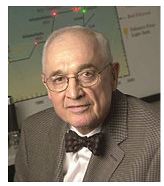
Handout 26

2D Nanostructures: Semiconductor Quantum Wells

In this lecture you will learn:

- Effective mass equation for heterojunctions
- Electron reflection and transmission at interfaces
- Semiconductor quantum wells
- Density of states in semiconductor quantum wells

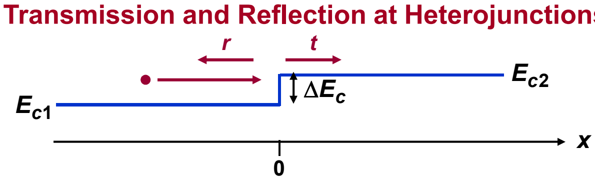
Leo Esaki (1925-)
Nobel Prize



Nick Holonyak Jr. (1928-)

Charles H. Henry (1937-)

Transmission and Reflection at Heterojunctions



The solution is:

$$t = \frac{2}{1 + m_{x1}k_{x2}/m_{x2}k_{x1}} \qquad r = \frac{1 - m_{x1}k_{x2}/m_{x2}k_{x1}}{1 + m_{x1}k_{x2}/m_{x2}k_{x1}}$$

Where:

$$\frac{\hbar^2 k_{x2}^2}{2m_{x2}} = \frac{\hbar^2 k_{x1}^2}{2m_{x1}} - \Delta E_c - \frac{\hbar^2 k_y^2}{2}\left(\frac{1}{m_{y2}} - \frac{1}{m_{y1}}\right) - \frac{\hbar^2 k_z^2}{2}\left(\frac{1}{m_{z2}} - \frac{1}{m_{z1}}\right)$$

$$\Rightarrow \frac{\hbar^2 k_{x2}^2}{2m_{x2}} = \frac{\hbar^2 k_{x1}^2}{2m_{x1}} - \Delta V_{eff}\left(k_y, k_z\right)$$

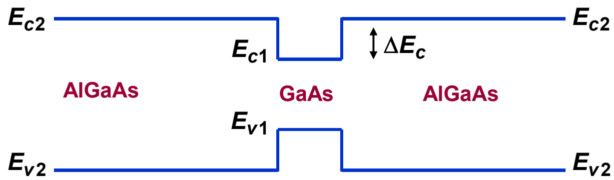
Special case: If the RHS in the above equation is negative, then k_{x2} becomes imaginary and the wavefunction decays exponentially for x>0 (in semiconductor 2). In this case:

$$|r| = 1$$

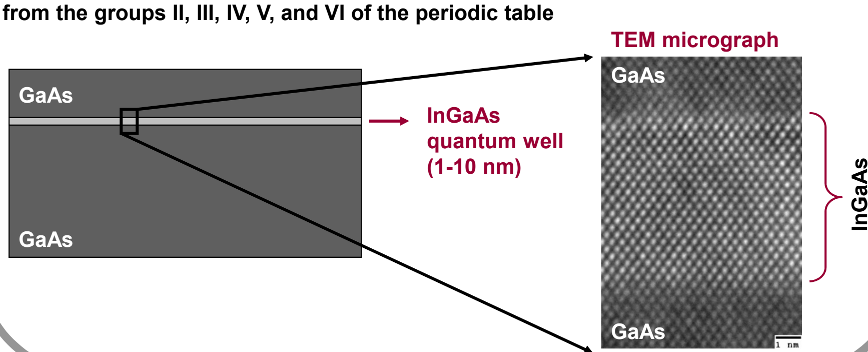
and the electron is completely reflected from the hetero-interface

Semiconductor Quantum Wells

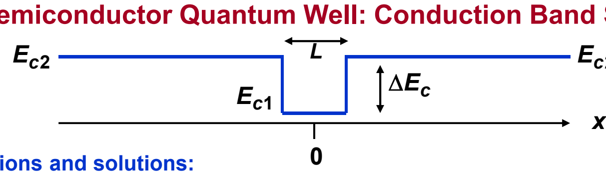
A thin (~1-10 nm) narrow bandgap material sandwiched between two wide bandgap materials



Semiconductor quantum wells can be composed of pretty much any semiconductor from the groups II, III, IV, V, and VI of the periodic table



Semiconductor Quantum Well: Conduction Band Solution



Assumptions and solutions:

$$E_{c1}(\vec{k}) = E_{c1} + \frac{\hbar^2 k^2}{2m_e}$$

$$\left[\hat{E}_{c1}(-i\nabla)\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2\nabla^2}{2m_e} + E_{c1}\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

$$\phi_1(\vec{r}) = A\begin{cases}\cos(k_x x)e^{i(k_y y + k_z z)} \\ \sin(k_x x)e^{i(k_y y + k_z z)}\end{cases}$$

