Handout 27

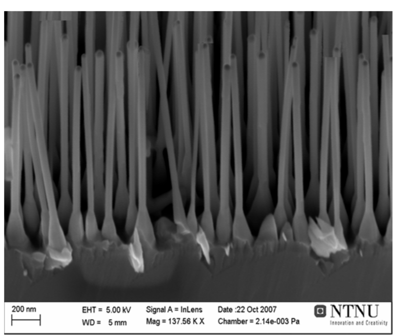
1D and 0D Nanostructures: Semiconductor Quantum Wires and Quantum Dots

In this lecture you will learn:

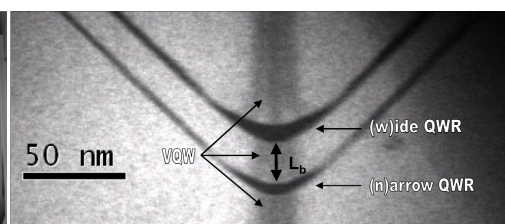
- Semiconductor quantum wires and dots
- Density of states in semiconductor quantum wires and dots

Charles H. Henry (1937-)

1D Nanostructures: Semiconductor Quantum Wires

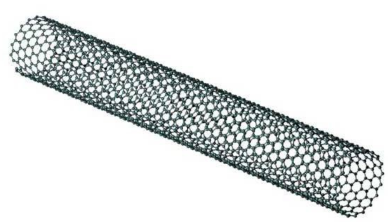


SEM of 20 nm diameter GaAs nanowires

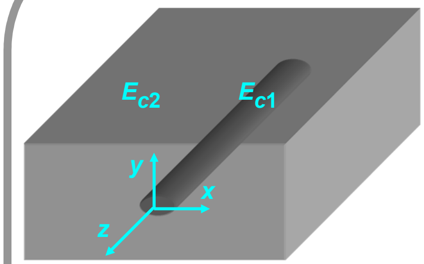


GaAs/AlGaAs quantum wires grown by electron waveguide confinement

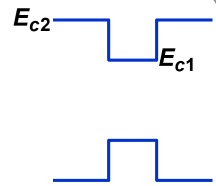
A carbon nanotube (rolled up graphene):



Semiconductor Quantum Wires



$$\Delta E_c = E_{c2} - E_{c1}$$



Inside:

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

Outside:

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

Inside:

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

Outside:

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

Assumed solutions:

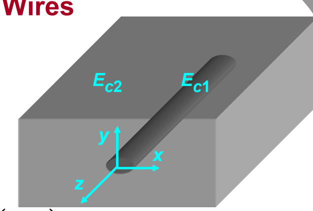
Inside:

$$\phi_1(\vec{r}) = A\ f_1(x,y)\,e^{i\,k_z\,z}$$

Outside:

$$\phi_2(\vec{r}) = A\ f_2(x,y)\,e^{i\,k_z\,z}$$

Semiconductor Quantum Wires



Inside:

Plug in the assumed solution:

$$\left[E_{c1} - \frac{\hbar^2\nabla^2}{2m_e}\right] f_1(x,y)\,e^{ik_z z} = E\ f_1(x,y)\,e^{ik_z z}$$

$$\Rightarrow \left[E_{c1} + \frac{\hbar^2 k_z^2}{2m_e} - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial y^2}\right] f_1(x,y) = E\ f_1(x,y)$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial y^2}\right] f_1(x,y) = \left(E - E_{c1} - \frac{\hbar^2 k_z^2}{2m_e}\right) f_1(x,y)$$

Outside:

$$\left[-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial y^2}\right] f_2(x,y) = \left(E - E_{c2} - \frac{\hbar^2 k_z^2}{2m_e}\right) f_2(x,y)$$

Boundary conditions at the inside-outside boundary:

$$f_1(x,y)\big|_{\text{boundary}} = f_2(x,y)\big|_{\text{boundary}}$$

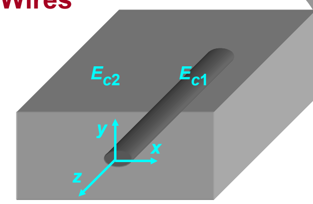
$$\frac{1}{m_e}\nabla f_1(x,y).\hat{n}\,\Big|_{\text{boundary}} = \frac{1}{m_e}\nabla f_2(x,y).\hat{n}\,\Big|_{\text{boundary}}$$

$\hat{n}$ is the unit vector normal to the boundary

Semiconductor Quantum Wires

Solve these with the boundary conditions to get for the energy of the confined states:

$$E_c(p,k_z) = E_{c1} + E_p + \frac{\hbar^2 k_z^2}{2m_e} \qquad \{ \quad p = 1,2,3........$$

