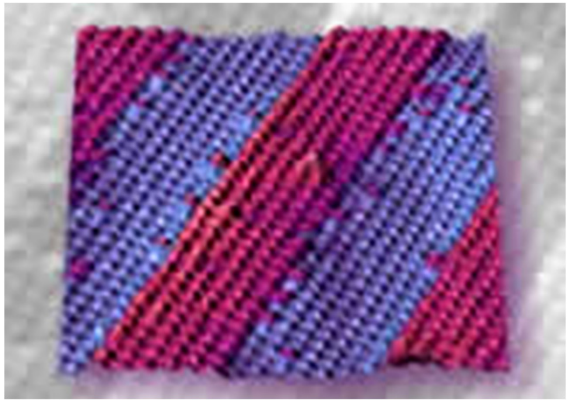
Lecture 2 – 26/02/2025

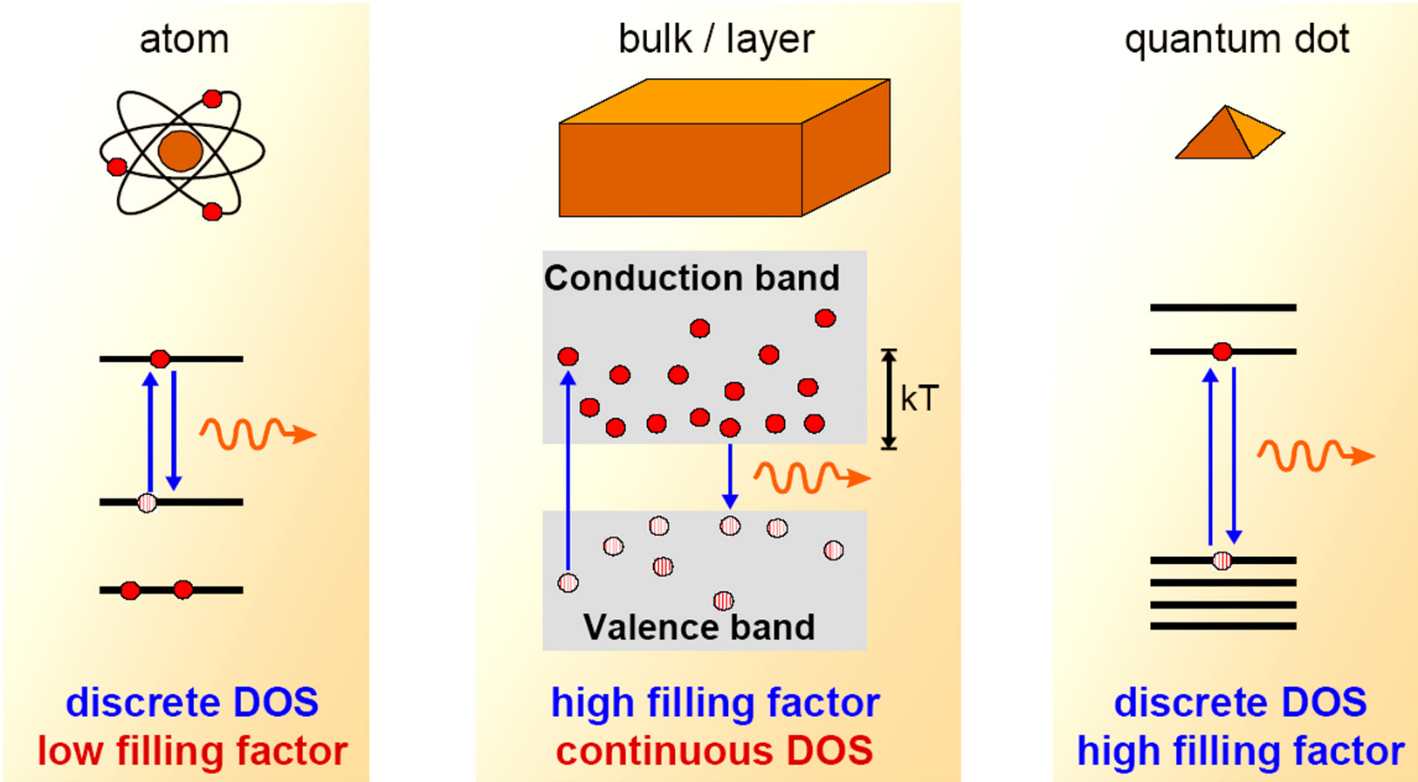
Quantum nanostructures

- Growth and fabrication: a brief overview
- Electronic states: determination of quantum well energy levels



Quantum nanostructures

Why reducing the dimensions?



Quantum dots ≡ artificial atoms

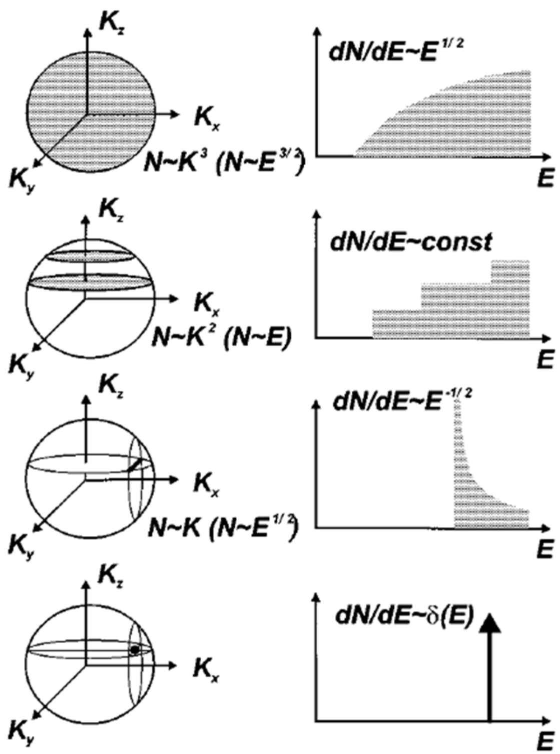
Quantum nanostructures

3D
Bulk

2D
Quantum well

1D
Quantum wire

0D
Quantum dot



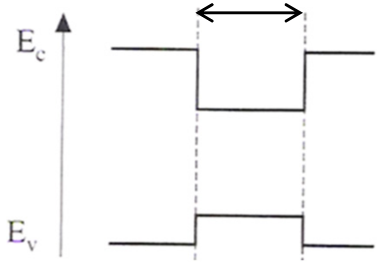
Density of states decreases with the dimensionality

Quantum nanostructures

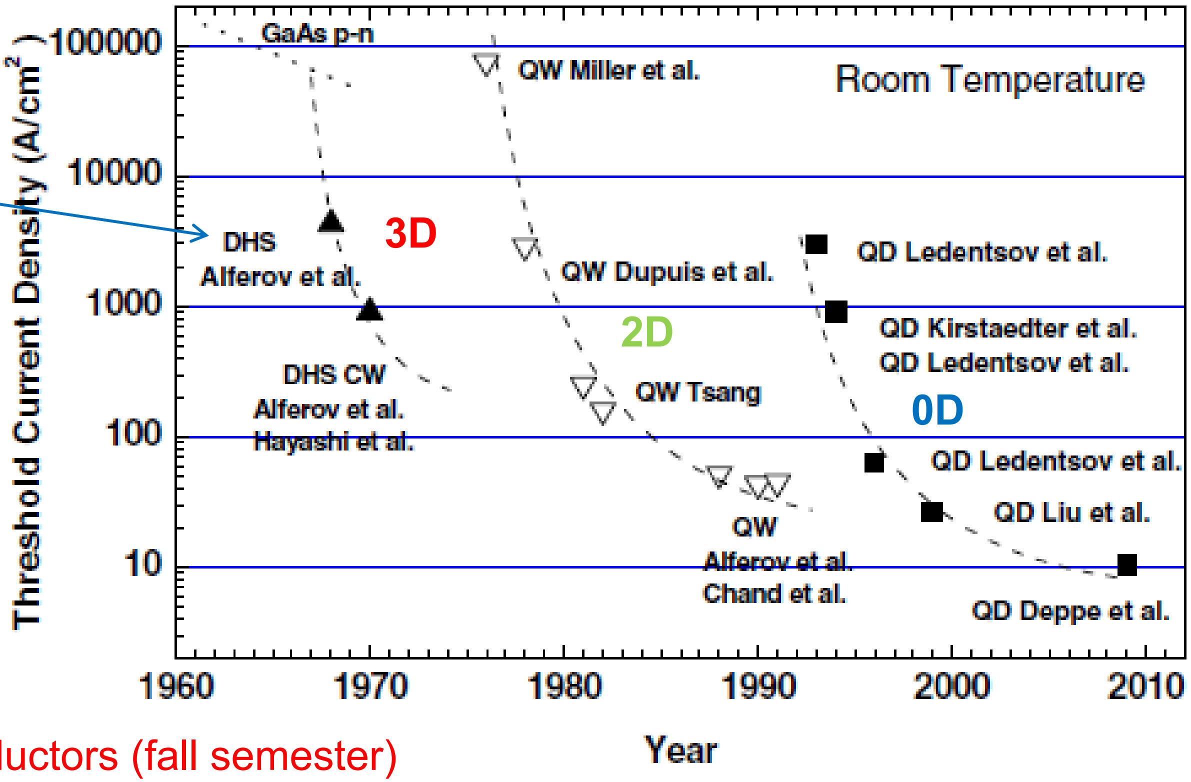
Threshold current density in laser diodes over the years

Double heterostructure (DHS)

$d \in$ 0.1-1 μm



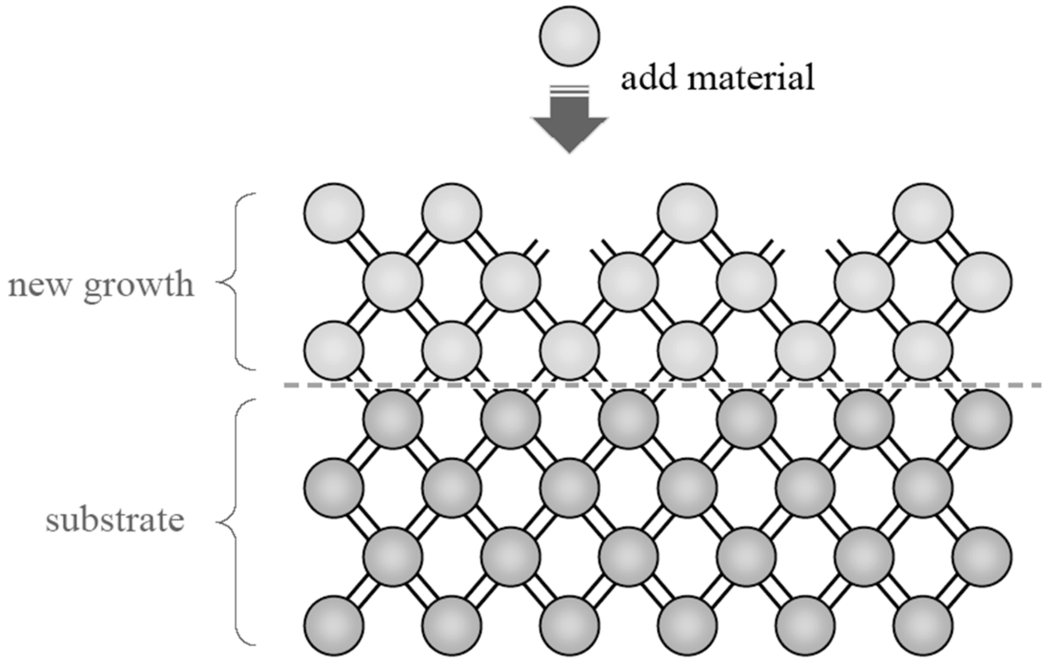
No quantization phenomena at play in a DHS!



