Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.6.09 Lecture 09

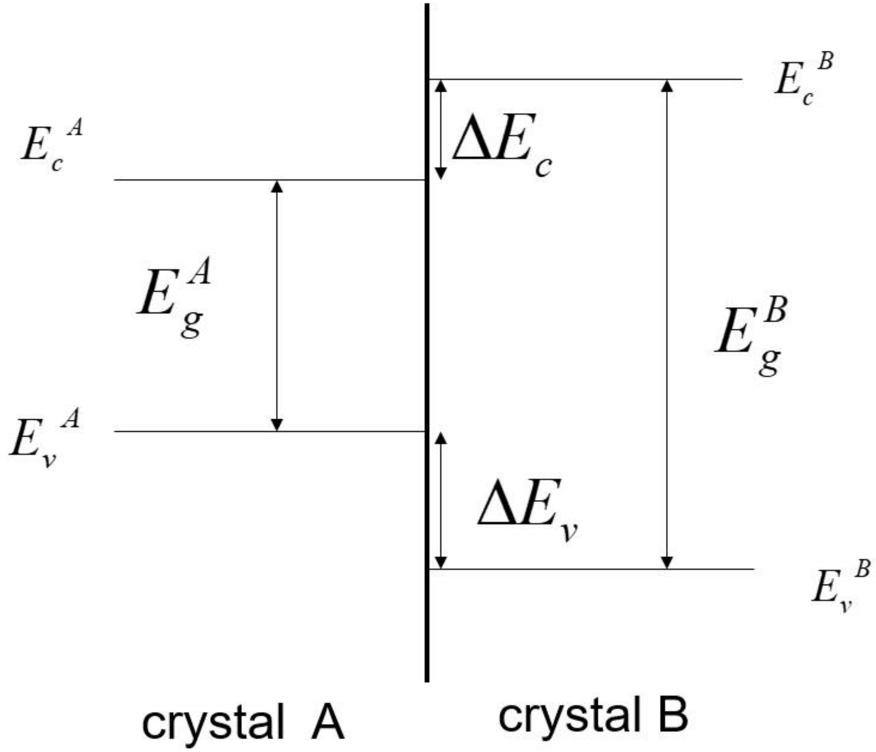
10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