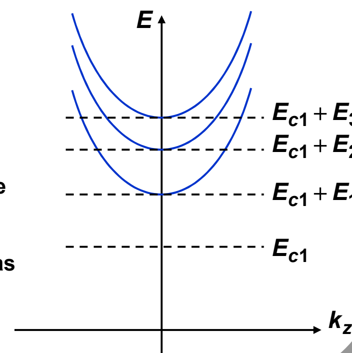


The electron is free in the z-direction but its energy due to motion in the *x-y* plane is quantized and can take on only discrete set of values

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

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

Electrons in each subband constitute a 1D Fermi gas



Semiconductor Quantum Wires: Density of States

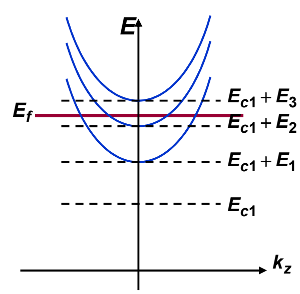
Suppose, given a Fermi level position E_f, we need to find the electron density:

We can add the electron present in each subband as follows:

$$n = \sum_p 2 \times \int_{-\infty}^{\infty} \frac{dk_z}{(2\pi)} f(E_c(p,k_z) - E_f)$$

If we want to write the above as:

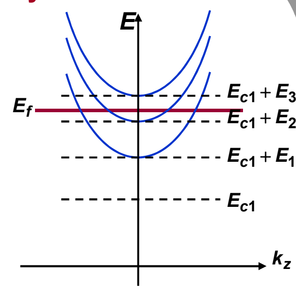
$$n = \int_{E_{c1}}^{\infty} dE \; g_{QW}(E)\, f(E - E_f)$$



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

Semiconductor Quantum Wires: Density of States

$$E_c(p,k_z) = E_{c1} + E_p + \frac{\hbar^2 k_z^2}{2m_e}$$



Start from:

$$n = \sum_p 2 \times \int_{-\infty}^{\infty} \frac{dk_z}{(2\pi)} f\left(E_c(p,k_z) - E_f\right)$$

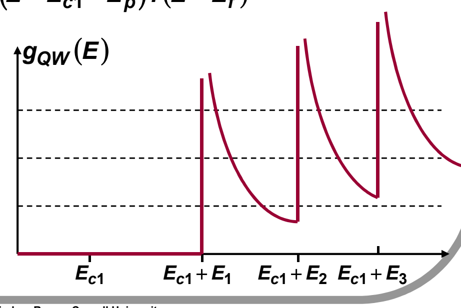
And convert the k-space integral to energy space:

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

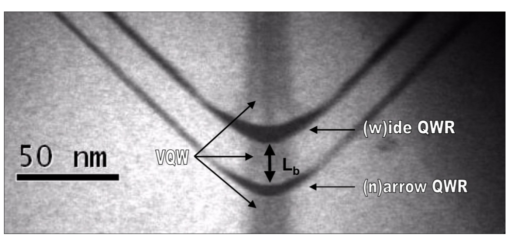
$$= \int_{E_{c1}}^{\infty} dE \sum_p \sqrt{\frac{2m_e}{\pi^2\hbar^2\left(E - E_{c1} - E_p\right)}}\, \theta\left(E - E_{c1} - E_p\right) f(E - E_f)$$

This implies:

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

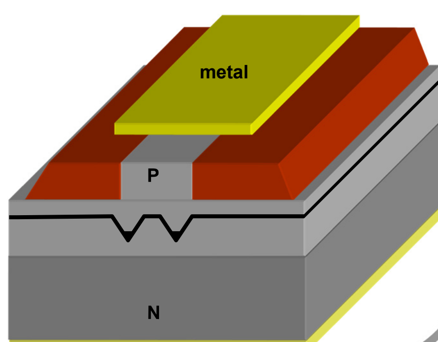


Semiconductor Quantum Wire Lasers

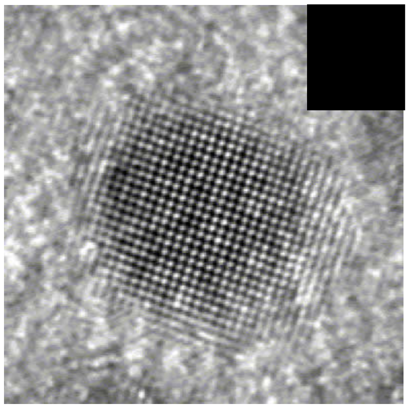


GaAs/AlGaAs quantum wires grown by electron waveguide confinement

A Ridge Waveguide Laser Structure

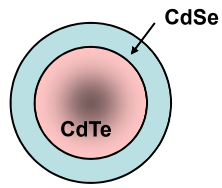


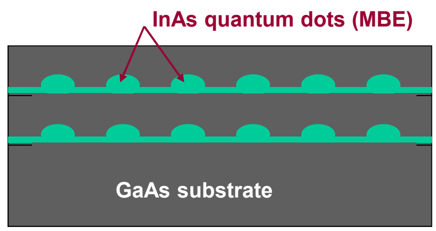
0D Nanostructures: Semiconductor Quantum Dots