≡ Transparency condition for semiconductors (fall semester)

Dimensionality reduction ⇨ laser threshold decrease (Bernard-Duraffourg condition is more easily fulfilled)

Epitaxial growth



Epitaxy: crystal growth proceeds layer-by-layer and the layer structure complies with the substrate lattice

Growth on a foreign substrate: **heteroepitaxy**

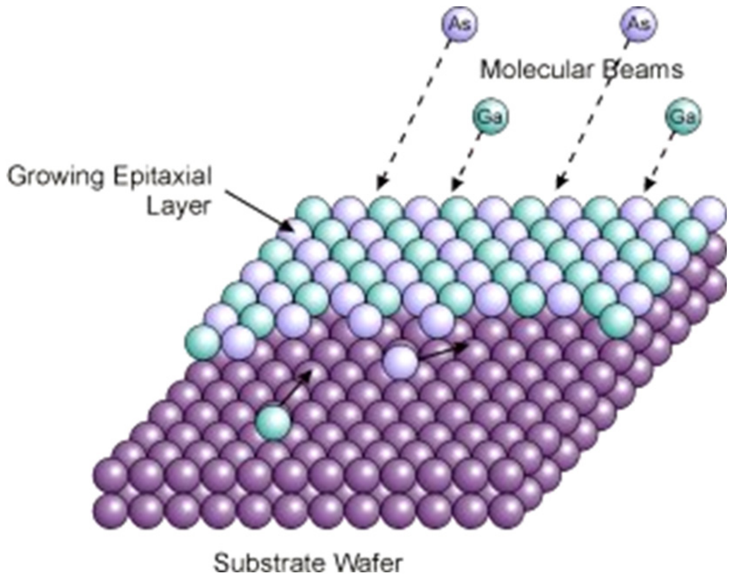
Epitaxial growth

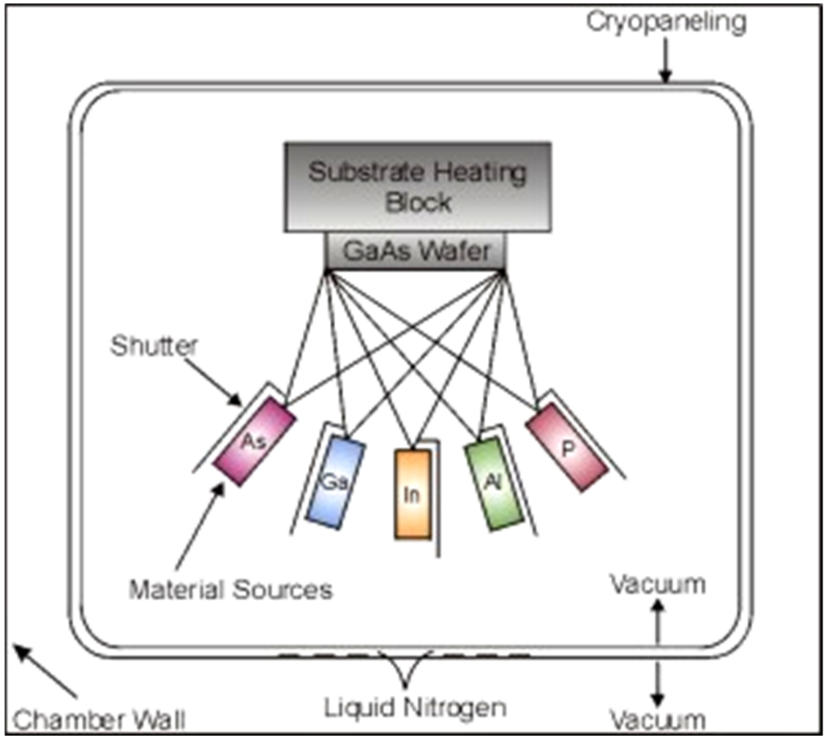
Two main growth techniques:

- Molecular beam epitaxy (MBE)

- Metal organic vapor phase epitaxy (MOVPE)
  Metal organic chemical vapor deposition (MOCVD)

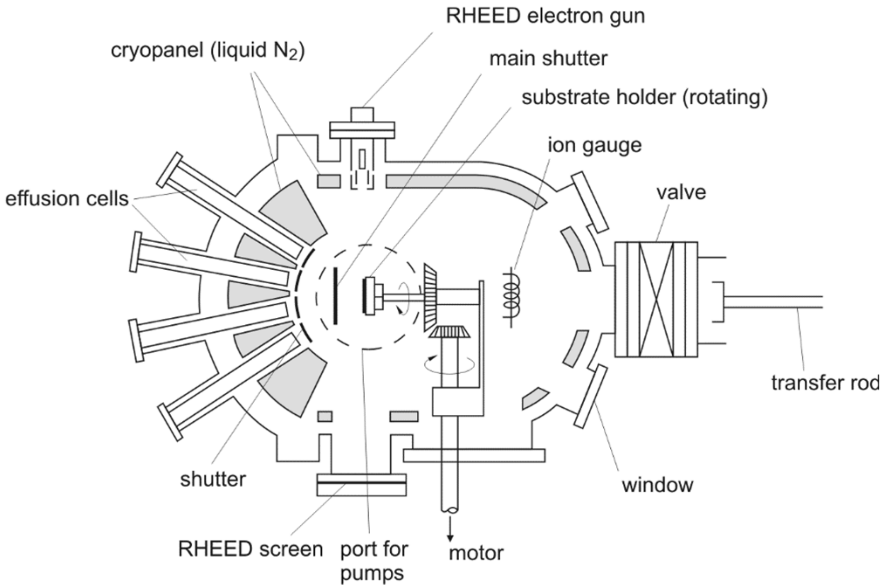
Molecular beam epitaxy (MBE) growth

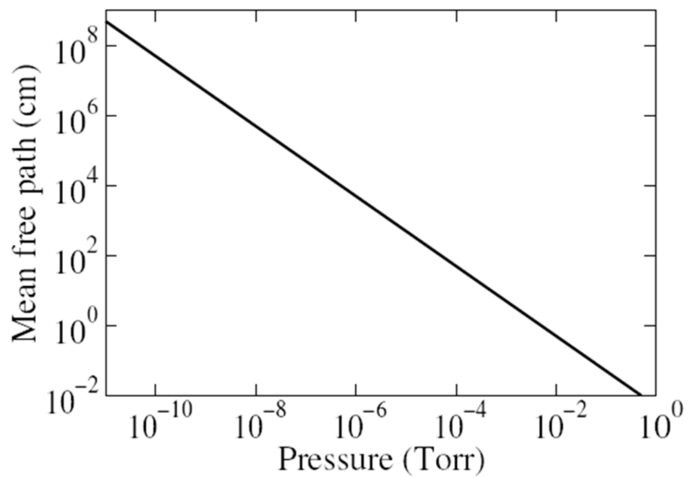




UHV growth technique

MBE growth



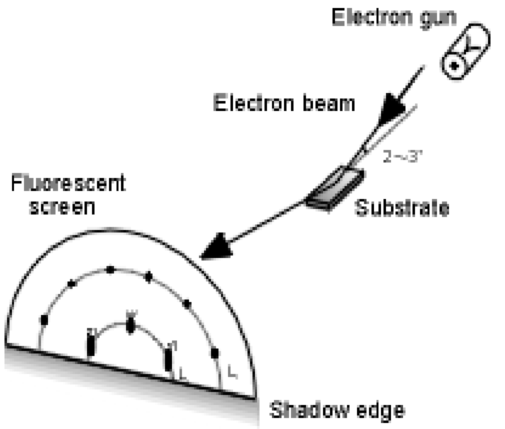


- No interaction between fluxes (⇒ long mean free path)
- High vacuum enables the use of an electron beam probe (RHEED)

RHEED: reflection high energy electron diffraction

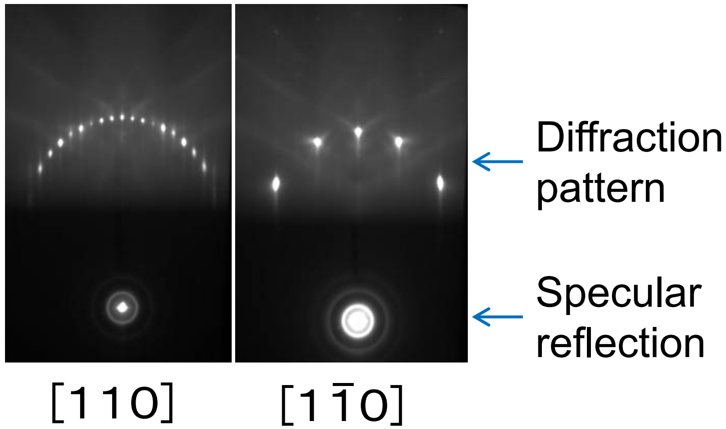
MBE growth

In situ monitoring via reflection high energy electron diffraction (RHEED)



