Chair of Condensed Matter Physics
Institute of Theoretical Physics
Faculty of Physics, Universityof Warsaw

Semester Zimowy 2011/2012

Wykład

Modelowanie Nanostruktur

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Modeling Nanostructures

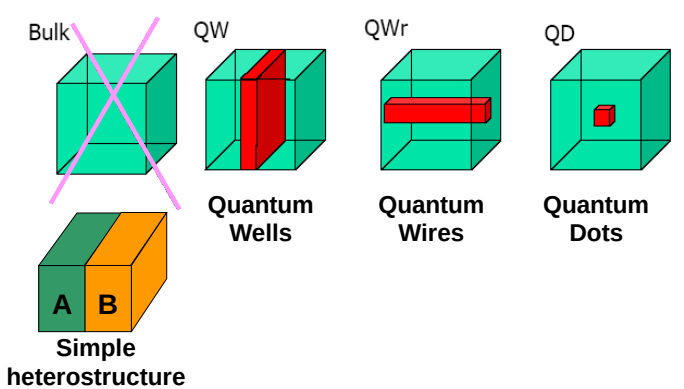
Modelowanie Nanostruktur, 2011/2012
Jacek A. Majewski

Wykład 4 – *25 X 2011*

Continuous Methods for Modeling Electronic Structure of Nanostructures

Effective Mass Approximation

Nanotechnology – Low Dimensional Structures



What about realistic nanostructures ?

Inorganics

3D (bulks) : **1-10** atoms in the unit cell

2D (quantum wells): **10-100** atoms in the unit cell

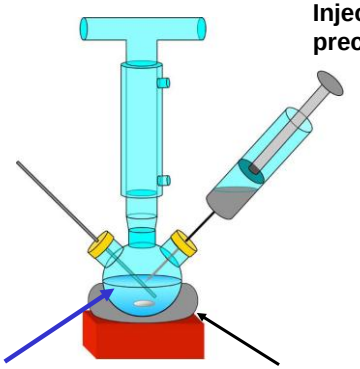
1D (quantum wires): **1 K-10 K** atoms in the unit cell

0D (quantum dots): **100K-1000 K** atoms in the unit cell

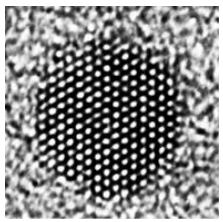
Organics

Nanotubes, DNA: **100-1000** atoms (or more)

Synthesis of colloidal nanocrystals



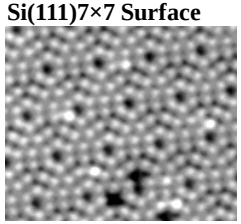
Injection of organometallic precursors



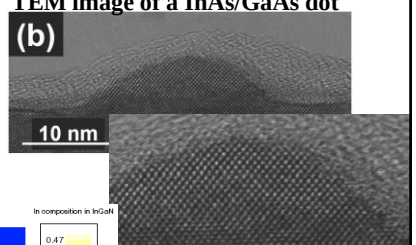
Mixture of surfactants **Heating mantle**

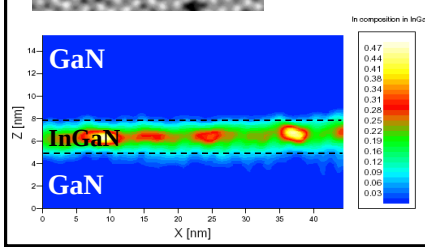
Examples of Nanostructures

Si(111)7×7 Surface



TEM image of a InAs/GaAs dot





HRTEM image: segregation of Indium in GaN/InGaN Quantum Well

Nanostructures: colloidal crystals

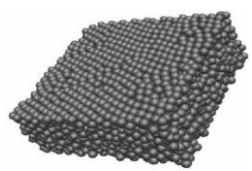
-Crystal from sub-µm spheres of PMMA (perpex) suspended in organic solvent;

- self-assembly when spheres density high enough;