TEM of a PbS quantum dot

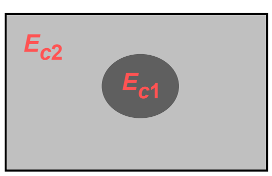
Core-shell colloidal quantum dots
(Mostly II-VI semiconductors)

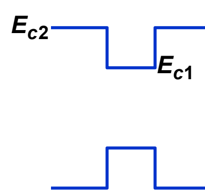




Semiconductor Quantum Dots

$$\Delta E_c = E_{c2} - E_{c1}$$





Inside:

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

Outside:

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

Inside:

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

Outside:

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

Assumed solutions:

Inside:

$$\phi_1(\vec{r}) = A\, f_1(x,y,z)$$

Outside:

$$\phi_2(\vec{r}) = A\, f_2(x,y,z)$$

Semiconductor Quantum Dots

Boundary conditions at the inside-outside boundary:

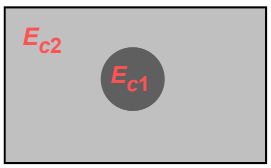
$$f_1(x,y,z)\big|_{\text{boundary}} = f_2(x,y,z)\big|_{\text{boundary}}$$

$$\frac{1}{m_e}\nabla f_1(x,y,z).\hat{n}\,\Big|_{\text{boundary}} = \frac{1}{m_e}\nabla f_2(x,y,z).\hat{n}\,\Big|_{\text{boundary}}$$

$\hat{n}$ is the unit vector normal to the boundary

Solve these with the boundary conditions to get for the energy of the confined states:

$$E_c(p) = E_{c1} + E_p \quad \{ \quad p = 1,2,3........$$



In the limit $\Delta E_c \rightarrow \infty$ the lowest energy level value for a spherical dot of radius R is:

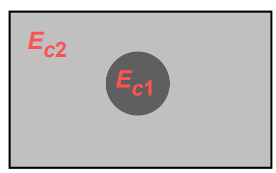
$$E_1 = \frac{\hbar^2}{2m_e}\left(\frac{\pi}{R}\right)^2$$

The electron is not free in any direction and its energy due to motion is quantized and can take on only discrete set of values

Semiconductor Quantum Dots: Density of States

Suppose, given a Fermi level position E_f, we need to find the electron number N:

We can add the electron present in each level as follows:



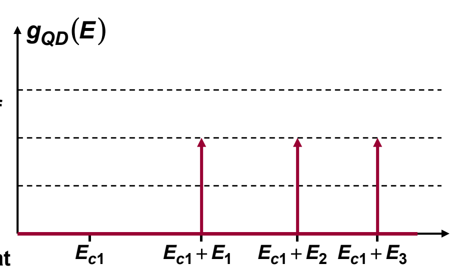
$$N = \sum_p 2 \times f(E_c(p) - E_f)$$

If we want to write the above as:

$$N = \int_{E_{c1}}^{\infty} dE\; g_{QD}(E)\, f(E - E_f)$$

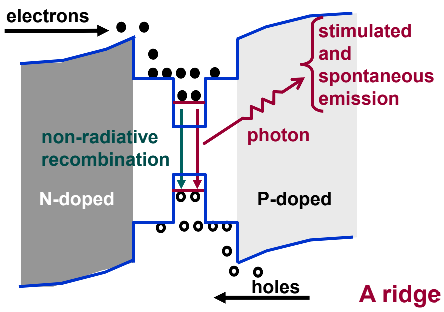
Then the question is what is the density of states $g_{QW}(E)$?

$$g_{QD}(E) = 2 \times \sum_p \delta(E - E_c(p))$$



Because the dot is such a small system, at many times concept of a Fermi level may not even be appropriate!!