Energy ~10 keV

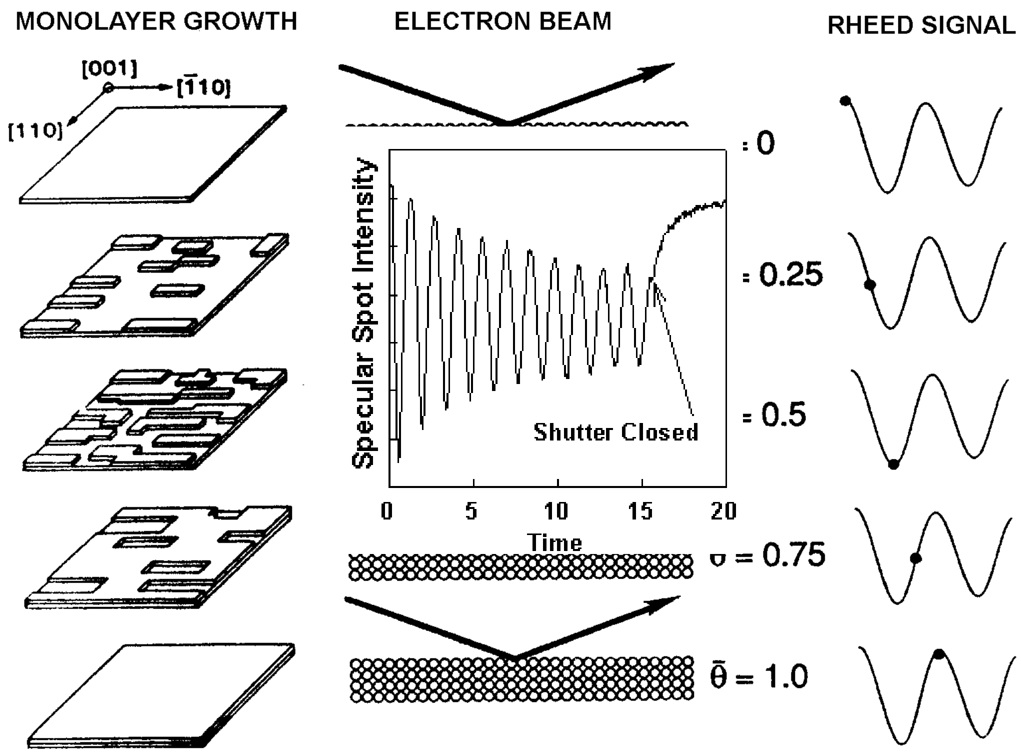
RHEED pattern



Twofold advantage of the RHEED technique:

- Specular reflection ⇒ access to the growth rate
- Diffraction pattern ⇒ surface reconstruction and growth mode (e.g., 2D vs 3D)

MBE growth: *in situ* monitoring

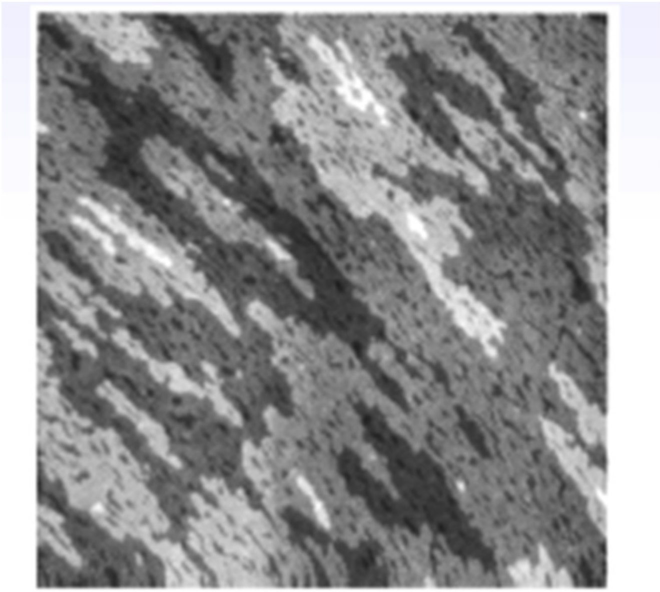


Oscillations ⇒ absolute measurement of growth rate

Damping of oscillations due to surface roughening (dynamical effect)

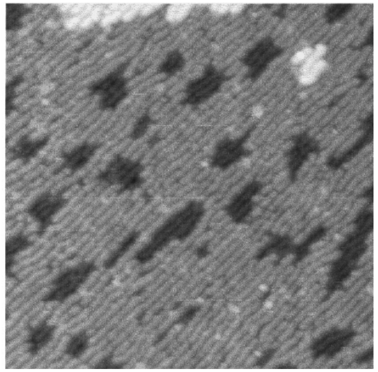
MBE growth: surface properties

GaAs surface probed by scanning tunneling microscopy (STM)

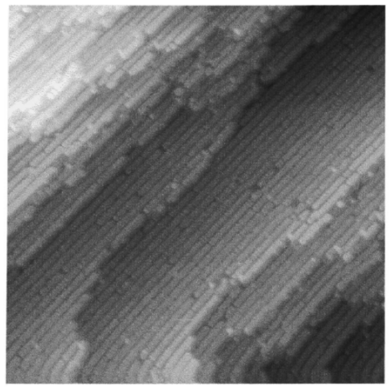


400 × 400 nm²

“Nominal”



“Vicinal” (misoriented)



75 × 75 nm²

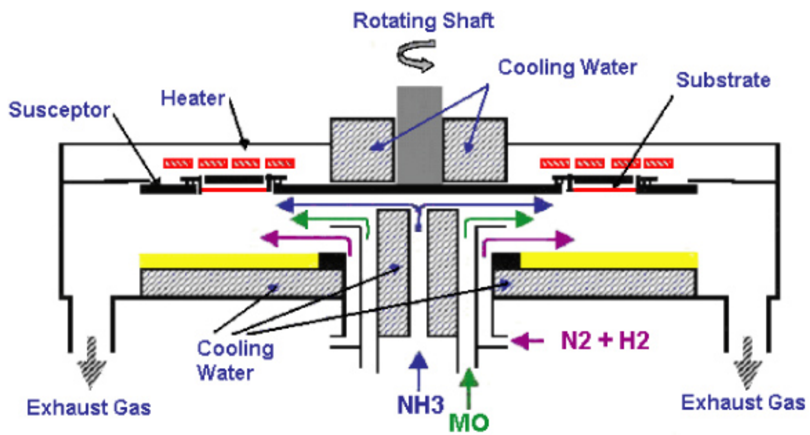
MBE growth

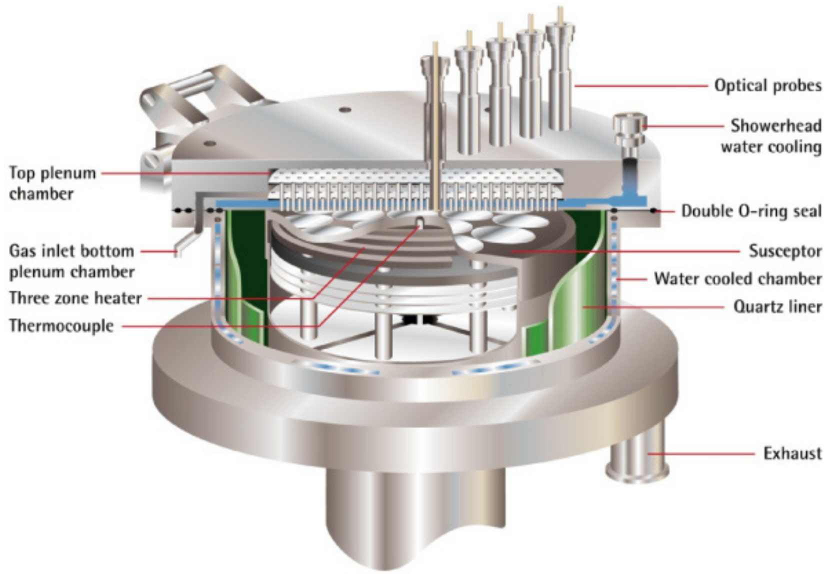
Production system (7 × 6 in.)

Mainly for GaAs based HEMTs and HBTs

Metalorganic vapor phase epitaxy (MOVPE) growth

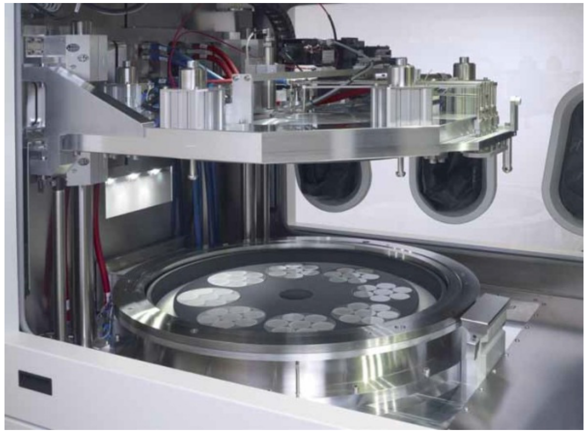
Organo-metallic precursors [MO $(CH_3)_3$-III for example] are first transported by a carrier gas (hydrogen, nitrogen) into the growth chamber where they decompose at the vicinity of a high-temperature substrate surface. Group-V elements are also provided by the high-temperature decomposition of other gas species like arsine (AsH_3) for GaAs or NH_3 for GaN.



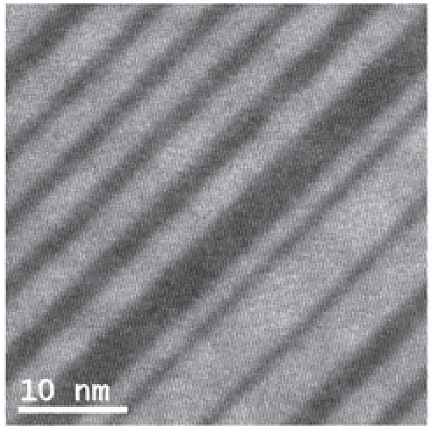


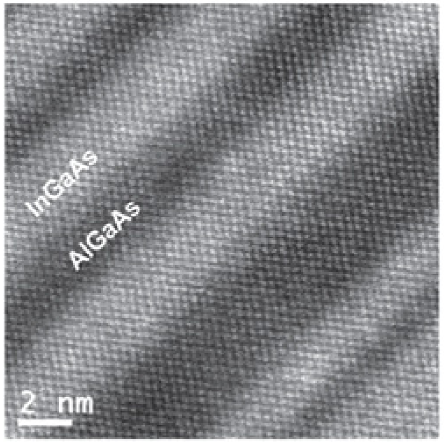
MOVPE growth

Production system

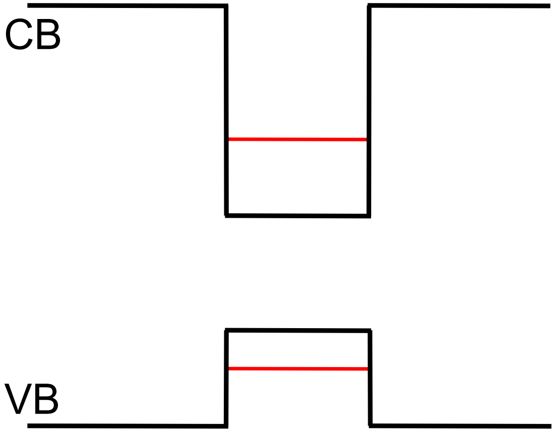


Prototypical heterostructure: the quantum well



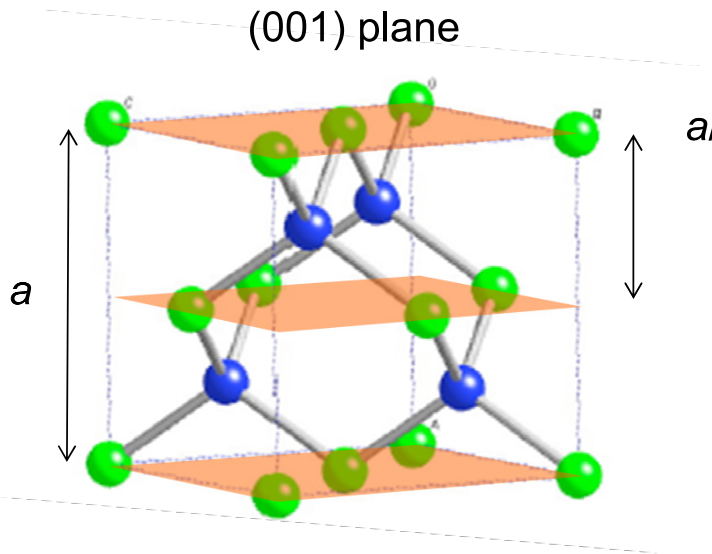


High resolution transmission electron microscopy (HRTEM)