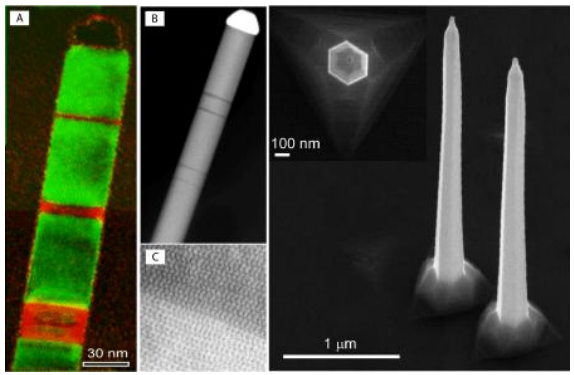
illuminated with white light ⟹

Bragg's law ⟹ different crystals ⟹ different orientation

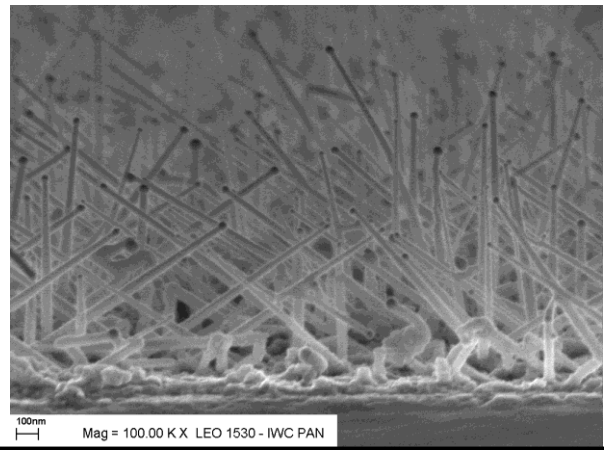
different λ



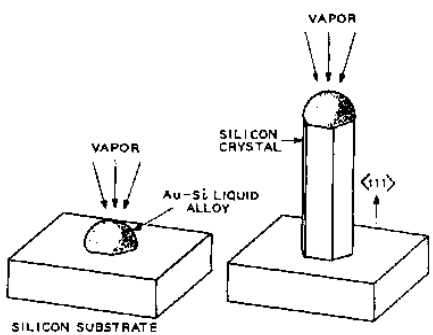
Hot topic (to come) – The curious world of nanowires



SEM of ZnTe nanowires grown by MBE on GaAs with Au nanocatalyst

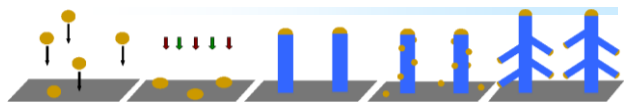


Self-organized growth of nanowires: catalytic VLS growth

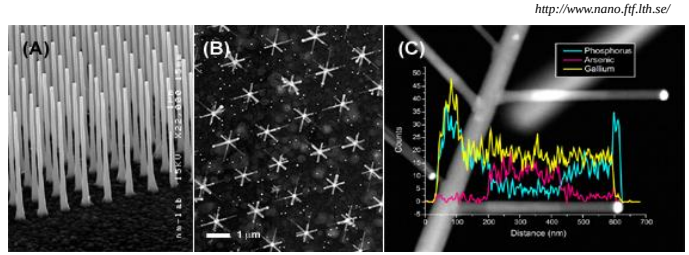


Mechanizm Vapor-Liquid-Solid VLS (Wagner 1964)

Nanowire site control and branched NW structures: nanotrees and nanoforests



http://www.nano.ftf.lth.se/

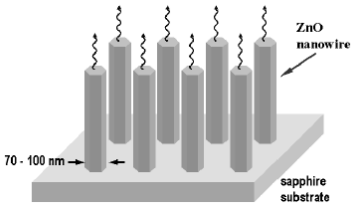


(A) Nanowires can be accurately positioned using lithographic methods such as EBL and NIL. **(B)** Subsequent seeding by aerosol deposition produces nanowire branches on an array as in panel (A). Shown here is a top view of such a 'nanoforest' where the branches grow in the <111>B crystal directions out from the stems. **(C)** Dark field STEM image and EDX line scan of an individual nanotree. **An optically active heterosegment of GaAsP in GaP has been incorporated into the branches.**

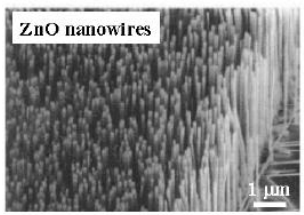
Nanowire nanolasers

Room temperature lasing action from chemically synthesized **ZnO** nanowires on sapphire substrate

Schematic illustration



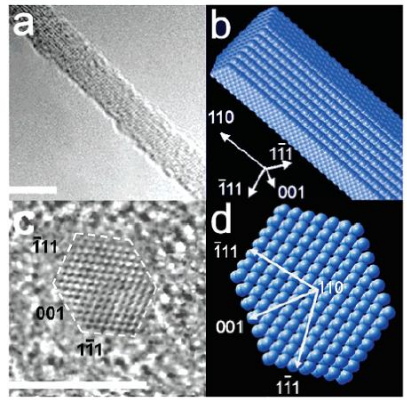
A SEM image



One end of the nanowire is the epitaxial interface between the sapphire
and ZnO, whereas ***the other end*** is the crystalline ZnO (0001) plane

Huang, M., Mao, S.S., *et al*., *Science* 292,

Controlled Growth and Structures of Molecular-Scale Silicon Nanowires



(a) TEM images of **3.8-nm** SiNWs grown along the <110> direction

(c) cross-sectional image

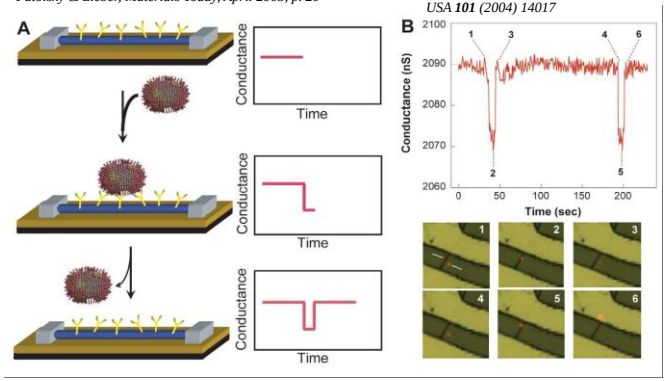
(b) & (d) models based on Wulff construction