Symmetric (cos), Anti-symmetric (sin)

$$E_{c2}(\vec{k}) = E_{c2} + \frac{\hbar^2 k^2}{2m_e}$$

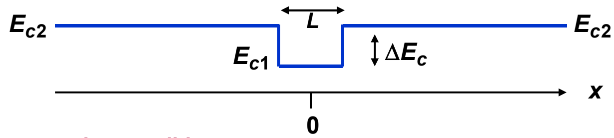
$$\left[\hat{E}_{c2}(-i\nabla)\right]\phi_2(\vec{r}) = E\,\phi_2(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2\nabla^2}{2m_e} + E_{c2}\right]\phi_2(\vec{r}) = E\,\phi_2(\vec{r})$$

$$\phi_2(\vec{r}) = B\begin{cases}e^{-\alpha(x-L/2)}\,e^{i(k_y y + k_z z)} \\ e^{-\alpha(x-L/2)}\,e^{i(k_y y + k_z z)}\end{cases} \quad x \geq L/2$$

$$\phi_2(\vec{r}) = B\begin{cases}e^{\alpha(x+L/2)}\,e^{i(k_y y + k_z z)} \\ -e^{\alpha(x+L/2)}\,e^{i(k_y y + k_z z)}\end{cases} \quad x \leq -L/2$$

Semiconductor Quantum Well: Conduction Band Solution



Energy conservation condition:

$$E = E_{c1} + \frac{\hbar^2\left(k_x^2 + k_\parallel^2\right)}{2m_e} = E_{c2} + \frac{\hbar^2\left(-\alpha^2 + k_\parallel^2\right)}{2m_e}$$

$$\Rightarrow \alpha = \sqrt{\frac{2m_e}{\hbar^2}\Delta E_c - k_x^2}$$

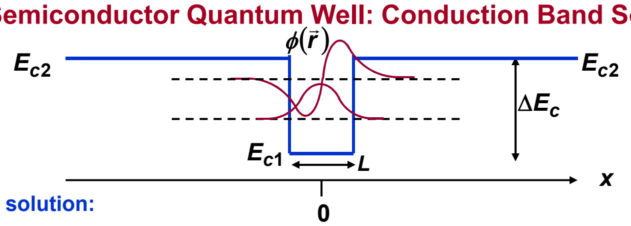
$$\left\{ k_\parallel^2 = k_y^2 + k_z^2 \right.$$

The two unknowns A and B can be found by imposing the continuity of the wavefunction condition and the probability current continuity condition to get the following conditions for the wavevector k_x:

$$\begin{cases} \tan\left(\dfrac{k_x L}{2}\right) = \dfrac{\alpha}{k_x} = \dfrac{\sqrt{\frac{2m_e}{\hbar^2}\Delta E_c - k_x^2}}{k_x} \\ -\cot\left(\dfrac{k_x L}{2}\right) = \dfrac{\alpha}{k_x} = \dfrac{\sqrt{\frac{2m_e}{\hbar^2}\Delta E_c - k_x^2}}{k_x} \end{cases}$$

Wavevector k_x cannot be arbitrary!
Its value must satisfy these transcendental equations

Semiconductor Quantum Well: Conduction Band Solution

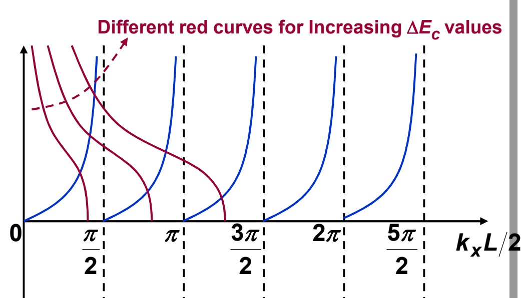


Graphical solution:

$$\begin{cases} \tan\left(\dfrac{k_x L}{2}\right) = \dfrac{\alpha}{k_x} = \dfrac{\sqrt{\frac{2m_e}{\hbar^2}\Delta E_c - k_x^2}}{k_x} \\ -\cot\left(\dfrac{k_x L}{2}\right) = \dfrac{\alpha}{k_x} = \dfrac{\sqrt{\frac{2m_e}{\hbar^2}\Delta E_c - k_x^2}}{k_x} \end{cases}$$