Prototypical heterostructure: the quantum well

Quantum well: crystal growth must be controlled at the atomic scale



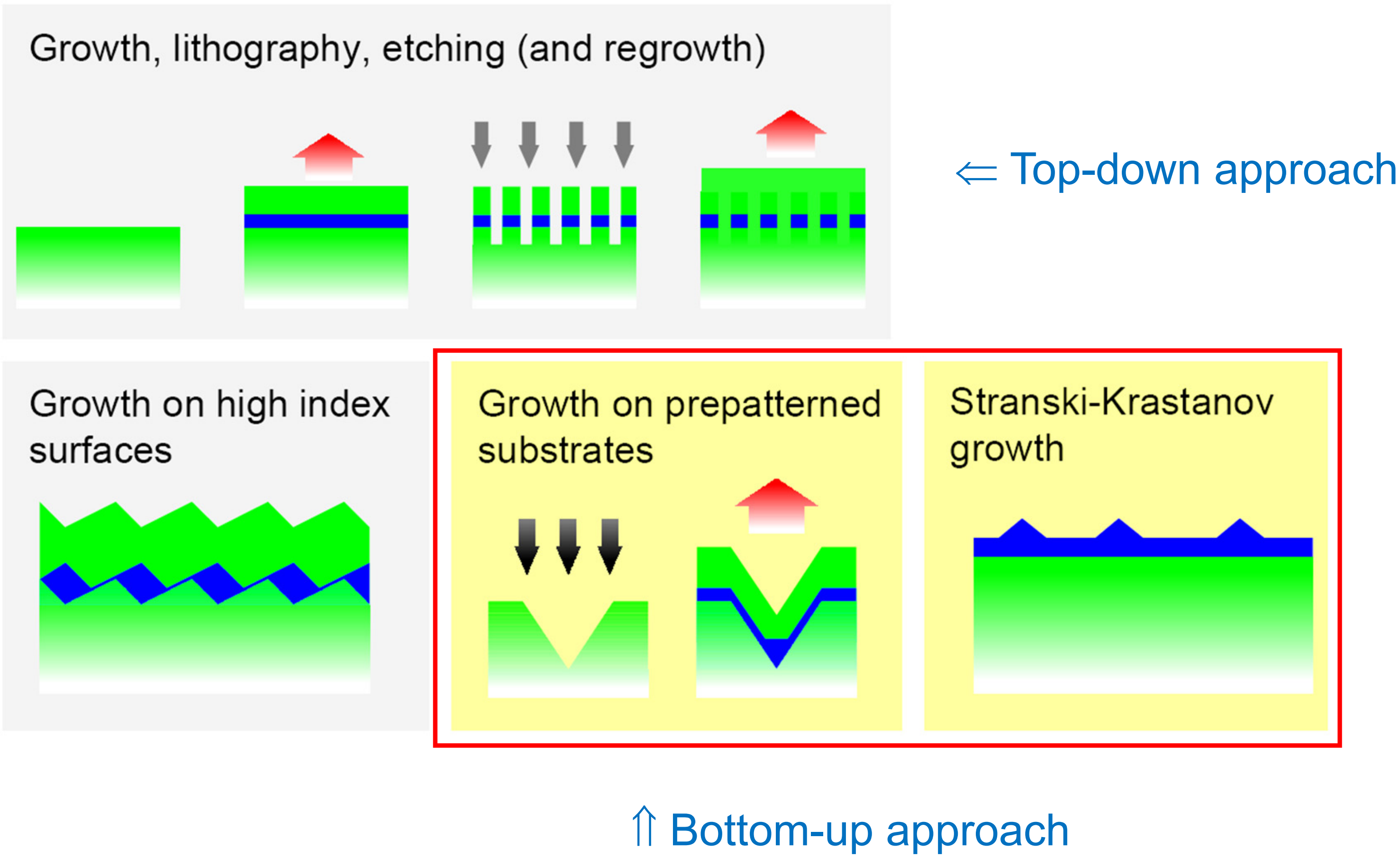
GaAs unit cell

a/2 ⇒ 1 molecular monolayer (ML)
= 1 Ga plane and 1 As plane

a = 5.65 Å for GaAs

1 ML = 2.83 Å

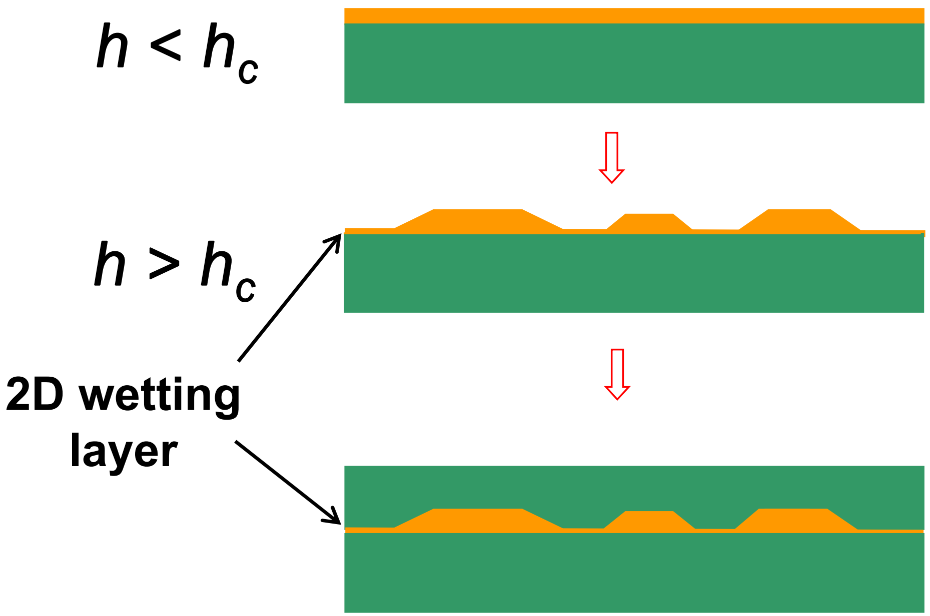
Quantum dot fabrication



Quantum dot fabrication

Stranski-Krastanov (SK) growth mode (strain-induced islanding)

2D-to-3D transition driven by the imbalance between elastic (strain) and surface energy



Pseudomorphic growth

Elastic energy relaxation by 3D island formation (visible in real time through RHEED)

3D islands are buried to form QDs

Lattice-mismatch

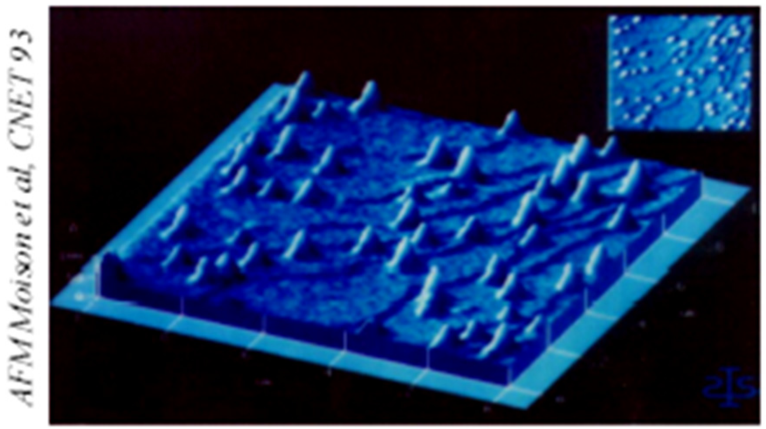
GaN/AlN ⇒ 2.5%

InAs/GaAs ⇒ 7.2% and Ge/Si ⇒ 4.2%

Stranski-Krastanov (SK) InAs/GaAs quantum dots

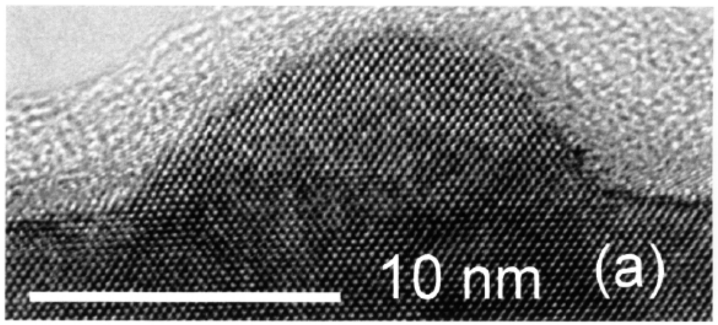
Self-organized quantum dots (SQDs)
Self-assembled quantum dots (SAQDs)

3D growth mode of
highly strained InAs on GaAs



AFM

Access to surface properties/morphology, e.g., QD size (apparent height + diameter) and density

