PHY404- Solid State Physics II

Semiconductor Heterostructures
and Low-Dimensional Quantum Structures

Assoc.Prof.Dr. Yeşim MOĞULKOÇ

Contents

- Low dimensional quantum structures
- Semiconductor crystal growth technology
  - Liquid-phase epitaxy (LPE)
  - Molecular beam epitaxy (MBE)
  - Metal-organic chemical vapor deposition (MOCVD)
- Energy Band Offsets

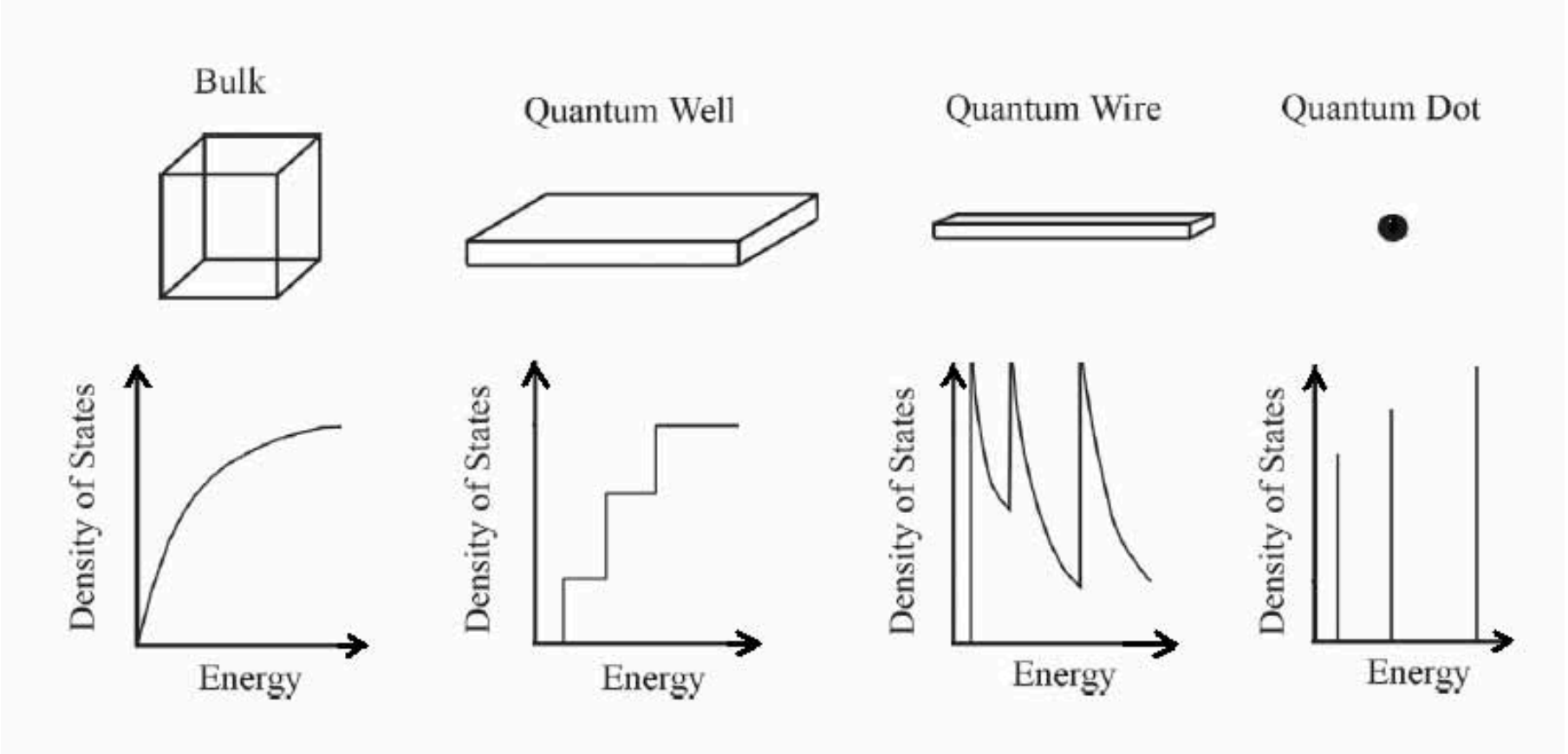
Low dimensional quantum structures

- In nanometer-scale structures in a crystal, **the motion of an electron** can be confined in one or more directions in space.