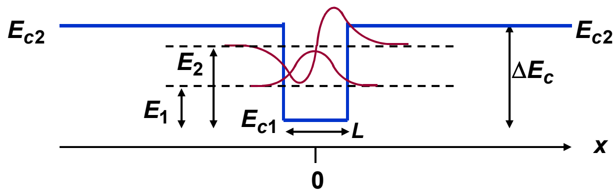
In the limit $\Delta E_c \to \infty$ the values of k_x are:

$$k_x = p\pi/L \quad (p = 1,2,3........$$



- Values of k_x are quantized
- Only a finite number of solutions are possible – depending on the value of ΔE_c

Electrons in Quantum Wells: A 2D Fermi Gas



Since values of k_x are quantized, the energy dispersion can be written as:

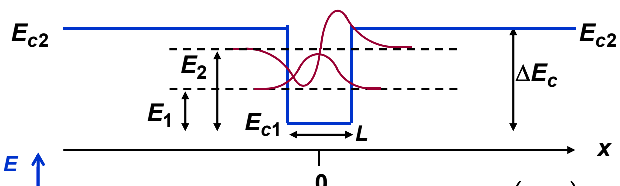
$$E = E_{c1} + \frac{\hbar^2 k_x^2}{2m_e} + \frac{\hbar^2 k_{||}^2}{2m_e} \qquad \left\{ k_{||}^2 = k_y^2 + k_z^2 \right.$$

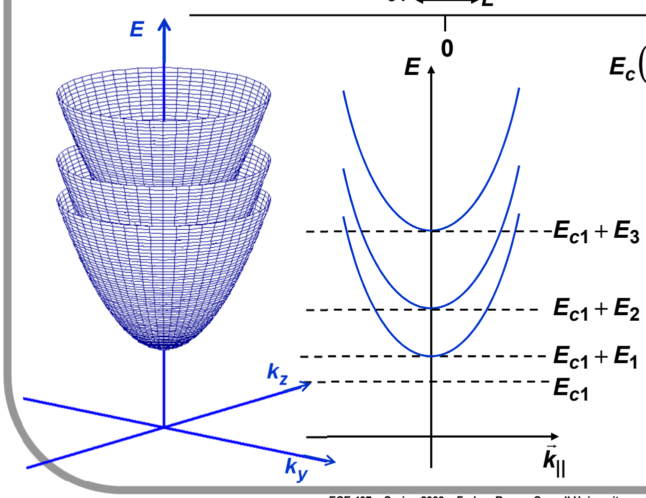
$$= E_{c1} + E_p + \frac{\hbar^2 k_{||}^2}{2m_e} \longrightarrow \qquad p = 1,2,3\ldots\ldots$$

In the limit $\Delta E_c \to \infty$ the values of E_p are: $E_p = \frac{\hbar^2}{2m_e}\left(\frac{p\pi}{L}\right)^2$ $\qquad p = 1,2,3\ldots\ldots$

- We say that the motion in the x-direction is quantized (the energy associated with that motion can only take a discrete set of values)
- The freedom of motion is now available only in the y and z directions (i.e. in directions that are in the plane of the quantum well)
- Electrons in the quantum well are essentially a two dimensional Fermi gas!

Energy Subbands in Quantum Wells





$$E_c\left(p, \vec{k}_{||}\right) = E_{c1} + E_p + \frac{\hbar^2 k_{||}^2}{2m_e}$$

$p = 1,2,3\ldots\ldots$

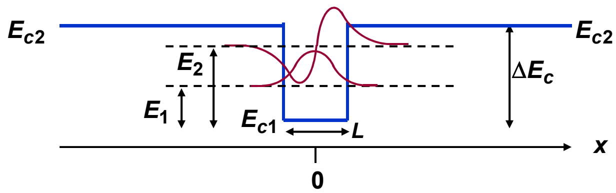
$k_{||}^2 = k_y^2 + k_z^2$

The energy dispersion for electrons in the quantum wells can be plotted as shown

It consists of energy subbands (i.e. subbands of the conduction band)

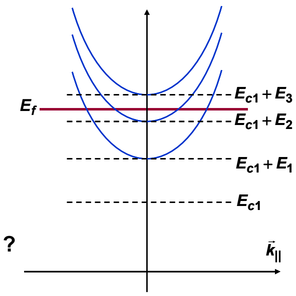
Electrons in each subband constitute a 2D Fermi gas

Density of States in Quantum Wells



Suppose, given a Fermi level position E_f, we need to find the electron density:
We can add the electron present in each subband as follows:

$$n = \sum_p 2 \times \int \frac{d^2\vec{k}_{||}}{(2\pi)^2} f\left(E_c\left(p,\vec{k}_{||}\right) - E_f\right)$$



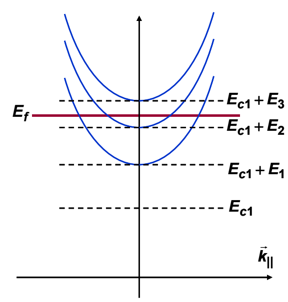
If we want to write the above as:

$$n = \int_{E_{c1}}^{\infty} dE\ g_{QW}(E)\, f(E - E_f)$$

Then the question is what is the density of states $g_{QW}(E)$?