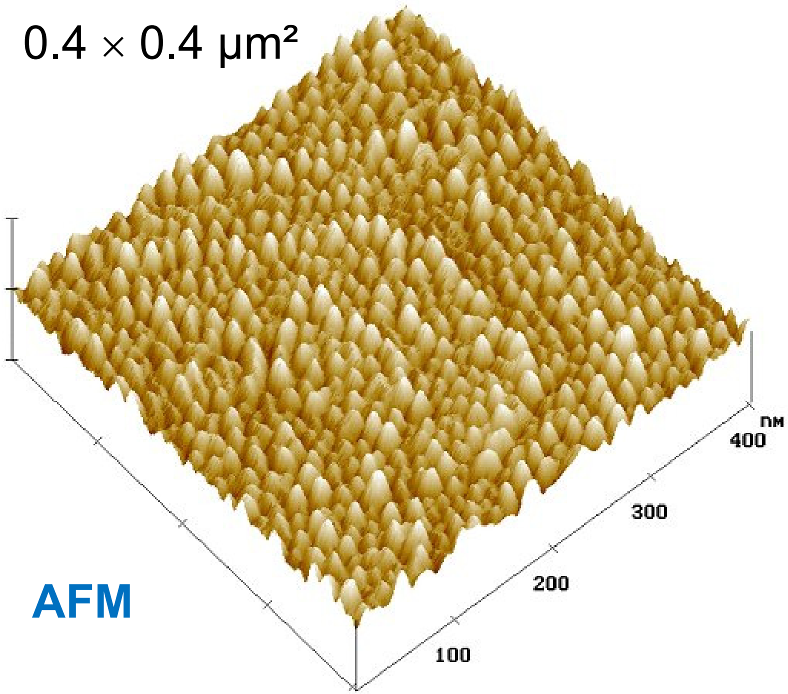


HRTEM

Access to atomic resolution thanks to electrons that are probing a volume

SK GaN/AlN QDs

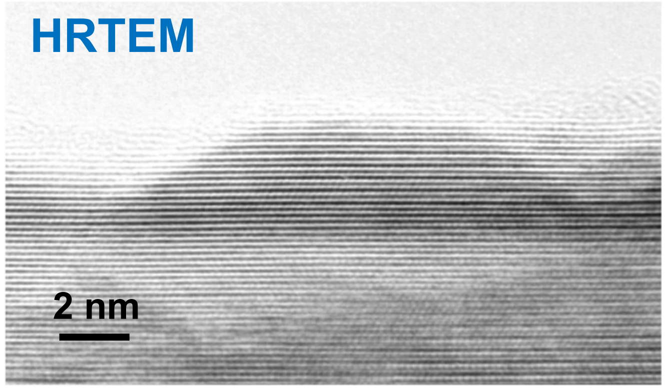
0.4 × 0.4 μm²

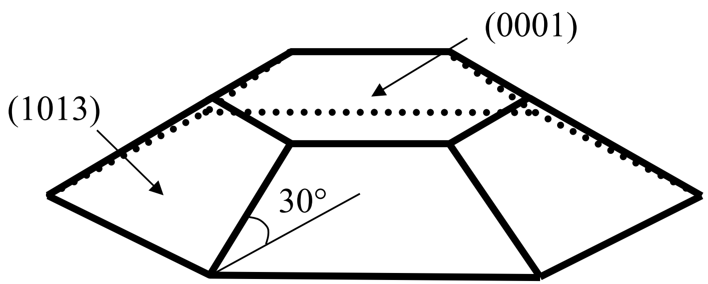


AFM

density: 3-5 × 10^{11} cm^{-2}

WL

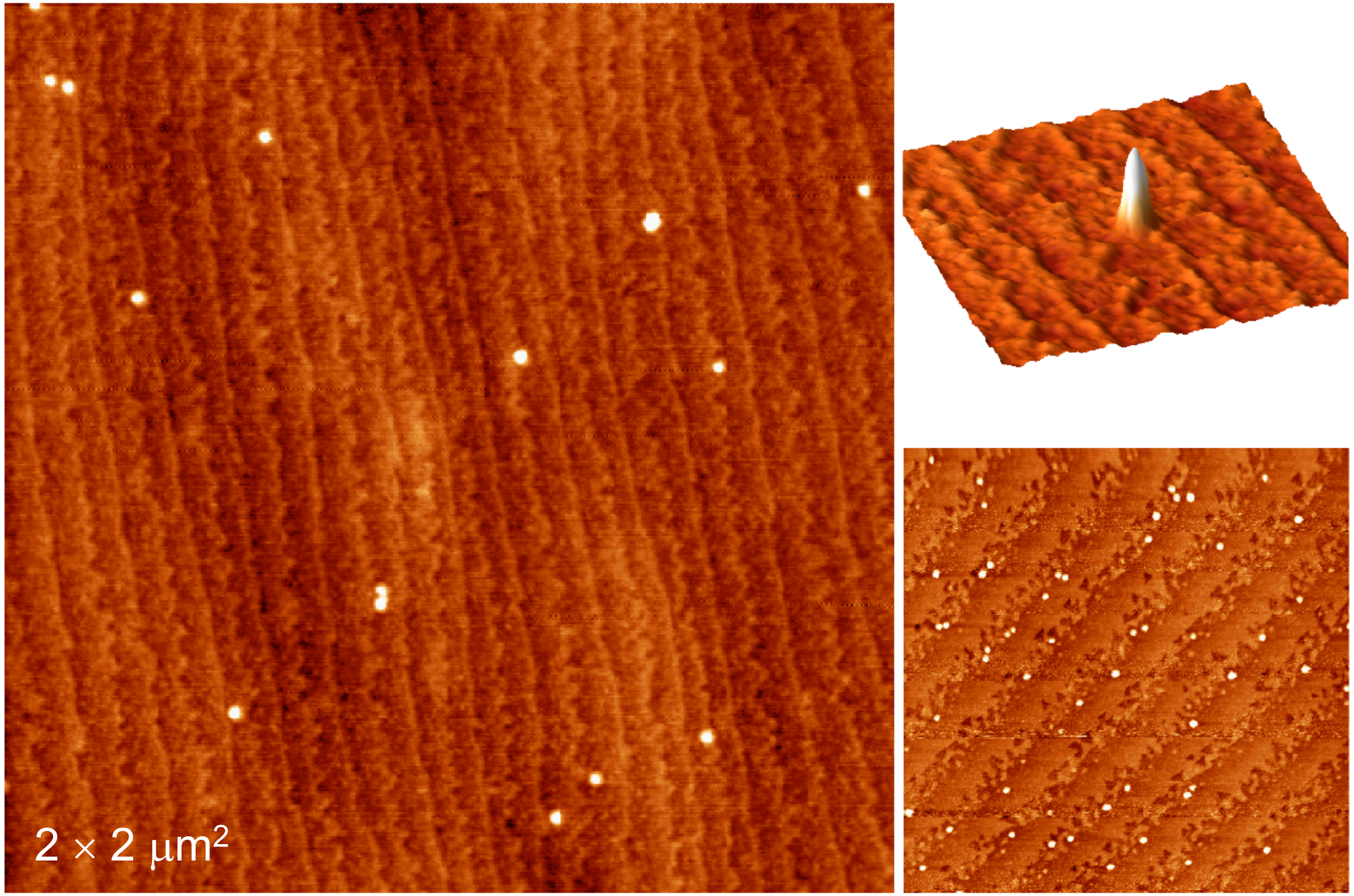




Critical thickness of 2-3 MLs

Sixfold symmetry

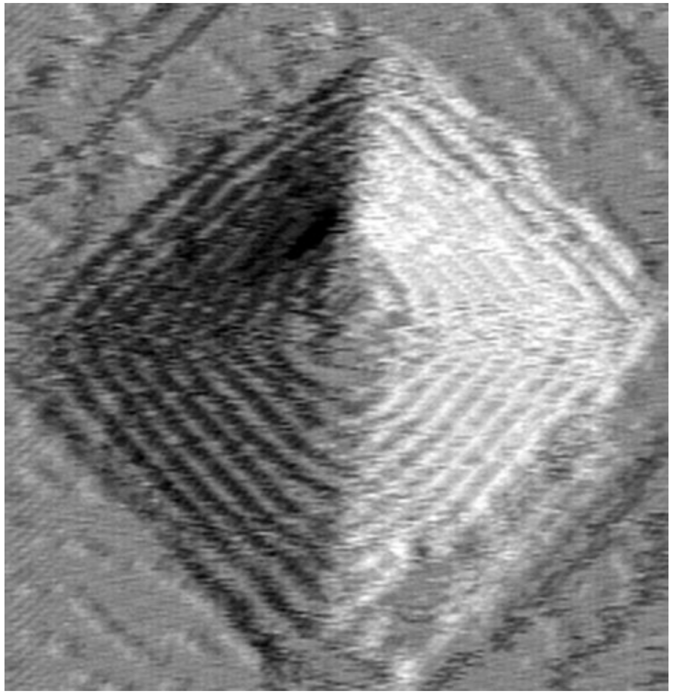
Stranski-Krastanov QDs



Density of QDs depends on the growth conditions (here GaN/AlN QDs)

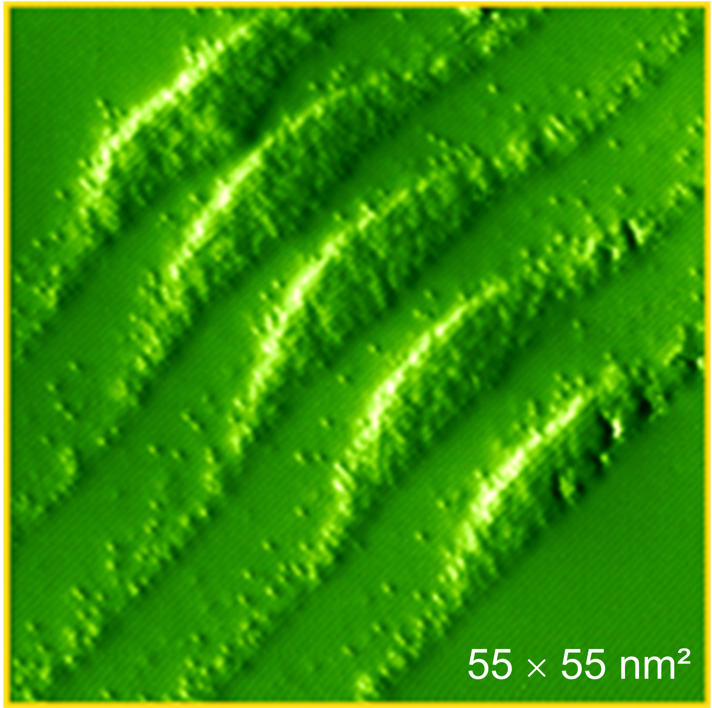
Quantum dots: scanning tunneling microscopy