- When **only one dimension is restricted** while the other two remain free, we talk about **a quantum well**; when **two dimensions are restricted**, we talk about **a quantum wire**; and when the motion in **all three dimensions is confined**, we talk about **a quantum dot**.

- In solid-state physics, these are *commonly called* **low-dimensional quantum structures**.

Low dimensional quantum structures



Semiconductor crystal growth technology

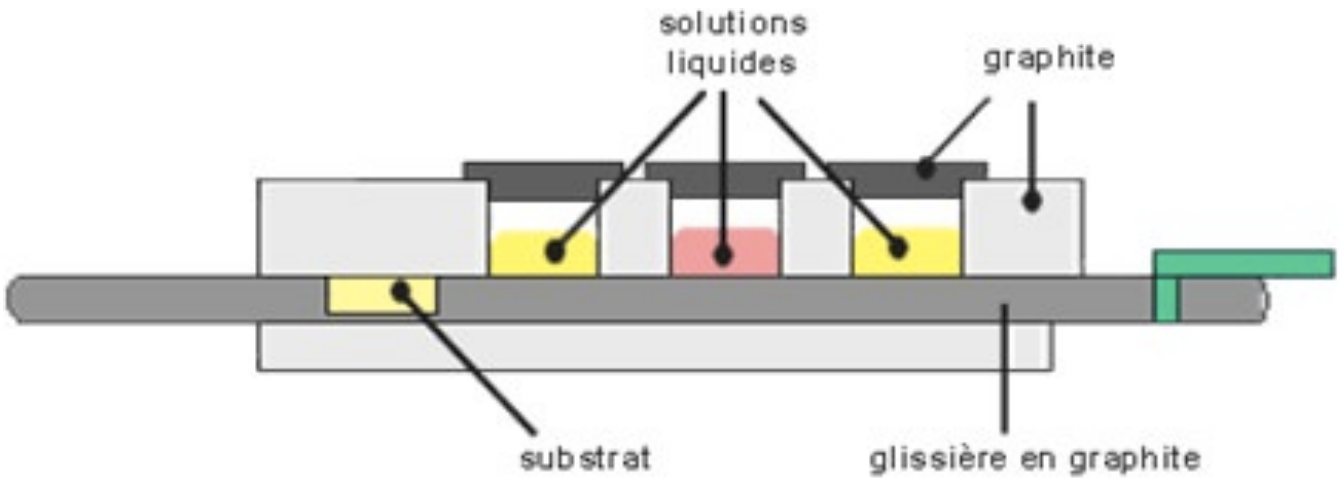
- Liquid-phase epitaxy (LPE)
- Molecular beam epitaxy (MBE)
- Metal-organic chemical vapor deposition (MOCVD)

This technology makes it possible:

- ➢ to control with atomic-scale precision of the dimensions of semiconductor structures
- ➢ to realize such low-dimensional quantum structures through the formation of heterojunctions or heterostructures.