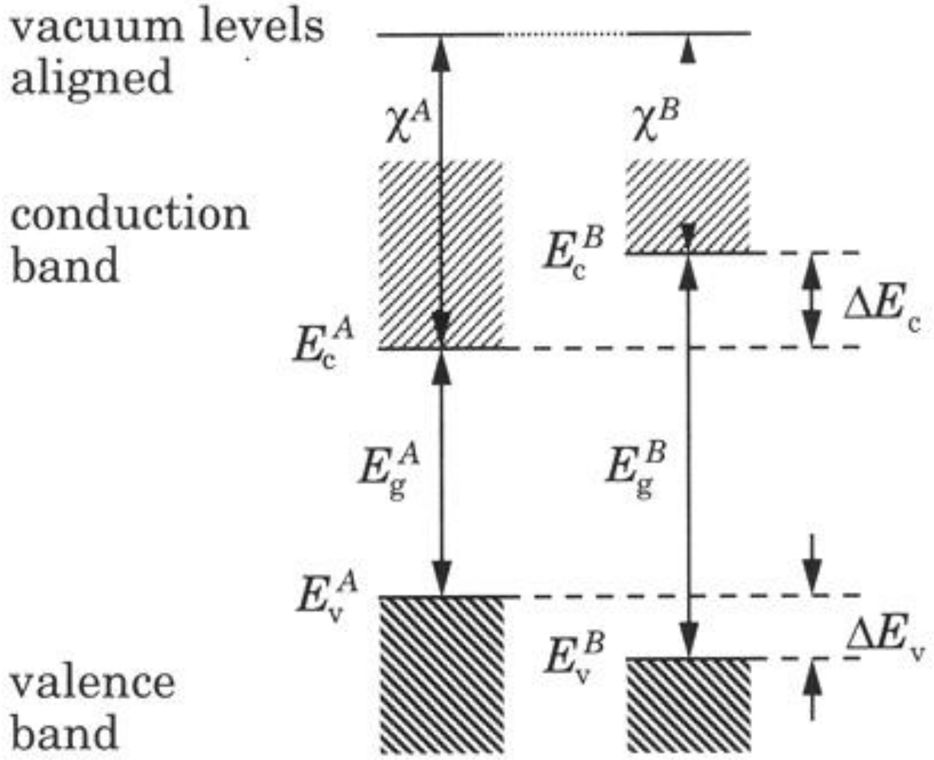
Shingo Katsumoto

Band discontinuity

Band discontinuity parameters

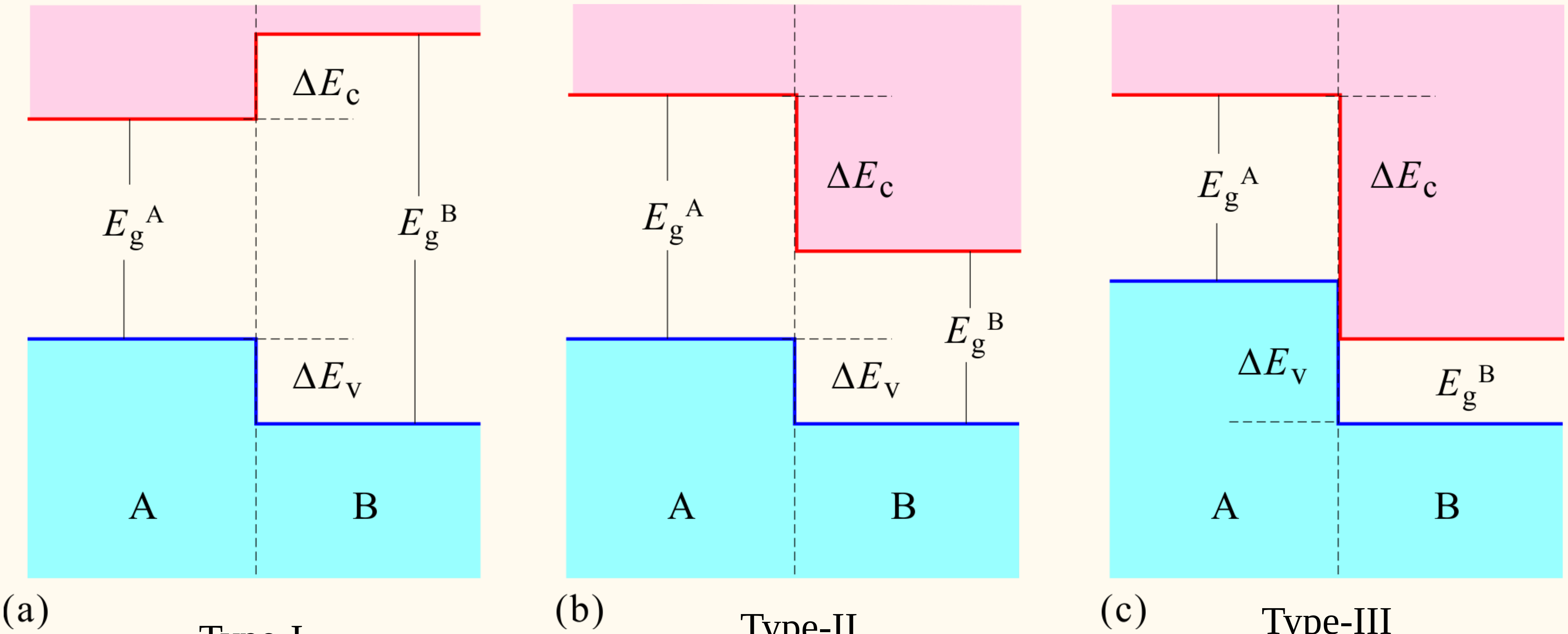


Anderson's rule: affinity from the vacuum level determines the alignment



R. L. Anderson, IBM J. Res. Dev. **4**, 283 (1960).

Heterojunction types



Type-I

Type-II

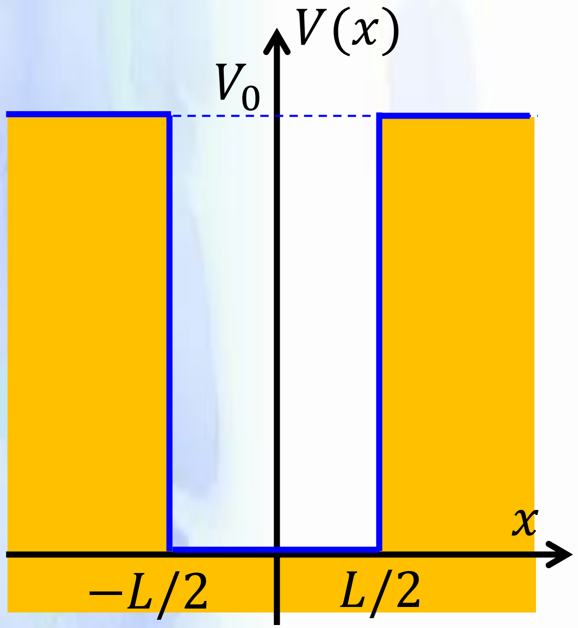
Type-III
(Type-II staggered)