Top view



Ge island on silicon

Cross section

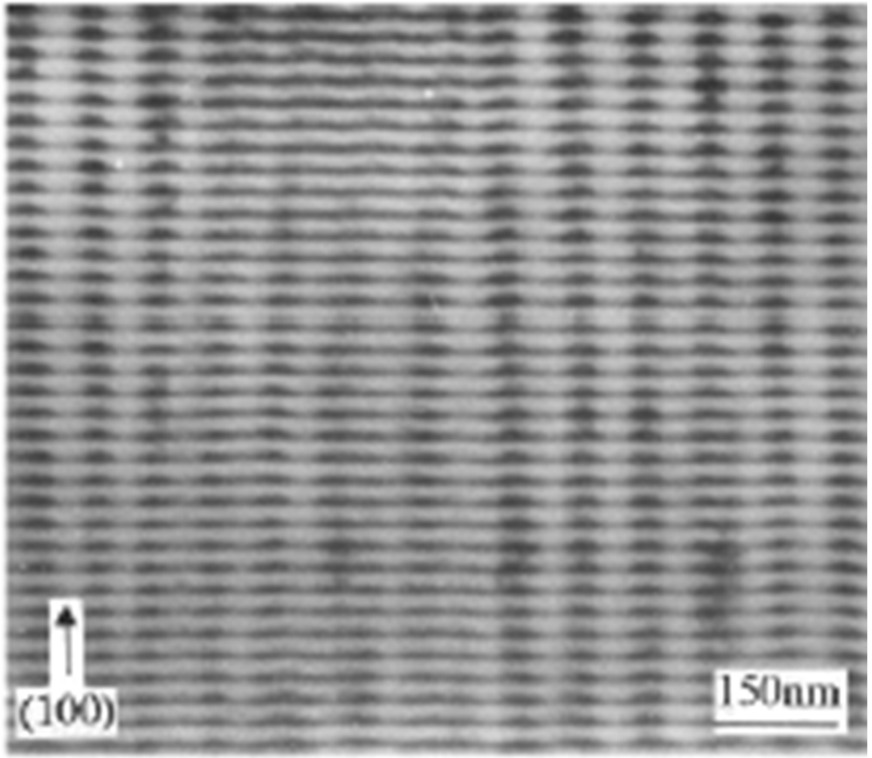


InAs/GaAs QDs

Protruding atoms (mostly indium)

SK InAs/GaAs QDs

QD plane stacking: self-organization

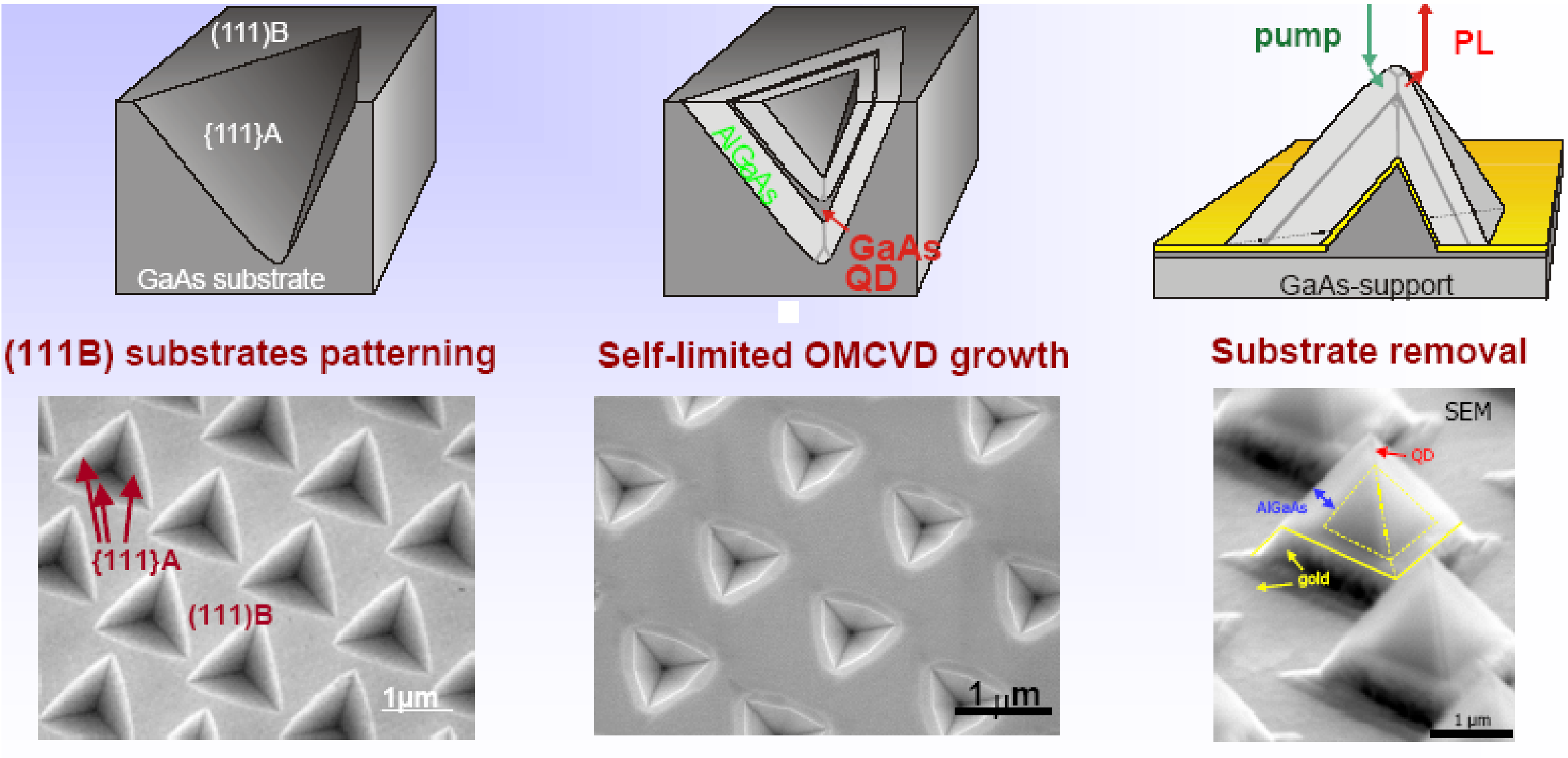


Cross section TEM

Example of coherent vertical alignment due to strain fields

GaAs/AlGaAs quantum dots

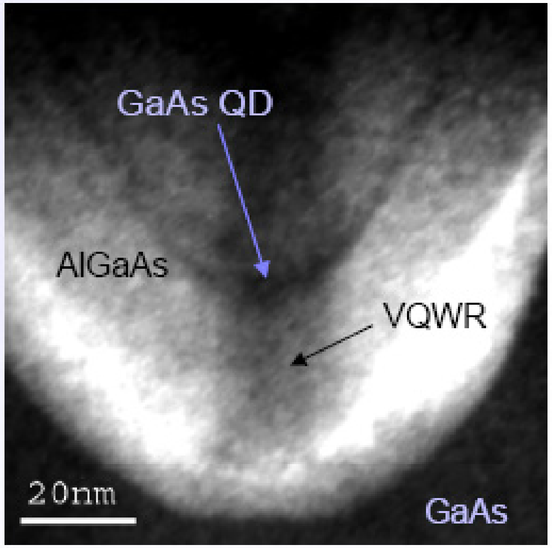
Growth on V-grooved surface

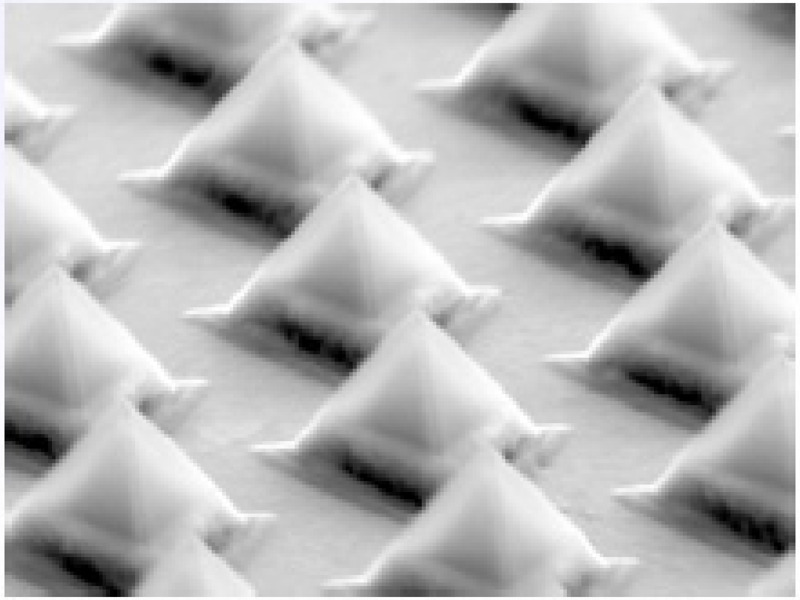


E. Kapon – LPN - EPFL

GaAs/AlGaAs quantum dots

Growth on V-grooved surface

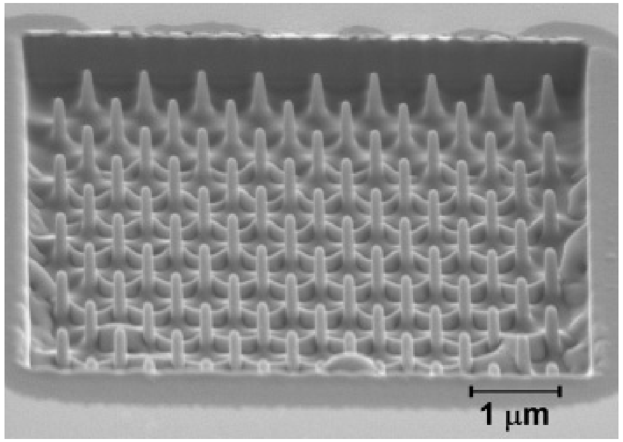


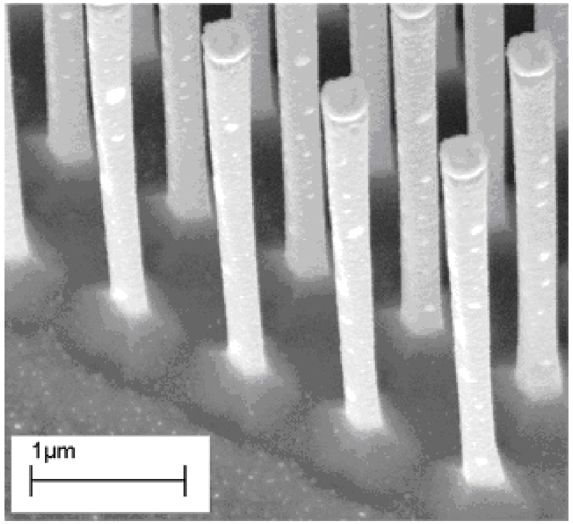


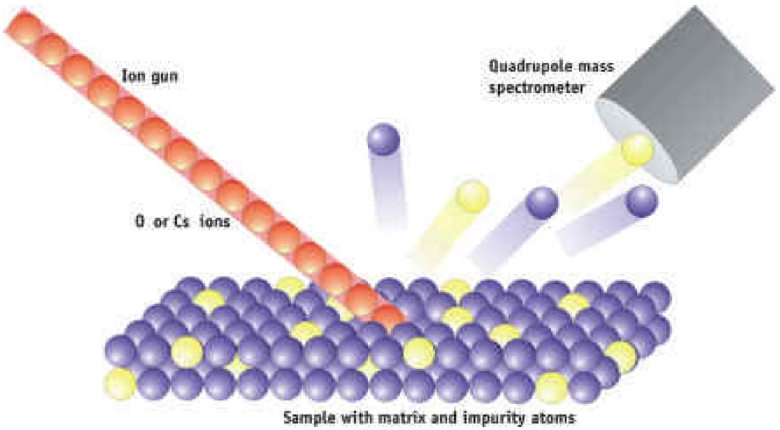
E. Kapon – LPN - EPFL

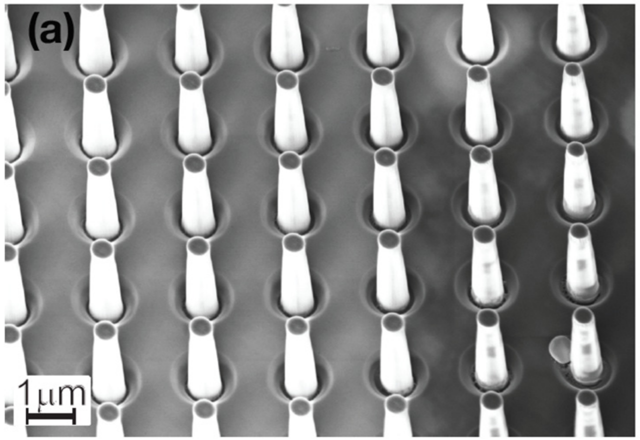
Nanowires: top-down approach

Focused ion beam (FIB)

