vec{k}_\perp \cdot \vec{r}_\perp}\, \psi_z(z) \qquad \vec{r}_\perp \equiv x\hat{x} + y\hat{y}$$
$$\vec{k}_\perp \equiv k_x\hat{x} + k_y\hat{y}$$

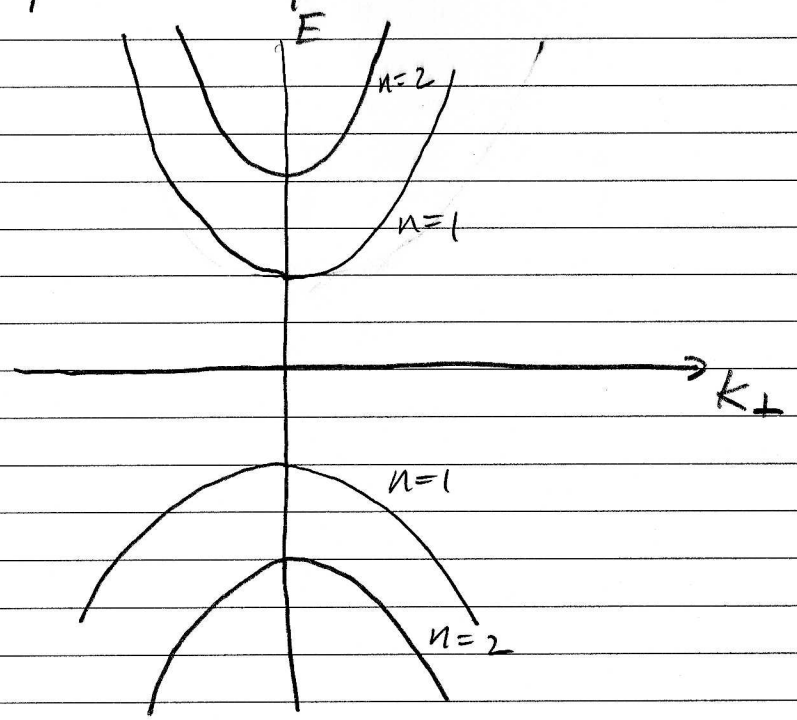
Thus there arise 2-dimensional bands for each quantum well "sublevel."

$$E_c^{tot} = \frac{\hbar^2 k_\perp^2}{2m_c^*} + E_{nc}$$

Similarly, in the valence band, with energy measured from the top of the valence band downward

$$E_v^{tot} = \frac{\hbar^2 k_\perp^2}{2m_v^*} + E_{nv}$$

Band dispersion for quantum wells:



Density of states

If we impose periodic boundary conditions in the x and y directions, as before, then again we have

For each sub-band we have allowed k-states only within a plane. Counting states is analogous to 3D case. Here, we take area of a circle.

Each state takes up area $\left(\frac{2\pi}{L}\right)^2$.

Total # of states with $k < k_\perp$:

$A = L^2$

Define $E_\perp = \frac{\hbar^2 k_\perp^2}{2m_c^*}$

$$N(E) = \frac{A}{2\pi} \frac{2 m_c^* E_\perp}{\hbar^2}$$

So $D(E) = \frac{dN}{dE} = \frac{m_c^*}{\pi \hbar^2}$ is the density of states per unit area