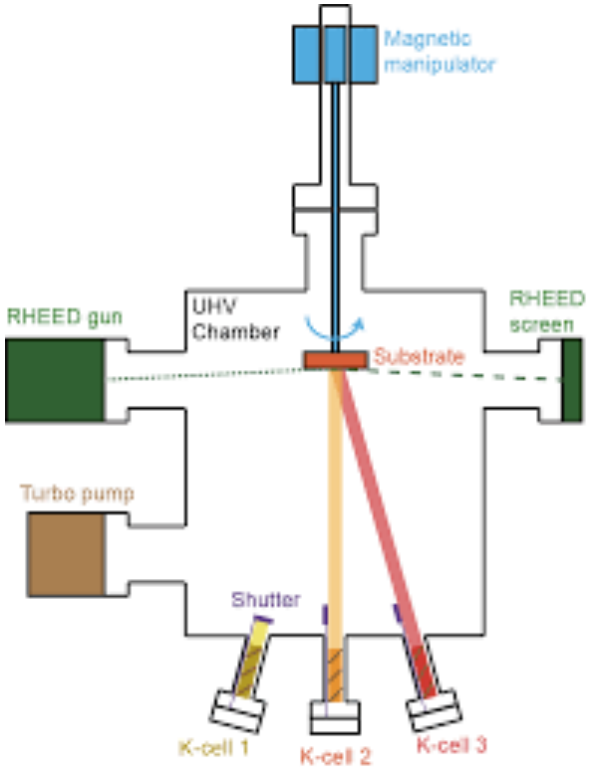
Liquid-phase epitaxy (LPE)

- This method is the most basic.
- A gas is cooled until it becomes a liquid, which is then cooled further until it becomes a solid.
- Polycrystalline solids are typically produced by this method unless special techniques are employed.



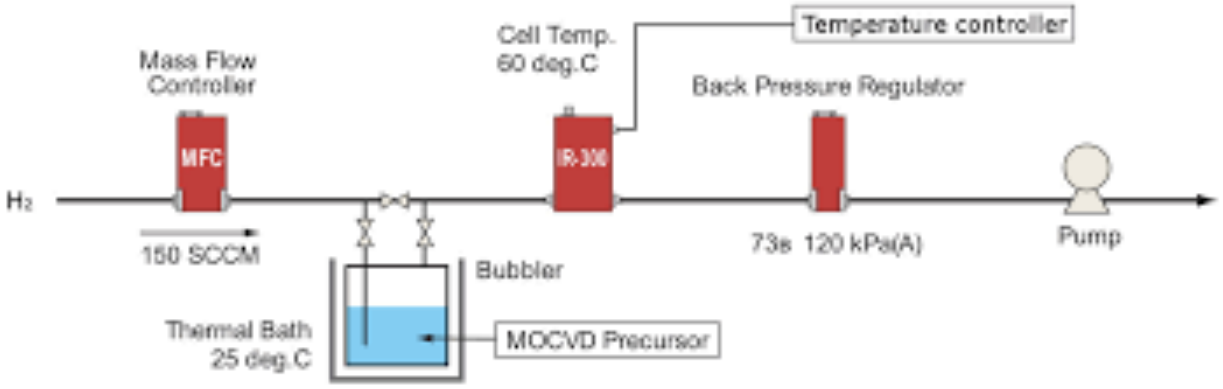
Molecular beam epitaxy (MBE)

- The term "molecular beam" describes a unidirectional kinematic flow of atoms or molecules with no collisions among them, as opposed to a viscous, fluid-like flow.
- Molecular beam epitaxy is unique in two respects: it is performed in UHV, and it is based on the reaction of atomic and/or molecular beams with a crystalline surface, relying on kinetic processes such as adsorption, desorption, dissociation, migration, reaction, and incorporation.
- These features allow real-time, in situ monitoring and control during the substrate preparation and film growth, to ensure the best conditions for stoichiometry and epitaxy.



Metal-organic chemical vapor deposition (MOCVD)

- In the metal organic chemical vapor deposition (MOCVD) technique, reactant gases are combined at elevated temperatures in the reactor to cause a chemical interaction, resulting in the deposition of materials on the substrate.
- A reactor is a chamber made of a material that does not react with the chemicals being used. It must also withstand high temperatures.
- A substrate sits on a *susceptor* which is at a controlled temperature.



A semiconductor heterojunction formation

- A semiconductor heterojunction is formed when two different semiconducting materials are brought into direct contact with each other, while heterostructures can be defined as materials that incorporate one or more heterojunctions and can describe more complicated device architectures such as multiple quantum wells, superlattices, and other low-dimensional quantum structures.
- First proposed by Shockley in 1951 in a heterojunction bipolar transistor (HBT) (Shockley 1951), heterojunctions have been used heavily in a variety of applications.
- Many conventional devices take advantage of the special properties of heterostructures including semiconductor lasers, light-emitting diodes, photodetectors, etc.