Yue Wu *et al*., NANO LETTERS **4**, 433

Detection of single viruses with NW-FET

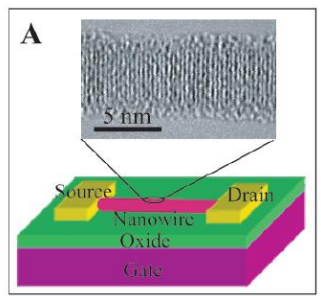
Patolsky & Lieber, Materials Today, April 2005, p. 20

*Patolsky et al., Proc. Natl. Acad. Sci. USA **101** (2004) 14017*



Simultaneous conductance and optical data recorded for a Si nanowire device after the introduction of **influenza A**

High Performance Silicon Nanowire Field Effect Transistors

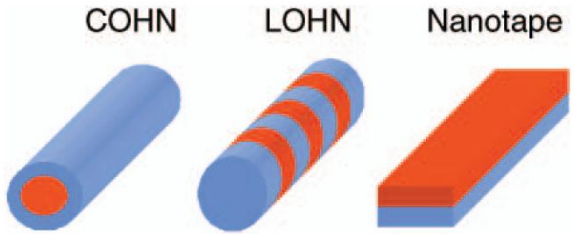


Comparison of SiNW FET transport parameters with those for state-of-the-art planar MOSFETs show that

- "SiNWs have the potential to exceed substantially conventional devices, and thus could be ideal building blocks for future nanoelectronics."

Yi Cui, *et al*. NANO LETTERS **3**, 149

Heterostructured Nanowires



coaxial heterostructured nanowire

longitudinal heterostructured nanowire

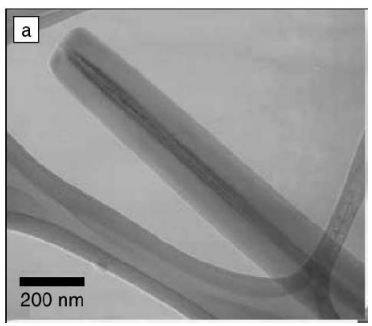
Simulation methods

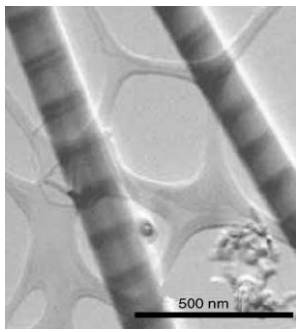
Heterostructured Nanowires

Transmission electron microscopy images of

a **GaN/AlGaN** core–sheath nanowire

two **Si/SiGe** superlattice nanowires





Atomistic methods for modeling of nanostructures

- ***Ab initio* methods** (up to few hundred atoms)

Density Functional Theory (DFT)

- One particle density determines the ground state energy of the system for arbitrary external potential

$$E[\rho] = \int d^3\vec{r}\,\rho(\vec{r})v_{ext}(\vec{r}) + F[\rho]$$

$E[\rho_0] = E_0$ — ground state energy

ground state density

Total energy functional | Kinetic energy | Exchange energy | Correlation energy

$$E[\rho] = \int d\vec{r}\,v_{ext}(\vec{r})\rho(\vec{r}) + T_S[\rho] + U[\rho] + E_x[\rho] + E_c[\rho]$$

External energy | Classic Coulomb energy | unknown!!!

Tight-Binding Hamiltonian

$$H = \sum_{\alpha i} \varepsilon_{i\alpha} c_{i\alpha}^{\dagger} c_{i\alpha} + \sum_{\alpha i,\beta j} t_{i\alpha,j\beta} c_{i\alpha}^{\dagger} c_{j\beta}$$

creation & anihilation operators

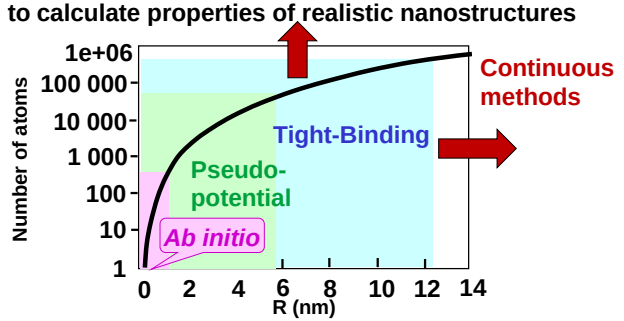
- *On-site energies* are not atomic eigenenergies
  They include on average the effects of neighbors
  ⇒ Problem: *Transferability*
  E.g., Si in diamond lattice (4 nearest neighbors) & in fcc lattice (12 nearest neighbors)
- Dependence of *the hopping energies* on the distance between atoms