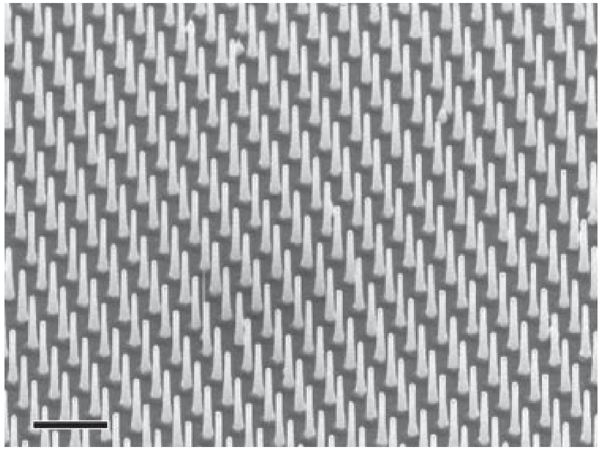




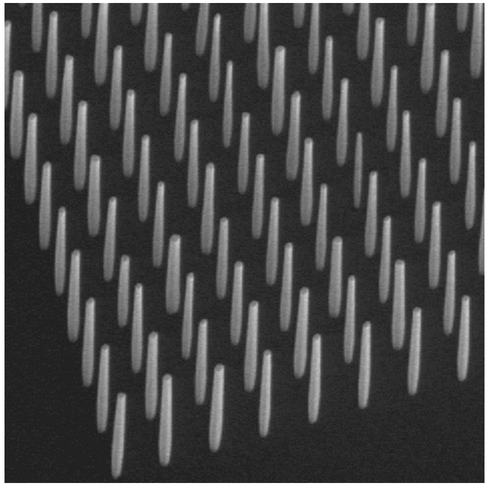




Nanowires: bottom-up approach

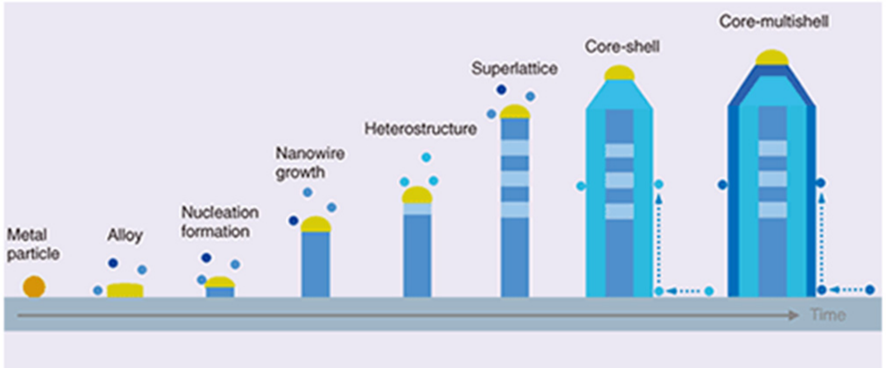


TU Eindhoven
Ordered InP
NW array

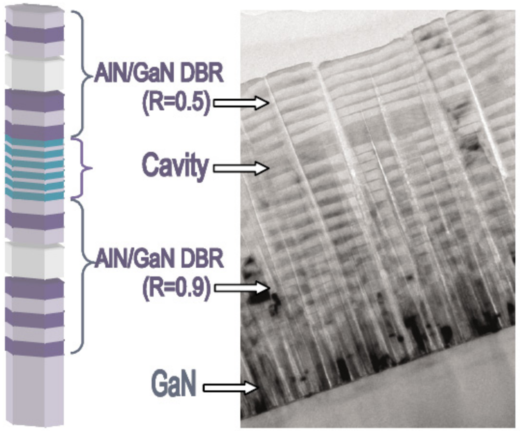


NIST
Ordered GaN
NW array

NTT technical review

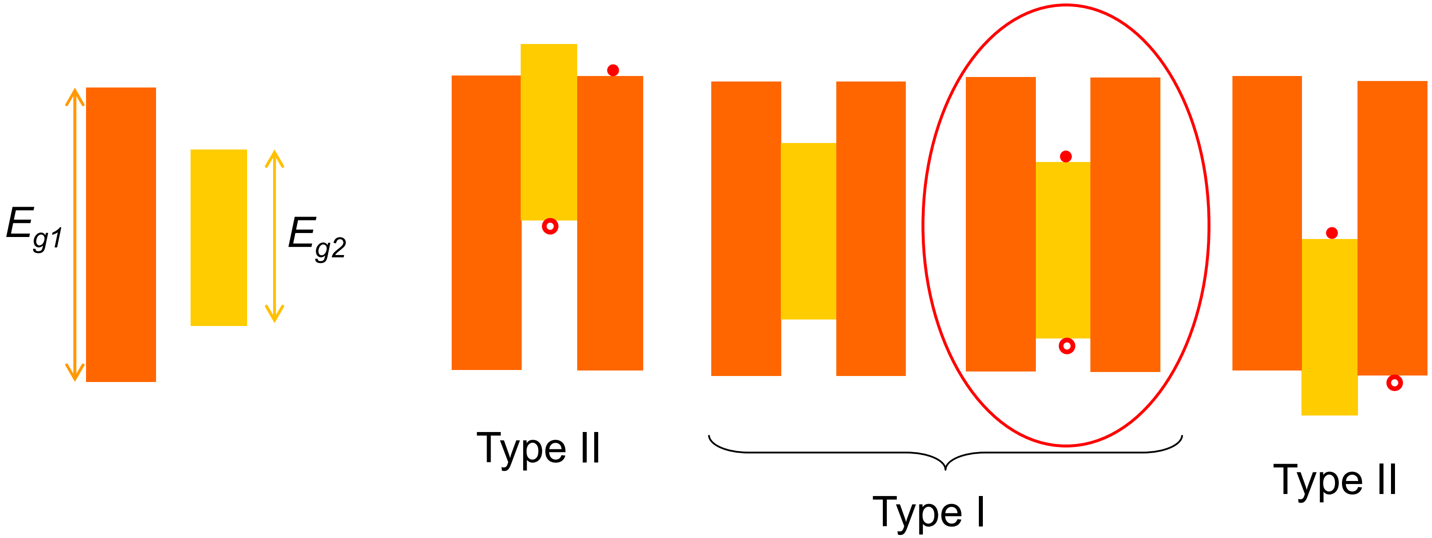


Univ. Politcn. Madrid



Heterostructures: band offset

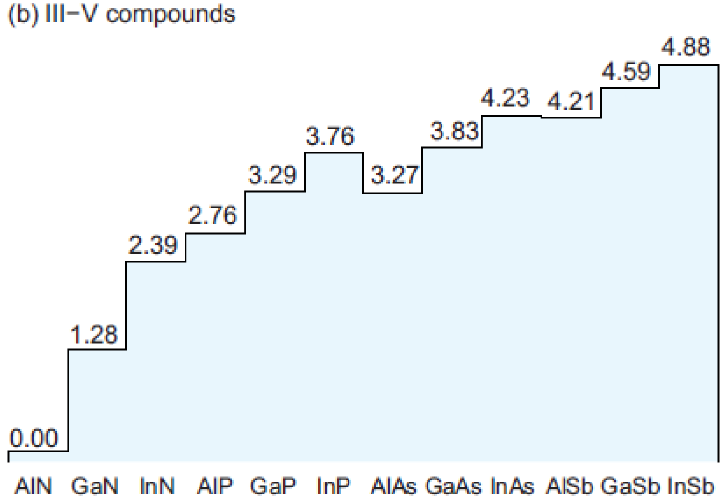
Different configurations



In III-V semiconductor compounds sharing the same anion: $\Delta V_{VB} = 0.3 \times \Delta E_g$