Energy Band Offsets

- When a heterojunction is formed, the conduction and valence band alignment is dependent upon the properties of the constituent materials such as their bandgap, the doping, and the electron affinity.

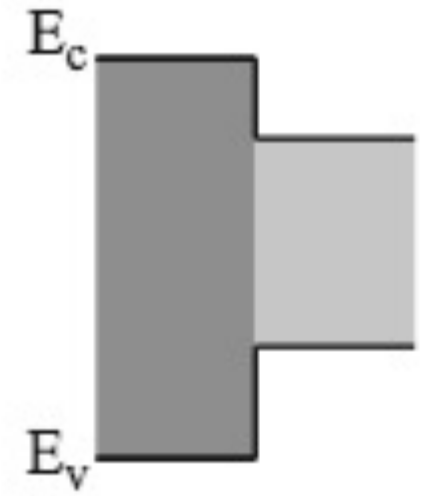
- Heterostructures can be classified depending on the band alignment formation between the two semiconductor materials.

- The possible band alignment combinations include “type I,” “type II staggered,” and “type II broken gap”.

Type I Alignment

- When the valence and conduction band of one material “straddles” the bands of the narrow-gap material, the heterojunction band alignment is termed type I.

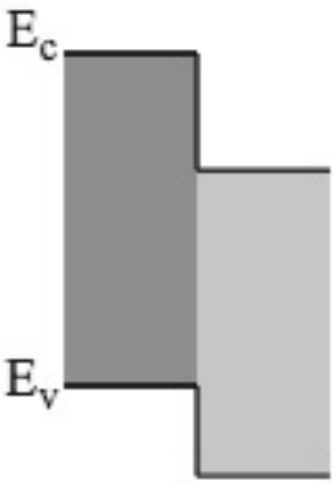
- The heavily investigated AlGaAs/GaAs heterojunction exhibits this band lineup with the aluminum-containing material having its conduction band above and valence band below the corresponding GaAs band energies.



Type II Alignment-I

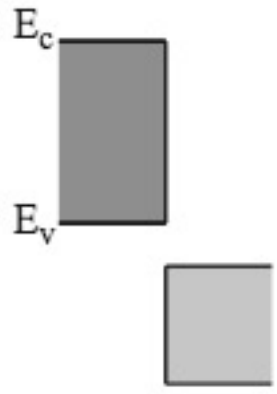
- Semiconductor heterojunctions may also form where the conduction and valence bands in one material are both slightly below the corresponding band energies in the adjacent semiconductor. This band alignment is termed type II staggered and is shown in Fig.

- One example of a heterojunction material system that can be generally classified as type II staggered is InAs/AlSb.