Atomistic methods for modeling of nanostructures

- *Ab initio* methods (up to few hundred atoms)
- **Semiempirical methods** (up to 1M atoms)
  - Tight-Binding Methods

Atomistic vs. Continuous Methods

- Microscopic approaches can be applied to calculate properties of realistic nanostructures



Number of atoms in a spherical Si nanocrystal as a function of its radius R.
Current limits of the main techniques for calculating electronic structure.
Nanostructures commonly studied experimentally lie in the size range 2-15 nm.

Atomistic methods for modeling of nanostructures

- *Ab initio* methods (up to few hundred atoms)
- **Semiempirical methods** (up to 1M atoms)
  - (Empirical Pseudopotential)
  - **Tight-Binding Methods**
- **Continuum Methods**
  (e.g., effective mass approximation)

Electron in an external field

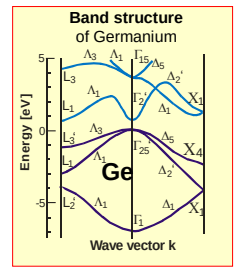
$$\left[\frac{\hat{p}^2}{2m} + V(\vec{r}) + U(\vec{r})\right]\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

Periodic potential of crystal

Non-periodic external potential

- Strongly varying on atomic scale
- Slowly varying on atomic scale

$U(\vec{r}) = 0 \Rightarrow \varepsilon_n(\vec{k})$ **Band Structure**



Continuum theory- Envelope Function Theory

Electron in an external field

$$\left[\frac{\vec{p}^2}{2m} + V(\vec{r}) + U(\vec{r})\right]\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

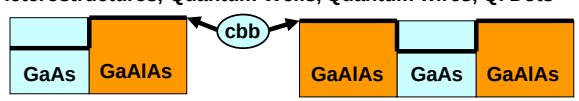
Periodic potential of crystal

Non-periodic external potential

- Strongly varying on atomic scale
- Slowly varying on atomic scale

Which external fields ?

- Shallow impurities, e.g., donors $U(\vec{r}) = -\frac{e^2}{\kappa|\vec{r}|}$
- Magnetic field B, $\vec{B} = curl\vec{A} = \vec{\nabla}\times\vec{A}$
- Heterostructures, Quantum Wells, Quantum wires, Q. Dots



- Does equation that involves the effective mass and a slowly varying function exist ?

$$\left(\frac{\vec{p}^2}{2m^*} + U(\vec{r})\right)F(\vec{r}) = \varepsilon F(\vec{r}) \qquad F(\vec{r}) = ?$$

Envelope Function Theory – Effective Mass Equation

J. M. Luttinger & W. Kohn, Phys. Rev. B **97**, 869 (1955).

$$[\varepsilon(-i\vec{\nabla}) + U(\vec{r}) - \varepsilon]F_n(\vec{r}) = 0$$ (EME)

EME does not couple different bands

$$\psi(\vec{r}) = F_n(\vec{r})u_{n0}(\vec{r})$$

"True" wavefunction — Envelope Function — Periodic Bloch Function

- Special case of constant (or zero) external potential

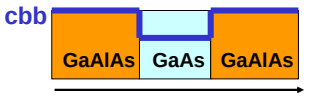
$U(\vec{r}) = 0 \Rightarrow F_n(\vec{r}) = \exp(i\vec{k}\cdot\vec{r}) \Rightarrow \psi(\vec{r})$ Bloch function

- $U(z) \Rightarrow F_n(\vec{r}) = \exp[i(k_x x + k_y y)]F_n(z)$

Envelope Function Theory- Electrons in Quantum Wells

Effect of Quantum Confinement on Electrons

- Let us consider an electron in the conduction band near Γ point



Potential $U(\vec{r})$?

$$U(\vec{r}) = U(z) = \begin{cases} \varepsilon_{c0} & z \in \text{GaAs} \\ \varepsilon_{c0} + \Delta E_c & z \in \text{GaAlAs} \end{cases}$$

Growth direction (z – direction)

$\varepsilon_c(\vec{k}) = \varepsilon_{c0} + \frac{\hbar^2}{2m^*}\vec{k}^2$ $U(\vec{r})$ is constant in the xy plane

Effective Mass Equation for the Envelope Function F

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)F(x,y,z)+U(z)F(x,y,z) = EF(x,y,z)$$

Separation Ansatz $F(x,y,z) = F_x(x)F_y(y)F_z(z)$

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2 F_x}{\partial x^2}F_yF_z+\frac{\partial^2 F_y}{\partial y^2}F_xF_z+\frac{\partial^2 F_z}{\partial z^2}F_xF_y\right)+U(z)F_xF_yF_z = EF_xF_yF_z$$