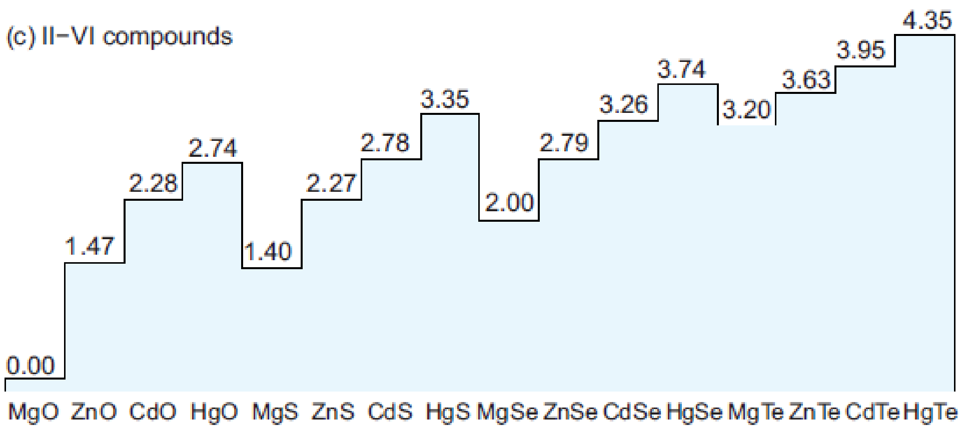
$\Rightarrow$ Common anion rule

Heterostructures: band offset

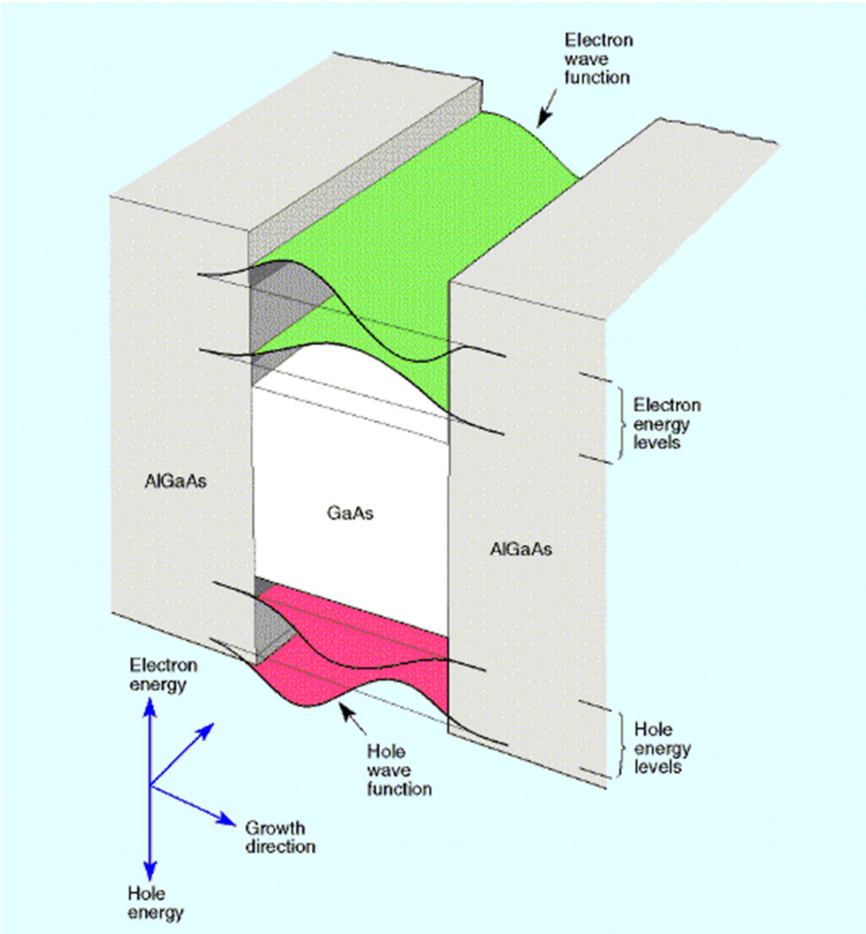


Valence band edge offsets

Numbers are expressed in eV!



Heterostructures: electronic states



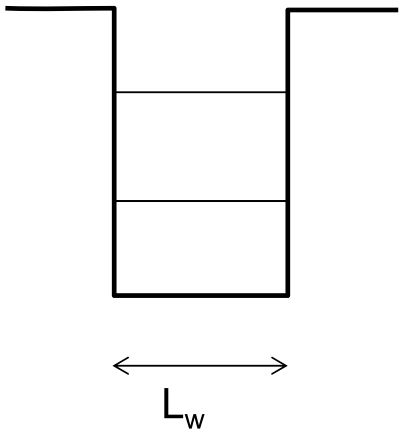
Rectangular quantum well

Quantized energy levels in CB and VB

Parameters to be considered:

- Well thickness
- Barrier height
- Carrier effective mass
- Dielectric mismatch

The quantum well: confinement effects



What should be the well thickness to ensure a strong quantum confinement?

1. $$E = \frac{\hbar^2 k^2}{2m^*} \Rightarrow \lambda_{dB} = \frac{h}{\sqrt{2m^* E}}$$ (with $E \approx 5$ eV)

↑ Typical ionization energy for e^-

$\lambda_{dB} \approx 21$ Å for GaAs

$\lambda_{dB} \approx 12$ Å for GaN

2. 3D Bohr radius $\Rightarrow$ extent of the excitonic wavefunctions

$a_{3D,GaAs} \approx 11$ nm, $a_{3D,GaN} \approx 3$ nm

Quantum confinement effects significant only for very small objects (1-20 nm)

Quantum well energy levels

Conduction electron energy levels

Approximation of the envelope wavefunction

in-plane wavefunction ↘ envelope wavefunction ↙

$$\psi = \sum_{A,B} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} u_{c\mathbf{k}}^{A,B}(\mathbf{r}) \chi_n(z)$$

↑ Periodic part of Bloch wavefunction

Separation of in-plane (x-y) and vertical (z) components

1D Schrödinger-like equation

$$\left(-\frac{\hbar^2}{2m_e^*(z)} \frac{\partial^2}{\partial z^2} + V_c(z) \right) \chi_n(z) = \varepsilon_n \chi_n(z)$$

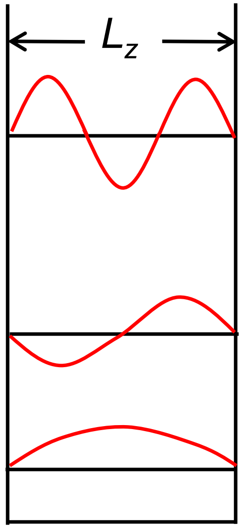
↑ electron effective mass

↑ confinement energy of the carriers

Continuity at the interfaces of (i) $\chi_n(z)$ and (ii) particle current $(1/m_e^*)(\partial\chi_n/\partial z)$

Quantum well energy levels

Infinite barrier height (1D case), $V_c = \infty$



$$-\frac{\hbar^2}{2m}\frac{\partial^2 \chi_n}{\partial z^2} = \varepsilon_n \chi_n \quad \text{i.e.} \quad \frac{\partial^2 \chi_n}{\partial z^2} + k_n^2 \chi_n = 0 \quad \text{with} \quad k_n^2 = \frac{2m\varepsilon_n}{\hbar^2}$$

Solutions have the general expression:

$$\chi_n(z) = A\sin(k_n z) + B\cos(k_n z)$$

with the boundary conditions:

$$\chi_n(0) = \chi_n(L_z) = 0$$

hence $\chi_n(z) = A\sin(k_n z)$ with $k_n = \frac{n\pi}{L_z}$

$$\int_{-\infty}^{+\infty} |\chi_n(z)|^2 dz = 1 = A^2 \int_0^{L_z} \sin^2(k_n z) dz = A^2 \frac{L_z}{2} \quad \Rightarrow \quad A = \sqrt{\frac{2}{L_z}}$$

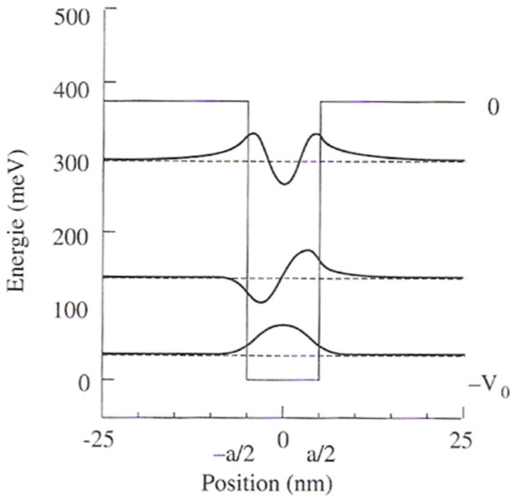
$$\varepsilon_n = \frac{n^2 \pi^2 \hbar^2}{2 m_e^* L_z^2}$$

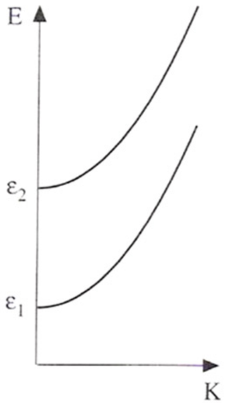
$$\chi_n = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n\pi z}{L_z}\right)$$

Dimension of the 1D wavefunction equal to $L^{-1/2}$!
$\Rightarrow \chi_n$ dimensionality $\propto L^{-d/2}$

Quantum well energy levels

Finite barrier height[1]





In-plane wavevector

$$-\nabla \frac{\hbar^2}{2m^*(z)} \nabla \psi(r) + V(z)\psi(r) = E\psi(r)$$

The function ψ can be written as follows

$$\psi(r) = \chi_n(z)\exp(i\mathbf{K}.\mathbf{R})$$

$$\left[-\frac{d}{dz}\frac{\hbar^2}{2m^*(z)}\frac{d}{dz} + V(z)\right]\chi_n(z) = \varepsilon_n \chi_n(z)$$

with $E_n = \varepsilon_n + \dfrac{\hbar^2 K^2}{2m^*}$

[1]G. Bastard, Phys. Rev. B **24**, 5693 (1981) (> 1200 citations) and Phys. Rev. B **25**, 7584 (1982) (> 600 citations).

Quantum well energy levels

Finite barrier height

Even wave function case

$$\chi_n(z) = A\cos kz, \quad \text{for } |z| < L/2$$
$$= B\exp\left[-\kappa(z - L/2)\right], \quad \text{for } z > L/2$$
$$= B\exp\left[+\kappa(z + L/2)\right], \quad \text{for } z < -L/2$$

where $\varepsilon_n = \dfrac{\hbar^2 k^2}{2m_A^*} - V_0, \quad \varepsilon_n = -\dfrac{\hbar^2 \kappa^2}{2m_B^*}, \quad -V_0 < \varepsilon < 0$

or

Odd wave function case

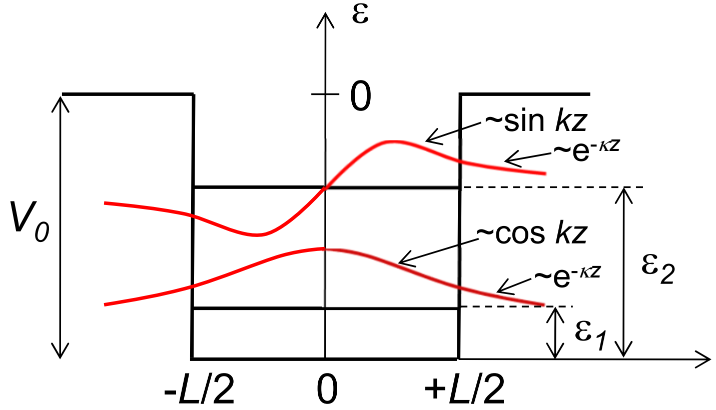
$$\chi_n(z) = A\sin kz, \quad \text{for } |z| < L/2$$
$$= B\exp\left[-\kappa(z - L/2)\right], \quad \text{for } z > L/2$$
$$= -B\exp\left[\kappa(z + L/2)\right], \quad \text{for } z < -L/2$$

Continuity conditions at *z* = ±*L*/2 yield

$$\left(k/m_A^*\right)\tan\left(kL/2\right) = \kappa/m_B^*$$
$$\left(k/m_A^*\right)\cot\left(kL/2\right) = -\kappa/m_B^*$$

Eqs. solved numerically or graphically

Inversion symmetry around the center of the well (⇒ parity of the wave function)



Number of bound states

$$1 + \text{Int}\left[\left(\frac{2m_A^* V_0 L^2}{\pi^2 \hbar^2}\right)^{1/2}\right] \quad \text{if } m_A^* = m_B^*$$