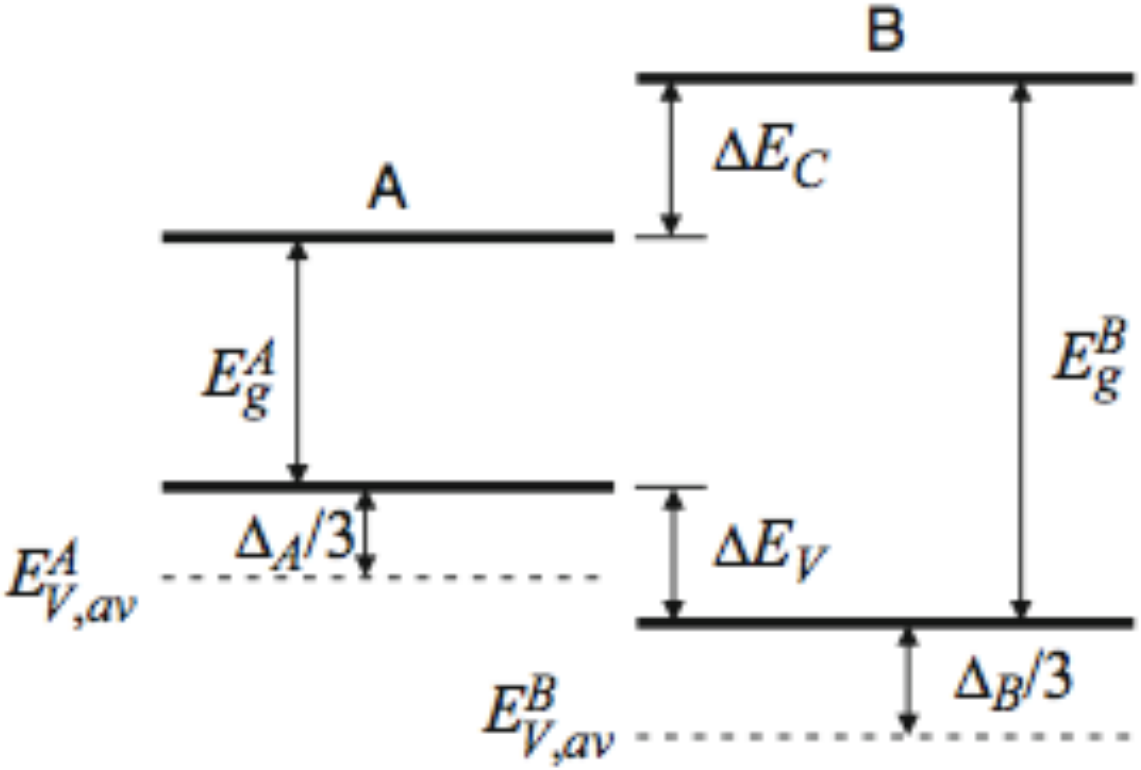


Type II Alignment-II

- The InAs/GaSb heterojunction is an example of a type II broken gap alignment.
- This occurs when the conduction of one material is at a lower energy than the valence band of the adjacent semiconductor.
- An example of broken-gap band alignment is shown in Figure.

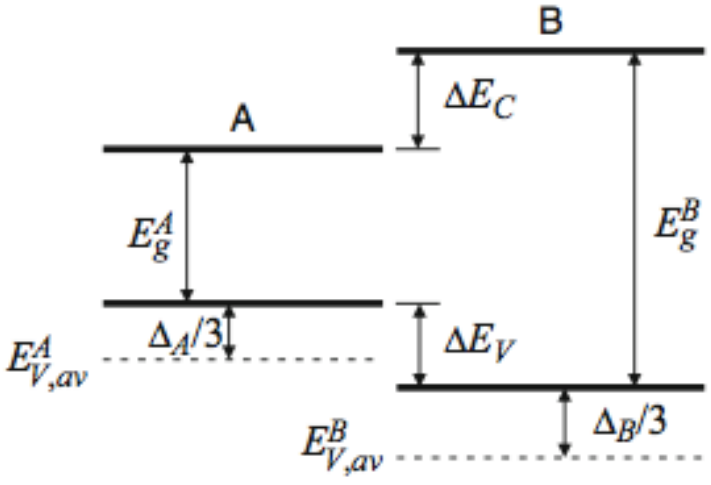


Band alignment diagram for calculation



Ex: Band alignment for III–V semiconductors

We assume A and B in this figure represents two III–V semiconductors that have the same lattice constant.



The valence band position can be calculated as:

$$E_V = E_{V,av} + \frac{\Delta}{3}$$

in which $E_{V,av}$ is the average valence band position which is obtained from theory and is referred to as the absolute energy level, E_V is the valence band position, and Δ is the spin-orbit splitting energy.

Band alignment for III–V semiconductors

The valence band offset between semiconductor A and B thus can be calculated as:

$$\Delta E_V = \left(E^A_{V,av} - E^B_{V,av}\right) + \frac{1}{3}\left(\Delta_A - \Delta_B\right)$$

The conduction band edge is obtained by adding the bandgap value to the valence band position:

$$E_C = E_V + E_g$$

Therefore the conduction band offset can be calculated as:

$$\Delta E_C = \left(E^A_{V,av} - E^B_{V,av}\right) + \frac{1}{3}\left(\Delta_A - \Delta_B\right) + \left(E^A_g - E^B_g\right)$$

Example: $GaAs/Al_{0.2}Ga_{0.8}As$ heterojunction

Question: Determine the band offset of a $GaAs/Al_{0.2}Ga_{0.8}As$ heterojunction.