Electronic states in Quantum Wells

Effective Mass Equation of an Electron in a Quantum Well

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2 F_x}{\partial x^2}F_yF_z+\frac{\partial^2 F_y}{\partial y^2}F_xF_z+\frac{\partial^2 F_z}{\partial z^2}F_xF_y\right)+U(z)F_xF_yF_z = EF_xF_yF_z$$

$$E = E_x + E_y + E_z$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2 F_x}{\partial x^2}F_yF_z = E_xF_xF_yF_z \qquad -\frac{\hbar^2}{2m^*}\frac{\partial^2 F_y}{\partial y^2}F_xF_z = E_yF_xF_yF_z$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2 F_z}{\partial z^2}F_xF_y+U(z)F_xF_yF_z = E_zF_xF_yF_z$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2 F_x}{\partial x^2} = E_xF_x \Rightarrow F_x \sim e^{ik_x x}, \quad E_x = \frac{\hbar^2}{2m^*}k_x^2$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2 F_y}{\partial y^2} = E_yF_y \Rightarrow F_y \sim e^{ik_y y}, \quad E_y = \frac{\hbar^2}{2m^*}k_y^2$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2 F_{zn}}{\partial z^2}+U(z)F_{zn} = E_{zn}F_{zn}$$

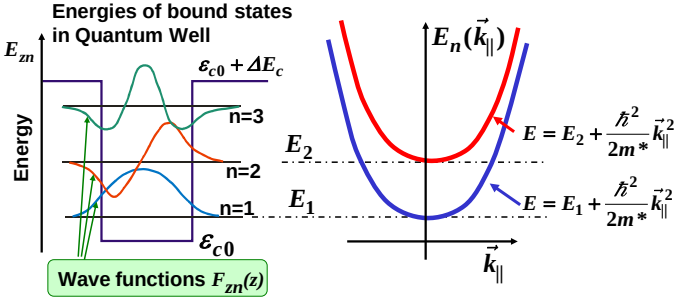
Conduction band states of a Quantum Well

$$F_{\vec{k}_\parallel}(\vec{r}_\parallel) = \frac{1}{A}\exp[i(k_x x + k_y y)] = \frac{1}{A}\exp(i\vec{k}_\parallel \cdot \vec{r}_\parallel)$$

$$F_{n,\vec{k}_\parallel}(\vec{r}) = F_{\vec{k}_\parallel}(\vec{r}_\parallel)F_{zn}(z) = \frac{1}{A}\exp(i\vec{k}_\parallel \cdot \vec{r}_\parallel)F_{zn}(z) \quad \leftarrow F_{zn}(z)$$

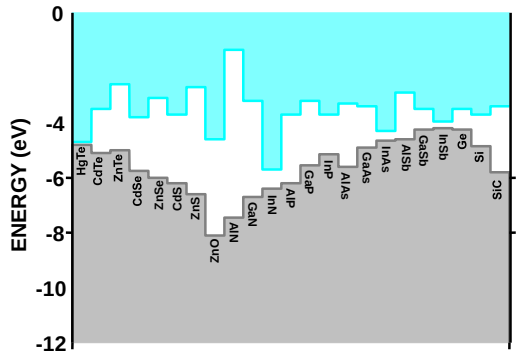
$$E_n(\vec{k}_\parallel) = \frac{\hbar^2}{2m^*}\vec{k}_\parallel^2 + E_{zn} \quad \leftarrow E_{zn} \quad -\frac{\hbar^2}{2m^*}\frac{\partial^2 F_{zn}}{\partial z^2} + U(z)F_{zn} = E_{zn}F_{zn}$$

Energies of bound states in Quantum Well



Wave functions $F_{zn}(z)$

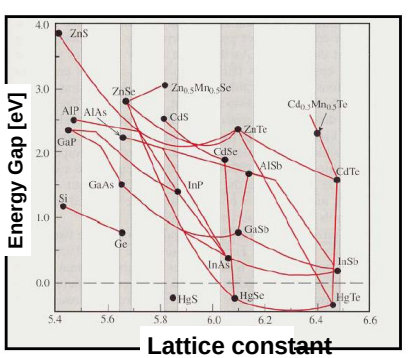
Band lineups in semiconductors

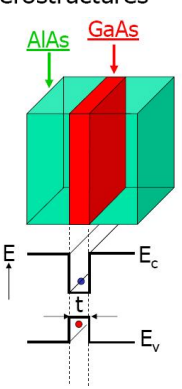


Band edges compile by: *Van de Walle (UCSB) Neugebauer (Padeborn), Nature'04*

Band structure Engineering

Semiconductor Multilayers → Heterostructures

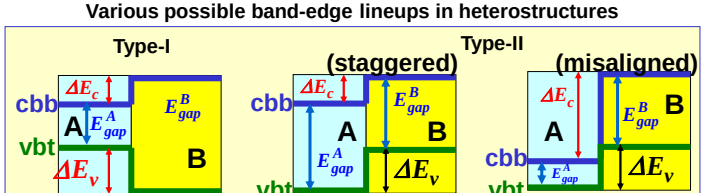




The major goal of the fabrication of heterostructures is the controllable modification of the energy bands of carriers