Density of States in Quantum Wells

$$E_c\left(p,\vec{k}_{||}\right) = E_{c1} + E_p + \frac{\hbar^2 k_{||}^2}{2m_e}$$



Start from:

$$n = \sum_p 2 \times \int \frac{d^2\vec{k}_{||}}{(2\pi)^2} f\left(E_c\left(p,\vec{k}_{||}\right) - E_f\right)$$

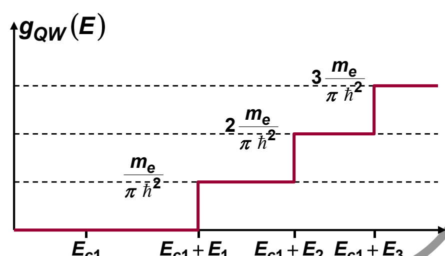
And convert the k-space integral to energy space:

$$n = \sum_p \int_{E_{c1}+E_p}^{\infty} dE \left(\frac{m_e}{\pi\hbar^2}\right) f(E - E_f)$$

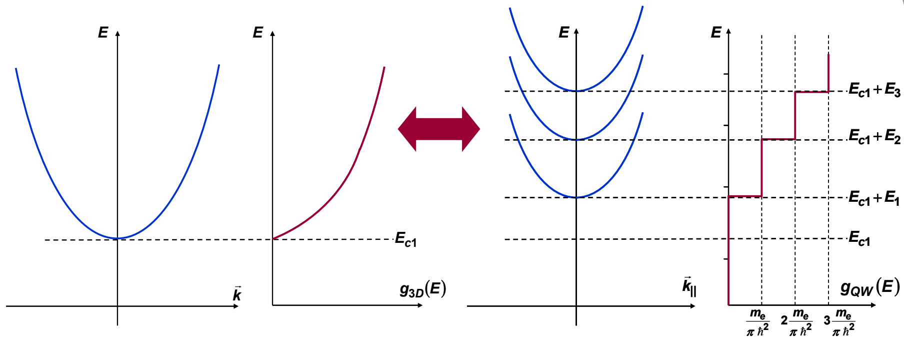
$$= \int_{E_{c1}}^{\infty} dE \sum_p \left(\frac{m_e}{\pi\hbar^2}\right) \theta\left(E - E_{c1} - E_p\right) f(E - E_f)$$

This implies:

$$g_{QW}(E) = \sum_p \left(\frac{m_e}{\pi\hbar^2}\right) \theta\left(E - E_{c1} - E_p\right)$$



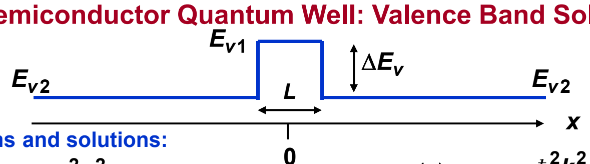
Density of States: From Bulk (3D) to QW (2D)



The modification of the density of states by quantum confinement in nanostructures can be used to:

i) Control and design custom energy levels for laser and optoelectronic applications
ii) Control and design carrier scattering rates, recombination rates, mobilities, for electronic applications
iii) Achieve ultra low-power electronic and optoelectronic devices

Semiconductor Quantum Well: Valence Band Solution



Assumptions and solutions:

$$E_{v1}(\vec{k}) = E_{v1} - \frac{\hbar^2 k^2}{2m_h}$$

$$\left[\hat{E}_{v1}(-i\nabla)\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

$$\Rightarrow \left[+\frac{\hbar^2\nabla^2}{2m_h} + E_{v1}\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2\nabla^2}{2m_h} - E_{v1}\right]\phi_1(\vec{r}) = -E\,\phi_1(\vec{r})$$

Symmetric

$$\phi_1(\vec{r}) = A\begin{cases}\cos(k_x x)e^{i(k_y y + k_z z)}\\ \sin(k_x x)e^{i(k_y y + k_z z)}\end{cases}$$