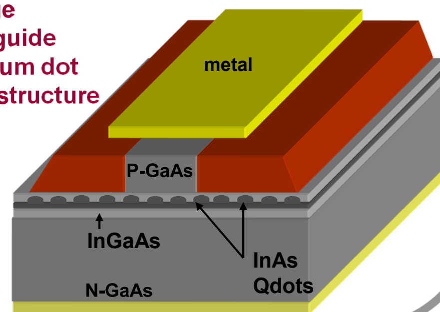
Semiconductor Quantum Dot Lasers (III-V Materials)



Some advantages of 0D quantum dots for laser applications:

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

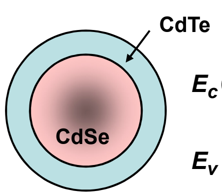
A ridge waveguide quantum dot laser structure



- Only 2 electrons can occupy a single quantum dot energy level in the conduction band

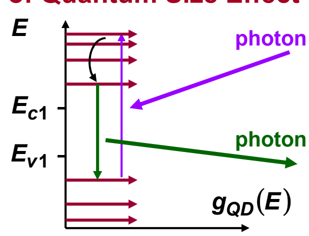
- Only 2 holes can occupy a single quantum dot energy level in the valence band

Colloidal Quantum Dots: Wonders of Quantum Size Effect



$$E_c(1) \approx E_c + \frac{\hbar^2}{2m_e}\left(\frac{\pi}{R}\right)^2$$

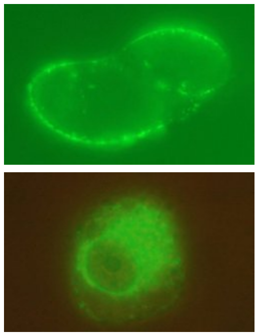
$$E_v(1) \approx E_v - \frac{\hbar^2}{2m_h}\left(\frac{\pi}{R}\right)$$



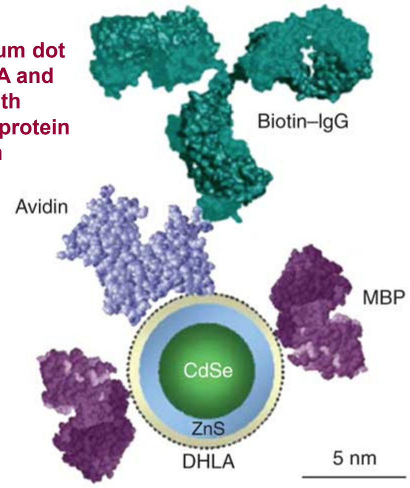
Photoluminescence from CdSe/ZnS (core-shell colloidal) quantum dots of different sizes (~2-6 nm) pumped with the same laser

Photoluminescence from CdTe/CdSe (core-shell colloidal) quantum dots of different sizes

Quantum Dots: Biology Applications



CdSe/ZnS quqntum dot coated with DHLA and functionalized with maltose binding protein (MBP) and Avidin

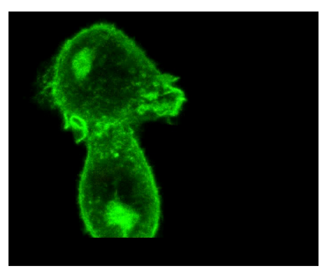


Motion of quantum-dot-attached-RNA into cells monitored by the luminescence (the quantum dots used are CdSe (core) and ZnS (shell))

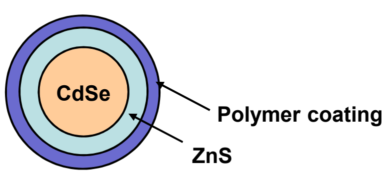
Quantum Dots: Biology Applications

Invitro microscopy of the binding of EGF to erbB1

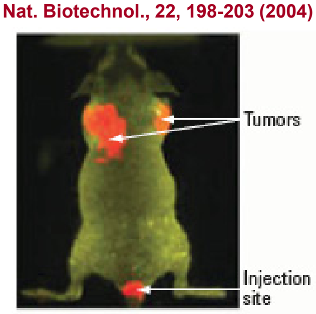
erB1 bound to eGFP (enhanced green fluorescent protein)
EGF (epidermal growth factor) bound to quantum dot
Movie shows binding of EGF tagged with fluorescent quantum dots to erB1 tagged with the green fluorescent protein



Nat. Biotechnol., 22, 198-203 (2004)

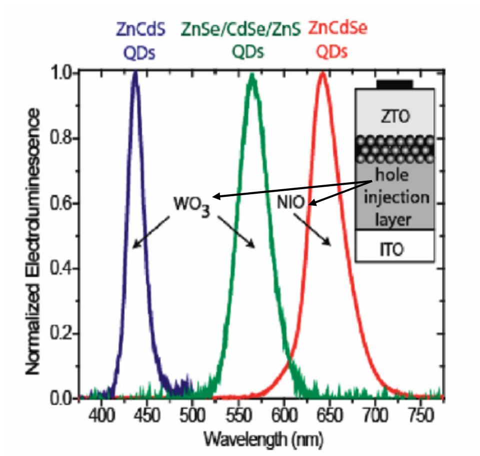


Imaging of antibody (PSMA) coated quantum dots targeting cancer tumors cells



Nat. Biotechnol., 22, 969 (2004)

Colloidal Quantum Dot Electrically Pumped LEDs



Bulovic et. al. (2010)