Envelope Function Theory- Electrons in Quantum Structures

Various possible band-edge lineups in heterostructures

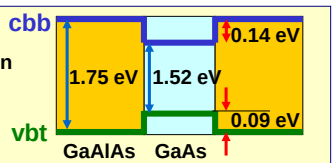


e.g., GaAs/GaAlAs | GaN/SiC | InAs/GaSb

ΔE_v - Valence Band Offset (VBO) ΔE_c - Conduction band offset

VBO's can be only obtained either from experiment or ab-initio calculatio

Band lineup in GaAs / GaAlAs Quantum Well with Al mole fraction equal 20%



Density of states

Density of States of a Two-Dimensional Electron Gas

A special function known as the *density of states G(E)* that gives the number of quantum states *dN(E)* in a small interval *dE* around energy *E*: $dN(E) = G(E)\,dE$

ν -the set of quantum numbers (discrete and continuous) corresponding to a certain quantum state

$$G(E) = \sum_{\nu} \delta(E - E_{\nu})$$

Energy associated with the quantum state ν

Spin quantum number

Continuous two-dimensional vector

For 2DEG: $\nu = \{s, n, \vec{k}_{\|}\}$

A quantum number characterizing the transverse quantization of the electron states

$$G(E) = 2 \sum_{n,k_x,k_y} \delta[E - E_n - \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)]$$

Density of States

G(E)dE - the number of electron states with energies *E* and *E + dE*

Generally, this quantity is proportional to the volume of the crystal

Convention: we define *G* to refer to the volume of a unit cell Ω

- We define G_σ to refer to a single direction of electron spin (denoted σ)

$$G_\sigma(E) = \frac{\Omega}{(2\pi)^3} \sum_n \int d^3\vec{k}\, \delta(E - \varepsilon_{n\sigma}(\vec{k}))$$

Band index

Of course, there is no contribution from a particular band at energy *E* unless there are states of energy *E* in that band

$$\varepsilon_n(\vec{k}) = \varepsilon_n(0) + \frac{\hbar^2 \vec{k}^2}{2m_n^*} \Rightarrow G^{(3D)}(E) = \left(\frac{m^*}{\hbar^2}\right)^{3/2} \frac{\sqrt{2}}{\pi^2} \sqrt{E}$$

Density of States of a Two-Dimensional Electron Gas

$$G(E) = 2 \sum_{n,k_x,k_y} \delta[E - E_n - \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)]$$

L_x, L_y - are the sizes of the system in x and y directions

$S = L_x L_y$ - the surface of the system $\sum_{k_x,k_y} (\ldots) = \frac{L_x L_y}{(2\pi)^2} \iint dk_x dk_y (\ldots)$

$$G(E) = 2\frac{L_x L_y}{(2\pi)^2} \sum_n \iint dk_x dk_y \delta[E - E_n - \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)] =$$

$$= \frac{L_x L_y}{2\pi^2} \sum_n \int_0^\infty 2\pi k_{\|} dk_{\|} \delta(E - E_n - \frac{\hbar^2}{2m^*} k_{\|}^2) =$$

$$= \frac{L_x L_y}{\pi} \frac{2m^*}{\hbar^2} \sum_n \int_0^\infty k_{\|} dk_{\|} \delta(E - E_n - k_{\|}^2)$$

$k_{\|}^2 = \varepsilon_{\|}$

$$G(E) = \frac{Sm^*}{\pi\hbar^2} \sum_n \int_0^\infty d\varepsilon_{\|} \delta(E - E_n - \varepsilon_{\|}) = \frac{Sm^*}{\pi\hbar^2} \sum_n \Theta(E - E_n)$$

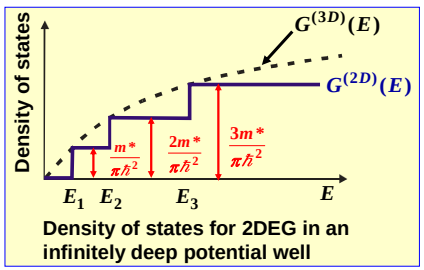
$\Theta(x)$ - Heaviside step function $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x < 0$

Density of States of a Two-Dimensional Electron Gas

$$G(E) = \frac{Sm^*}{\pi\hbar^2}\sum_n \Theta(E - E_n)$$

Often the density of states per unit area, $G(E)/S$, is used to eliminate the size of the sample

- Each term in the sum corresponds to the contribution from one subba
- The contributions of all subbands are equal and independent of energy
- The DOS of 2DEG exhibits a staircase-shaped energy dependence, with each step being associated with one of the energy states.