Answer: For GaAs, we have:

$$E_V^{GaAs} = E_{V,av}^{GaAs} + \frac{\Delta_{GaAs}}{3} = -6.807\text{eV}$$

For $Al_{0.2}Ga_{0.8}As$, we use the arithmetic average of 20% AlAs and 80% of GaAs:

$$\begin{aligned} E_V^{Al_{0.2}Ga_{0.8}As} &= 0.2 \times \left(E_{V,av}^{AlAs} + \frac{\Delta_{AlAs}}{3} \right) + 0.8 \times \left(E_{V,av}^{GaAs} + \frac{\Delta_{GaAs}}{3} \right) \\ &= -6.925\text{eV} \end{aligned}$$

$$E_g^{Al_{0.2}Ga_{0.8}As} = 0.2 \times E_g^{AlAs} + 0.8 \times E_g^{GaAs} = 1.842\text{eV}$$

Example: $GaAs/Al_{0.2}Ga_{0.8}As$ heterojunction

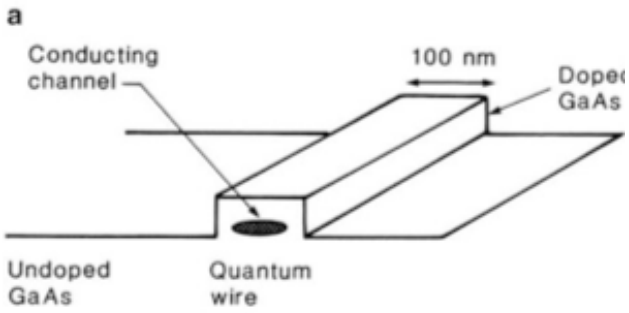
The material parameters for GaAs and AlAs are listed in Table.

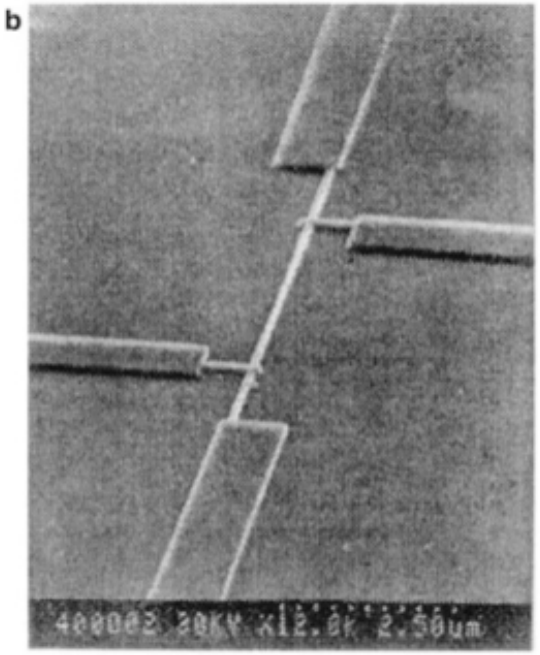
	$E_{V,av}$ (eV)	Δ(eV)	E_g(eV)
GaAs	−6.92	0.34	1.52
AlAs	−7.49	0.28	3.13

Therefore, we obtain the band offset as follows:

$$\begin{cases} \Delta E_V = E_V^{GaAs} - E_V^{Al_{0.2}Ga_{0.8}As} = (-6.807) - (-6.925) \\ \qquad = 0.118\text{eV} \\ \Delta E_C = \left(E_V^{Al_{0.2}Ga_{0.8}As} + E_g^{Al_{0.2}Ga_{0.8}As}\right) - \left(E_V^{GaAs} + E_g^{GaAs}\right) \\ \qquad = (-5.287) - (-5.555) \\ \qquad = 0.268\text{eV} \end{cases}$$