Anti-symmetric

$$E_{v2}(\vec{k}) = E_{v2} - \frac{\hbar^2 k^2}{2m_v}$$

$$\left[\hat{E}_{v2}(-i\nabla)\right]\phi_2(\vec{r}) = E\,\phi_2(\vec{r})$$

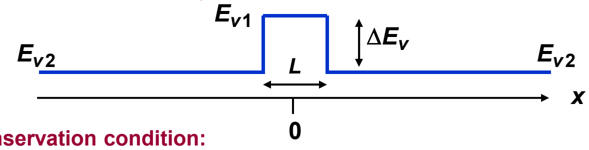
$$\Rightarrow \left[+\frac{\hbar^2\nabla^2}{2m_h} + E_{v2}\right]\phi_2(\vec{r}) = E\,\phi_2(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2\nabla^2}{2m_h} - E_{v2}\right]\phi_2(\vec{r}) = -E\,\phi_2(\vec{r})$$

$$\phi_2(\vec{r}) = B\begin{cases}e^{-\alpha(x-L/2)}\,e^{i(k_y y + k_z z)}\\ e^{-\alpha(x-L/2)}\,e^{i(k_y y + k_z z)}\end{cases} \quad x \geq L/2$$

$$\phi_2(\vec{r}) = B\begin{cases}e^{\alpha(x+L/2)}\,e^{i(k_y y + k_z z)}\\ -e^{\alpha(x+L/2)}\,e^{i(k_y y + k_z z)}\end{cases} \quad x \leq -L/2$$

Semiconductor Quantum Well: Valence Band Solution



Energy conservation condition:

$$E = E_{v1} - \frac{\hbar^2\left(k_x^2 + k_{||}^2\right)}{2mh} = E_{v2} - \frac{\hbar^2\left(-\alpha^2 + k_{||}^2\right)}{2m_e}$$

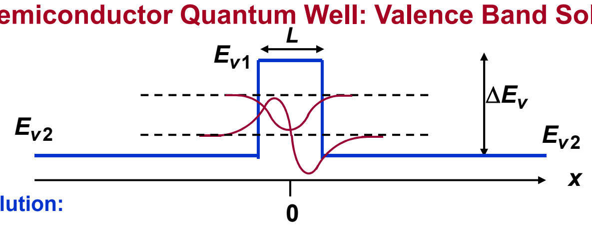
$$\Rightarrow \alpha = \sqrt{\frac{2m_h}{\hbar^2}\Delta E_v - k_x^2}$$

The two unknowns A and B can be found by imposing the continuity of the wavefunction condition and the probability current conservation condition to get the following conditions for the wavevector k_x:

$$\begin{cases} \tan\left(\frac{k_x L}{2}\right) = \frac{\alpha}{k_x} = \frac{\sqrt{\frac{2m_h}{\hbar^2}\Delta E_v - k_x^2}}{k_x} \\ -\cot\left(\frac{k_x L}{2}\right) = \frac{\alpha}{k_x} = \frac{\sqrt{\frac{2m_h}{\hbar^2}\Delta E_v - k_x^2}}{k_x} \end{cases}$$

Wavevector k_x cannot be arbitrary!

Semiconductor Quantum Well: Valence Band Solution

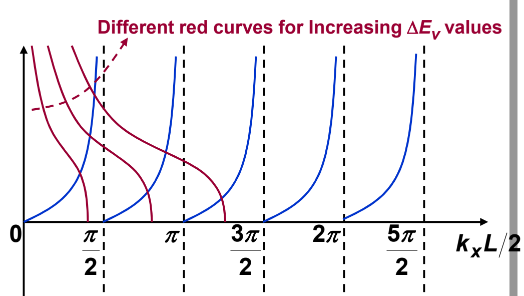


Graphical solution:

$$\begin{cases} \tan\left(\frac{k_x L}{2}\right) = \frac{\alpha}{k_x} = \frac{\sqrt{\frac{2m_h}{\hbar^2}\Delta E_v - k_x^2}}{k_x} \\ -\cot\left(\frac{k_x L}{2}\right) = \frac{\alpha}{k_x} = \frac{\sqrt{\frac{2m_h}{\hbar^2}\Delta E_v - k_x^2}}{k_x} \end{cases}$$

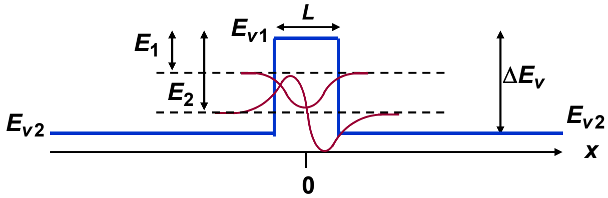
In the limit $\Delta E_v \rightarrow \infty$ the values of k_x are:

$$k_x = p\pi/L \quad (p = 1,2,3........$$



- Values of k_x are quantized
- Only a finite number of solutions are possible – depending on the value of ΔE_v