Density of states for 2DEG in an infinitely deep potential well

$$G^{(3D)}(E) = \left(\frac{m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{2}}{\pi^2}\sqrt{E}$$

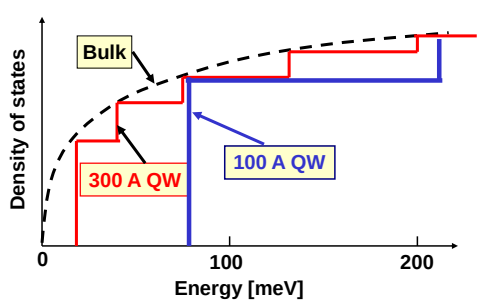
$$\varepsilon(\vec{k}) = \frac{\hbar^2}{2m^*}\vec{k}^2$$

For large n, the staircase function lies very close to the bulk curve $G^{(3D)}(E)$

Electronic states in Quantum Wires

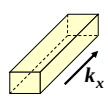
Density of States of a Two-Dimensional Electron Gas

Dependence on the width of Quantum Well



QW of large width ⟹ Bulk

Electron States in Quantum Wires



- Free movement in the x-direction,
- Confinement in the y, z directions
- Confinement potential $U(y,z)$

$$F(x,y,z) = e^{ik_x x}F_n(y,z)$$

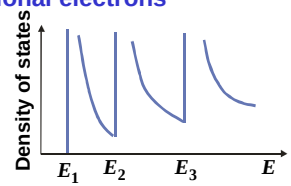
$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)F_n(y,z) + U(y,z)F_n(y,z) = E_n F_n(y,z)$$

$$E_n(k_x) = E_n + \frac{\hbar^2}{2m^*}k_x^2$$

Density of states for one-dimensional electrons

$$G^{(1D)}(E) = 2\sum_{n,k_x}\delta(E - E_n - \frac{\hbar^2 k_x^2}{2m^*})$$

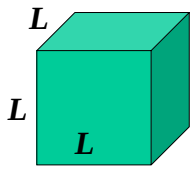
$$G^{(1D)}(E) = \frac{L_x}{\pi}\sqrt{\frac{2m^*}{\hbar^2}}\sum_n \frac{1}{\sqrt{E - E_n}}\Theta(E - E_n)$$



Electronic states in Quantum Dots

Confinement ➟ Quantization of energy levels

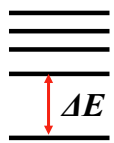
How small should be semiconductor system to see separate levels in room temperature?



$$k_x L = 2\pi n_x \qquad k_y L = 2\pi n_y \qquad k_z L = 2\pi n_z$$

$$E = \frac{\hbar^2}{2m^*}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$m^* = \tilde{m} * m_0$$

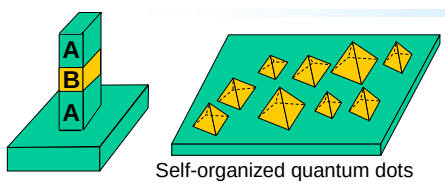


$$\Delta E > k_B \cdot 300K = 0.026eV$$

$$L^2 < \frac{1}{\tilde{m}^*} 173.55 \text{ nm}^2$$

GaAs	$\tilde{m}^* = 0.03$	$L < 76nm$
Si	$\tilde{m}^* = 0.2$	$L < 29nm$

Electron States in Quantum Dots



Self-organized quantum dots

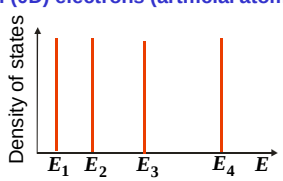
Electrons confined in all directions

$U(x,y,z)$

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)F_n(x,y,z)+U(x,y,z)F_n(x,y,z)=E_nF_n(x,y,z)$$

Density of states for zero dimensional (0D) electrons (artificial atoms)

$$G^{(0D)}(E)=\sum_\nu \delta(E-E_\nu)$$



Electronic states in Nanostructures Summary

Energy spectrum

1D: free motion in *x* direction, dimensional quantisation in *z,y*

$[H,p_x] = 0$ ➔

$\psi_{m,n}(r) = u_k(r)e^{ik_x x}F_{m,n}(y,z)/(L_x)^{1/2}$

2D: free motion in *x,y* directions,dimensional quantisation in *z*

$[H,p_x] = 0; [H,p_y] = 0$ ➔

$\psi_n(r) = u_k(r)e^{i(k_x x+k_y y)}F_n(z)/(L_x L_y)^{1/2}$

3D: free motion in *x,y,z* directions

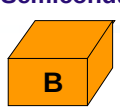
$[H,p] = 0$ ➔

$\psi_k(r) = u_k(r)e^{ikr}/(L_x L_y L_z)^{1/2}$

Position Dependent Effective Mass

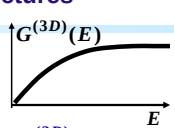
Density of States of Electrons in Semiconductor Quantum Structures