Ex: Quantum wires

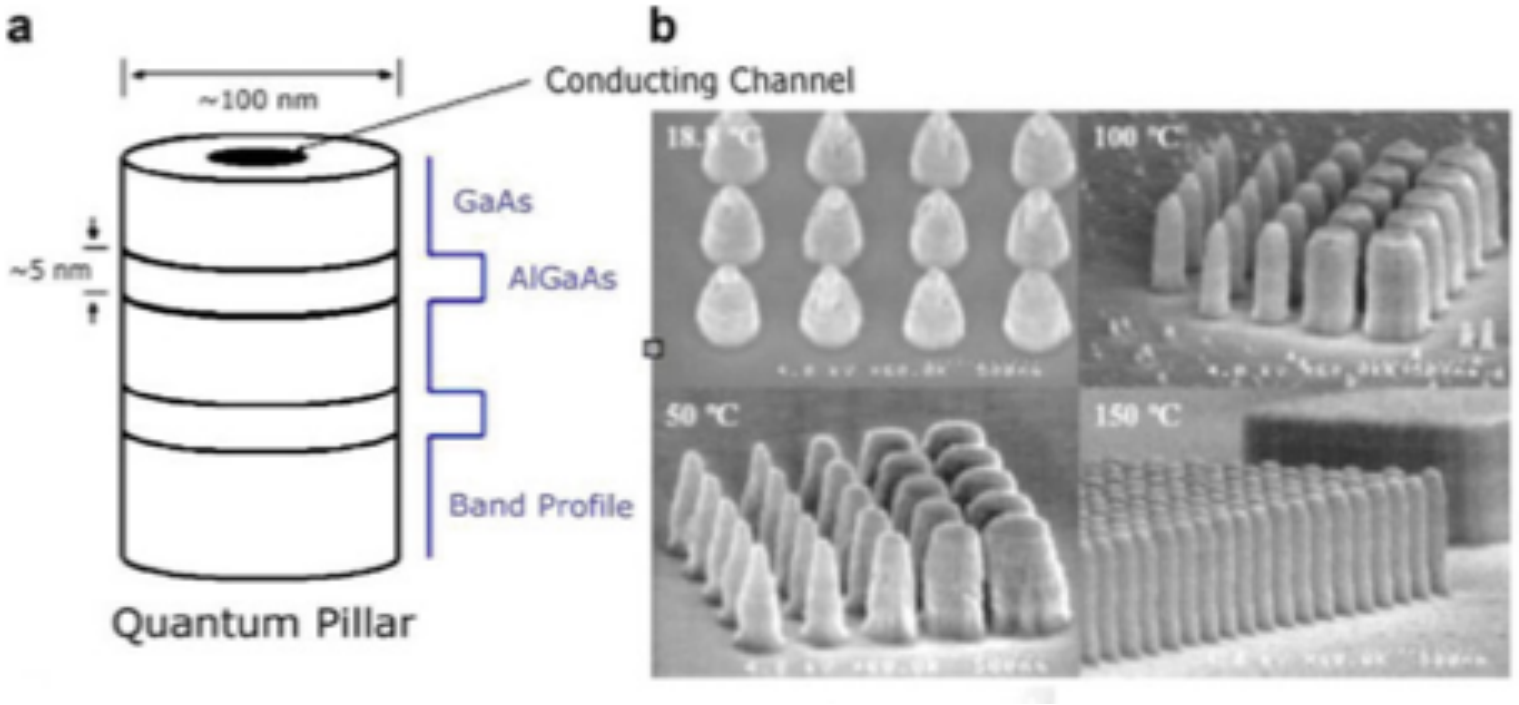




Quantum wire formed by etching away all but a thin strip of doped semiconductor on an undoped substrate: (a) schematic diagram; (b) practical example

Figure ref: Low-Dimensional Semiconductors: Materials, Physics, Technology, and Devices by M.J. Kelly; taken after Physica Scripta Vol. T45, Beaumont SP.

Ex: Quantum dots



A quantum pillar formed from resonant tunneling semiconductor multilayers showing (a) a schematic diagram of the pillar