Lecture 21 – Nanostructures (semiconductor)

Outline
- Electron in a box (again)
- Examples of nanostructures
- Created by Applied Voltages
  - Patterned metal gates on semiconductors
  - Create “dots” that confine electrons
- Created by material structures
  - Clusters of atoms, e.g., Si_{29}H_{36}, CdSe clusters
  - Clusters of atoms embedded in an insulator, e.g., Si clusters in SiO_{2}
  - Buckyballs, nanotubes, . . .
- How does one study nanosystems?
- What are novel properties?
- See Kittel Ch 18 and added material in the lecture notes

Probes to determine structures
- Transmission electron microscope (TEM)
- Scanning electron microscope (SEM)
- Scanning tunneling microscope (STM) – more later

How small – How large?
- “Nano” means size ~ nm
- Is this the relevant scale for “nano effects”? 
  - Important changes in chemistry, mechanical properties
  - Electronic and optical properties
  - Magnetism (later)
  - Superconductivity (later)
- Changes in chemistry, mechanical properties
  - Expect large changes if a large fraction of the atoms are on the surface
- Electronic and optical properties
  - Changes due to the importance of surface atoms
  - Quantum “size effects” – can be very large and significant

“Surface” vs “Bulk” in Nanosystems
- Consider atomic “clusters” with ~ 1 nm
- Between molecules (well-defined numbers and types of atoms – well-defined structures) and condensed matter (“bulk” properties are characteristic of the “bulk” independent of the size – surface effects separate)
- Expect large changes if a large fraction of the atoms are on the surface
- Typical atomic size ~ 0.3 nm
- Consider a sphere – volume 4πR^3/3, surface area 4πR^2

Quantum Size Effects
- We can make estimates using the “electron in a box” model of the previous lecture
- The key quantity that determines the quantum effects is the mass
- When can we use m = m_{\text{electron}}?
  - In typical materials (metals like Na, Cu, … the intrinsic electrons in semiconductors,…)
- When do we use the effective mass m^*
  - For the added electrons or holes in a semiconductor

Rough estimates
- R = 3 nm ⇒ ~ 10^3 atoms ~ 10^2 on the surface – 10%
- R = 1.2 nm ⇒ ~ 64 atoms ~ 16 on the surface – 25%
- R = 0.9 nm ⇒ ~ 27 atoms ~ 9 on the surface – 33%
Quantization for electrons in a box in one dimension

- \[ E_n = \left( \frac{\hbar^2}{2m} \right) k_z^2, k_z = n \pi/L, \quad n = 1, 2, ... \]
- Lowest energy solutions with \( \Psi_n(x) = 0 \) at \( x = 0, L \)

\[ \Psi_n(x) \]

Here we emphasize the case where the box is very small.

Electron in a box

- If the electrons are confined in a cubic box of size \( L \) in all three dimensions then the total energy for the electrons:

\[ E(n_x, n_y, n_z) = \left( \frac{\hbar^2}{4mL^2} \right) (n_x^2 + n_y^2 + n_z^2) \]

The wavefunction has this form in each direction.

Nanoscale clusters

- Estimate the quantum size effects using the electron in a box model
- The discrete energies for electrons are given by

\[ E = \left( \frac{\hbar^2}{4mL^2} \right) (n_x^2 + n_y^2 + n_z^2) \]

- The typical energy scale is \( \hbar^2/(4mL^2) = 3.7 \text{ eV}/L^2 \) where \( L \) is in nm
- Thus for 3 nm, the confinement energy is

\~ 3 \times 3.7 \text{ eV}/9 \sim 1 \text{ eV}

As large as the gap in Si!

Nanoscale clusters - II

- Example: Silicon clusters
  - Must have other atoms to "passivate" the "dangling bonds" at the surface – is ideal
  - Si_{29}H_{36} – bulk-like cluster with 18 surface atoms, each with 2 H attached
  - Si_{29}H_{24} – 5 bulk-like atoms at the center and 24 rebonded surface atoms, each with one H attached – shown in the figure

- Carbon “Buckyballs”
  - Sheet of graphite (graphene) rolled into a ball (C_{60} forms a soccer ball with diameter \~ 1 nm)
  - Graphene is a zero gap material, and the size effect causes C_{60} to have a gap of \~ 2 eV

Special Presentation

Prof. Munir Nayfeh

Semiconductor Quantum Dots

- Structures with electrons (holes) confined in all three directions

\[ E = \left( \frac{\hbar^2}{2mL^2} \right) (n_x^2 + n_y^2 + n_z^2) \]

- The energy scale factor is \( \hbar^2/(2mL^2) = 3.7 \text{ eV}(m_e/m^*)L^2 \) where \( L \) is in nm
- If \( m^* = 0.01 \ m_e \), then the confinement energy is

\~ 1 \text{ eV for } L \sim 30 \text{ nm}

\~ 0.04 \text{ eV for } L \sim 150 \text{ nm}

(note 300K \~ 0.025 eV)
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One dimensional nanowires
- The motion of the electrons is exactly like the “electron in a box” problems discussed in Kittel, ch. 6
- Except the electrons have an effective mass $m^*$
- And in this case, the box has length $L$ in two directions (the $y$ and $z$ directions) and large in the $x$ direction ($L_x$ very large)
- Key Point: For ALL “electron in a box” problems, the energy is given by
  $$E(k) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$$
  For this case $m = m^*$ and $k_y = \frac{\pi}{L} n_y$, $k_z = \frac{\pi}{L} n_z$

Quantized one-dimensional bands
- $E_n(k_x, k_y) = \frac{\hbar^2}{2m^*}(\frac{\pi}{L})^2 (n_y^2 + n_z^2) + \frac{\hbar^2}{2m^*} k_x^2$
- $n = 1, 2, ...$

Density of States in two-dimensions
- Density of states (DOS) for each band is constant
- Example - electrons fill bands in order
- The density of states in a nanotube have this form
  - See Kittel, Ch 18

Quantized one-dimensional bands
- What does this mean? One can make one-dimensional electron gas in a semiconductor!
- Example - electrons fill bands in order

Nanotubes
- Carbon nanotubes are similar except there is a special “zero gap” feature in some cases
- Electrons can be added using a FET

Eg: $k_x \times k_y$ 

Electrons can move in 1 dimension but are in one quantized state in the other dimensions

More description in Kittel Ch 18
### Summary

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### Next time

- Metals – start superconductivity