Semiconductor Quantum Wells: A 2D Fermi Gas



Since values of k_x are quantized, the energy dispersion can be written as:

$$E = E_{v1} - \frac{\hbar^2 k_x^2}{2m_h} - \frac{\hbar^2 k_{||}^2}{2m_h}$$

$$= E_{v1} - E_p - \frac{\hbar^2 k_{||}^2}{2m_h} \longrightarrow \qquad p = 1,2,3........$$

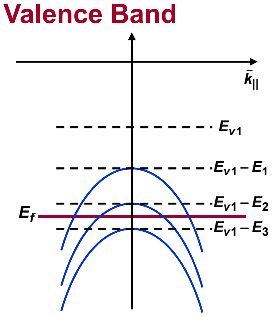
Light-hole/heavy-hole degeneracy breaks!

In the limit $\Delta E_v \rightarrow \infty$ the values of E_p are: $E_p = \frac{\hbar^2}{2m_h}\left(\frac{p\pi}{L}\right)^2$ $\qquad p = 1,2,3........$

- We say that the motion in the x-direction is quantized (the energy associated with that motion can only take a discrete set of values)
- The freedom of motion is now available only in the y and z directions (i.e. in directions that are in the plane of the quantum well)
- Electrons (or holes) in the quantum well are essentially a two dimensional Fermi gas!

Density of States in Quantum Wells: Valence Band

$$E_v(p,\vec{k}_{||}) = E_{v1} - E_p - \frac{\hbar^2 k_{||}^2}{2m_h}$$



Start from:

$$p = \sum_p 2 \times \int \frac{d^2\vec{k}_{||}}{(2\pi)^2}\left[1 - f\left(E_v(p,\vec{k}_{||}) - E_f\right)\right]$$

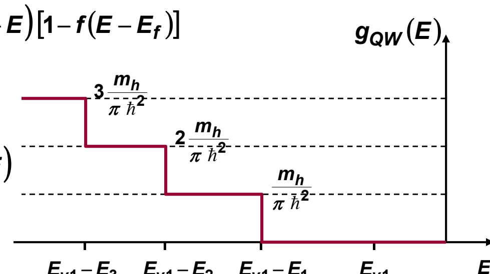
And convert the k-space integral to energy space:

$$p = \sum_p \int_{-\infty}^{E_{v1}-E_p} dE \left(\frac{m_h}{\pi\hbar^2}\right)\left[1 - f(E - E_f)\right]$$

$$= \int_{-\infty}^{E_{v1}} dE \sum_p \left(\frac{m_h}{\pi\hbar^2}\right)\theta\left(E_{v1} - E_p - E\right)\left[1 - f(E - E_f)\right]$$

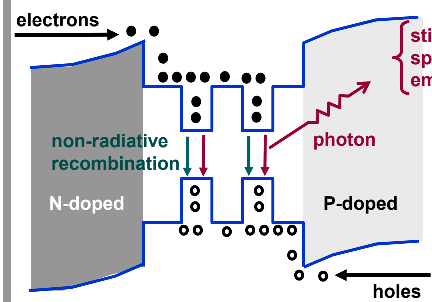
This implies:

$$g_{QW}(E) = \sum_p \left(\frac{m_h}{\pi\hbar^2}\right)\theta\left(E_{v1} - E_p - E\right)$$

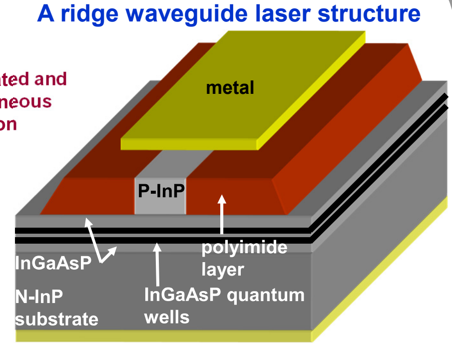


Example (Photonics): Semiconductor Quantum Well Lasers

A quantum well laser (band diagram)