3D Bulk

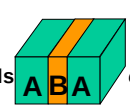


$\varepsilon_c(\vec{k}) = \varepsilon_{c0} + \frac{\hbar^2}{2m^*}\vec{k}^2$

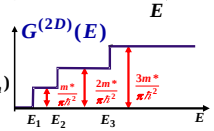
$G^{(3D)}(E) = \left(\frac{m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{2}}{\pi^2}\sqrt{E}$



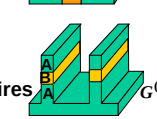
2D Quantum Wells



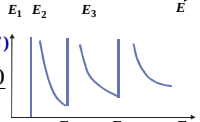
$G^{(2D)}(E) = \frac{m^*}{\pi\hbar^2}\sum_n \Theta(E-E_n)$



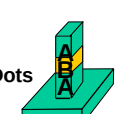
1D Quantum Wires



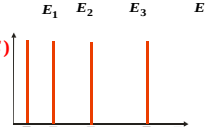
$G^{(1D)}(E) = \sqrt{\frac{2m^*}{\pi^2\hbar^2}}\sum_n \frac{\Theta(E-E_n)}{\sqrt{E-E_n}}$



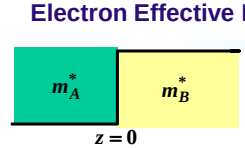
0D Quantum Dots



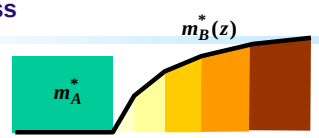
$G^{(0D)}(E) = \sum_n \delta(E-E_n)$



Effective Mass Theory with Position Dependent Electron Effective Mass



$m_A^* \neq m_B^*$



"Graded structures"

$-\frac{\hbar^2}{2m^*(z)}\frac{d^2}{dz^2}$ IS NOT HERMITIAN !!

Symetrization of the kinetic energy operator $-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz}$ IS HERMITIAN !

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m^*(z)}\frac{d}{dz}\right]F(z)+U(z)F(z) = EF(z)$$

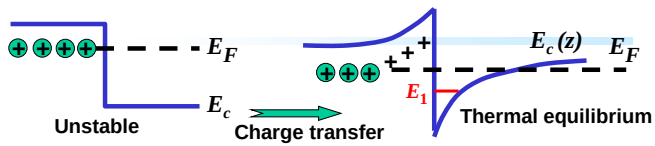
$F(z)$ and $\frac{1}{m^*(z)}\frac{dF(z)}{dz}$ ARE CONTINOUOS !

General form of the kinetic energy operator

$T = [m^*(z)]^\alpha \hat{p}_z [m^*(z)]^\beta \hat{p}_z [m^*(z)]^\alpha$ with $2\alpha+\beta = -1$

Doping in Semiconductor Low Dimensional Structures

Effects of Doping on Electron States in Heterostructures



Resulting electrostatic potential

Fermi distribution function

$$\nabla^2\Phi(\vec{r}) = \frac{4\pi e}{\varepsilon}\left[\sum_{(acc)}\delta(\vec{r}-\vec{R}_A) - \sum_{(don)}\delta(\vec{r}-\vec{R}_D) - \sum_{\nu} f_\nu |\psi_\nu(\vec{r})|^2\right]$$

should be taken into account in the Effective Mass Equation

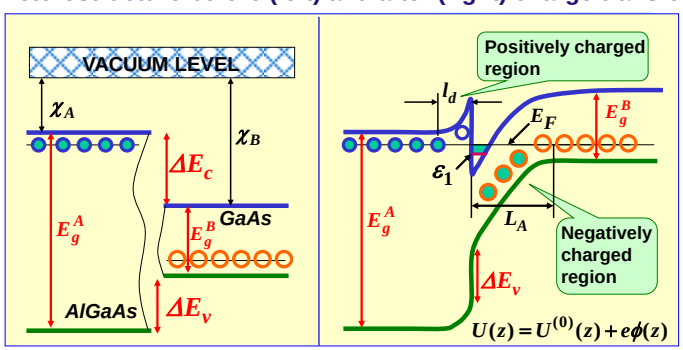
$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+U(x,y,z)-e\Phi(\vec{r})\right]\psi_\nu(\vec{r}) = E_\nu\psi_\nu(\vec{r})$$

Electrostatic potential can be obtained from the averaged acceptor and donor concentrations

$$\nabla^2\Phi(\vec{r}) = \frac{4\pi e}{\varepsilon}\left[N_A(\vec{r}) - N_D(\vec{r}) - \sum_{\nu} f_\nu |\psi_\nu(\vec{r})|^2\right]$$

- The self-consistent problem, so-called "Schrödinger-Poisson" problem

Energy band diagram of a selectively doped AlGAAs/GaAs Heterostructure before (left) and after (right) charge transfer



- χ_A and χ_B - The electron affinities of material A & B
- The Fermi level in the *GaAlAs* material is supposed to be pinned on the donor level.
- The narrow bandgap material GaAs is slightly p doped.

Thank you!