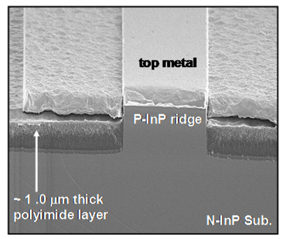


A ridge waveguide laser structure



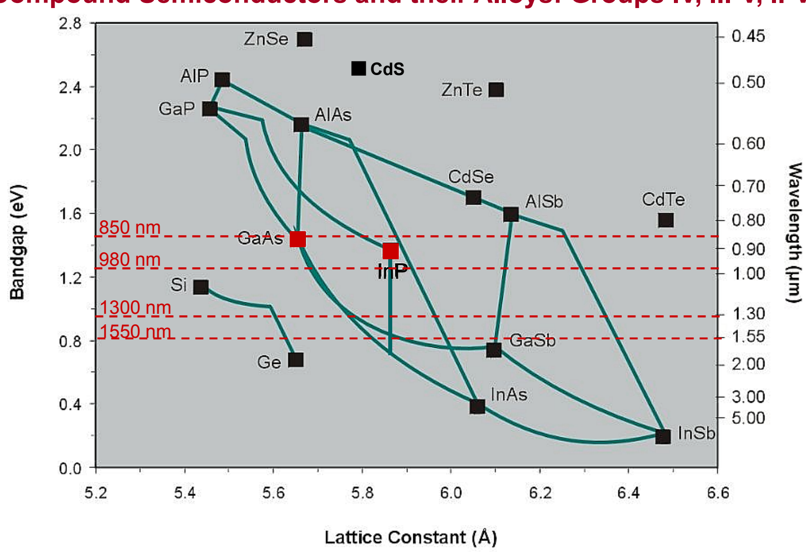
Some advantages of quantum wells for laser applications:

- Low laser threshold currents due to reduced density of states
- High speed laser current modulation due to large differential gain
- Ability to control emission wavelength via quantum size effect

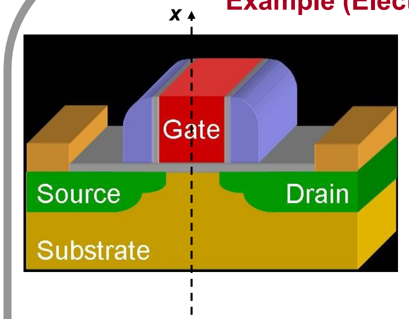


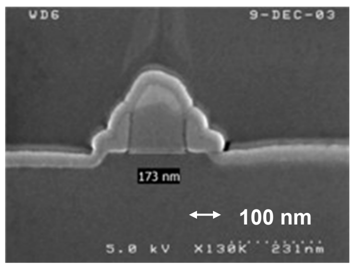
All lasers used in fiber optical communication systems are semiconductor quantum well lasers

Compound Semiconductors and their Alloys: Groups IV, III-V, II-VI

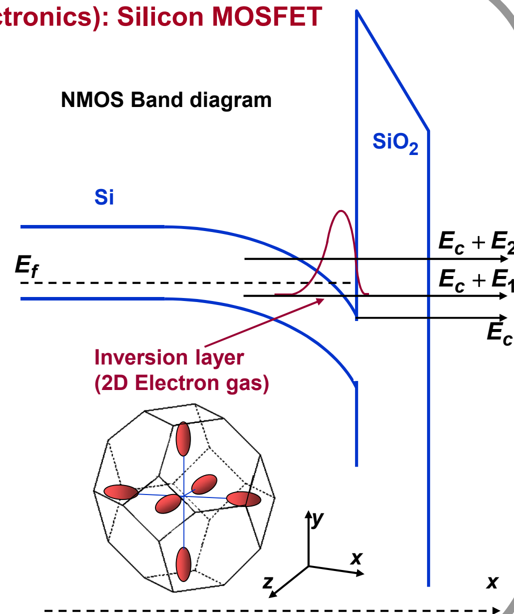


Example (Electronics): Silicon MOSFET





A 50 nm gate MOS transistor



Example (Electronics): Silicon MOSFET

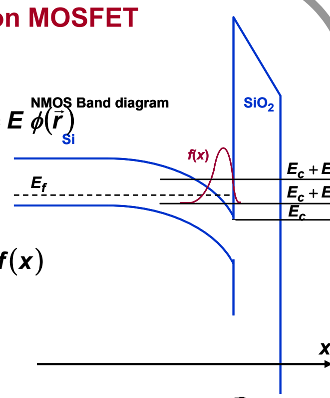
For minima 1 and 2:

$$\left[-\frac{\hbar^2}{2m_\ell}\frac{\partial^2}{\partial x^2}-\frac{\hbar^2}{2m_t}\frac{\partial^2}{\partial y^2}-\frac{\hbar^2}{2m_t}\frac{\partial^2}{\partial z^2}+E_c+\vec{U}(\vec{r})\right]\phi(\vec{r})=E\,\phi(\vec{r})$$

$$\phi(\vec{r})=f(x)e^{ik_y z+ik_z z}$$

$$\left[-\frac{\hbar^2}{2m_\ell}\frac{\partial^2}{\partial x^2}+U(\vec{r})\right]f(x)=\left(E-E_c-\frac{\hbar^2k_y^2}{2m_t}--\frac{\hbar^2k_z^2}{2m_t}\right)f(x)$$

$$\Rightarrow E=E_c+E_\ell+\frac{\hbar^2k_y^2}{2m_t}+\frac{\hbar^2k_z^2}{2m_t}$$

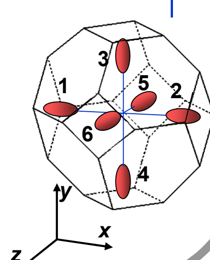


For minima 3 and 4:

$$\phi(\vec{r})=g(x)e^{ik_y z+ik_z z}$$

$$\left[-\frac{\hbar^2}{2m_t}\frac{\partial^2}{\partial x^2}+U(\vec{r})\right]g(x)=\left(E-E_c-\frac{\hbar^2k_y^2}{2m_\ell}--\frac{\hbar^2k_z^2}{2m_t}\right)g(x)$$

$$\Rightarrow E=E_c+E_t+\frac{\hbar^2k_y^2}{2m_\ell}+\frac{\hbar^2k_z^2}{2m_t} \longrightarrow \left\{E_t>E_\ell\right.$$



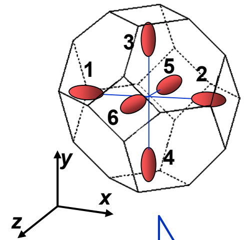
Example (Electronics): Silicon MOSFET

For minima 5 and 6:

$$\phi(\bar{r}) = g(x)\, e^{ik_y z + ik_z z}$$

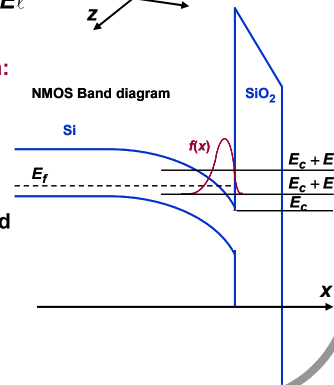
$$\left[-\frac{\hbar^2}{2m_t}\frac{\partial^2}{\partial x^2} + U(\bar{r})\right] g(x) = \left(E - E_c - \frac{\hbar^2 k_y^2}{2m_t} - - \frac{\hbar^2 k_z^2}{2m_\ell}\right) g(x)$$

$$\Rightarrow E = E_c + E_t + \frac{\hbar^2 k_y^2}{2m_t} + \frac{\hbar^2 k_z^2}{2m_\ell} \longrightarrow \left\{ E_t > E_\ell \right.$$

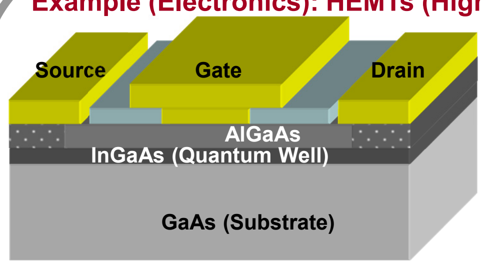


Advantage of Quantum Confinement and Quantization:

- As a result of quantum confinement the degeneracy among the states in the 6 valleys or pockets is lifted
- Most of the electrons (at least at low temperatures) occupy the two valleys (1 & 2) with the lower quantized energy (i.e. E_ℓ)
- Electrons in the lower energy valleys have a lighter mass (i.e. m_t) in the directions parallel to the interface (*y-z* plane) and, therefore, a higher mobility

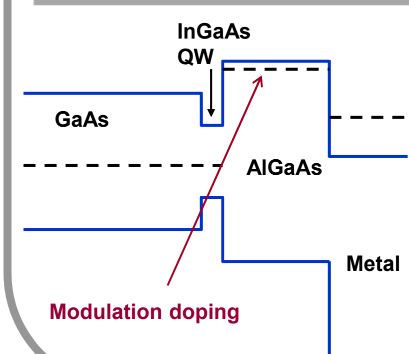


Example (Electronics): HEMTs (High Electron Mobility Transistors)

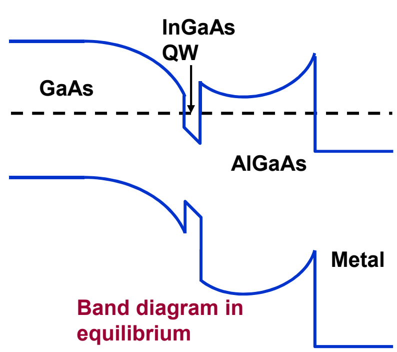


The HEMT operates like a MOS transistor:

The application of a positive or negative bias on the gate can increase or decrease the electron density in the quantum well channel thereby changing the current density



Modulation doping



Band diagram in equilibrium