Chapter 7 Quantum Structure (Quantum wells, wires, dots)

Zhores I. Alferov   Herbert Kroemer   Jack S. Kilby

The Nobel Prize in Physics 2000 was awarded *"for basic work on information and communication technology"* with one half jointly to Zhores I. Alferov and Herbert Kroemer *"for developing semiconductor heterostructures used in high-speed- and opto-electronics"* and the other half to Jack S. Kilby *"for his part in the invention of the integrated circuit"*.

Quantum well (elementary quantum mechanics)



Outside the well: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\right]\psi = E\psi, \quad x \le -\frac{L}{2}, \; \frac{L}{2} \le x, \quad \kappa \equiv \frac{\sqrt{2m|E-V_0|}}{\hbar}$

$$\psi(x) = \begin{cases} C_1 \exp(i\kappa x) + C_2 \exp(-i\kappa x) & E \ge V_0, \\ D_1 \exp(\kappa x) + D_2 \exp(-\kappa x) & E < V_0. \end{cases}$$

States localized inside the well: $E < V_0$ $\quad \frac{L}{2} < x \to D_1^+ = 0, \quad x < -\frac{L}{2} \to D_2^- = 0$

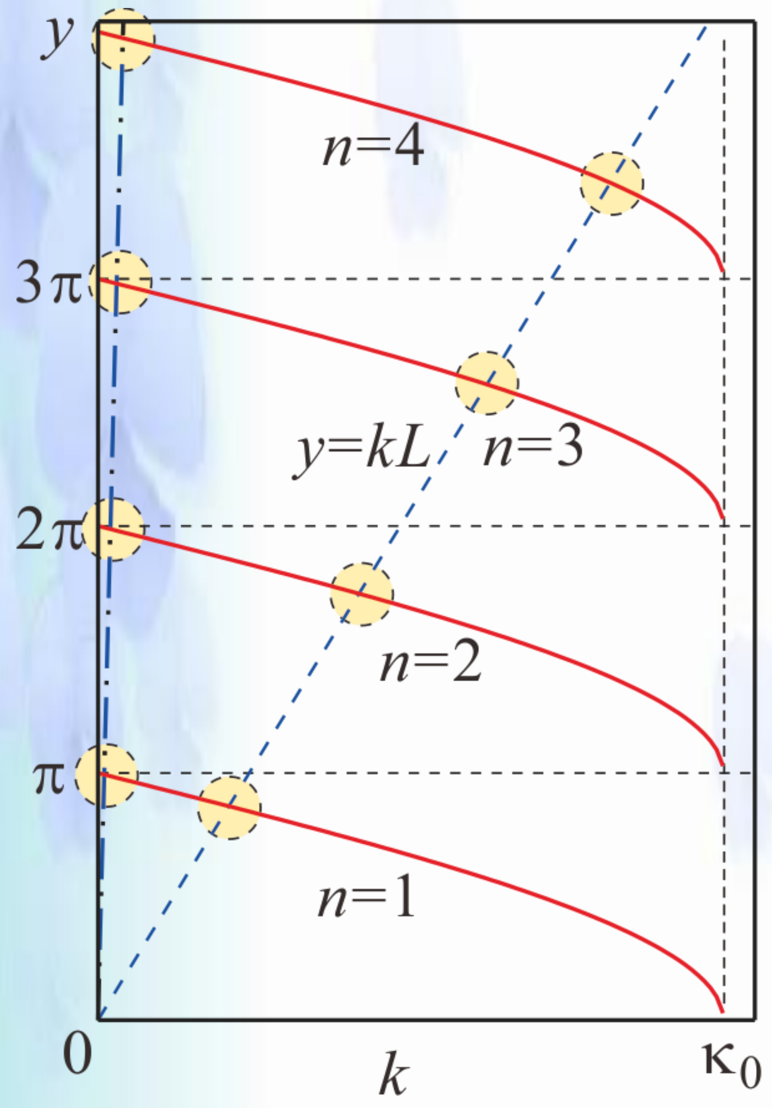
Inside the well: $\psi(x) = C_1 \exp(ikx) + C_2 \exp(-ikx), \; k \equiv \frac{\sqrt{2mE}}{\hbar}, \; x \in \left[-\frac{L}{2}, \frac{L}{2}\right]$

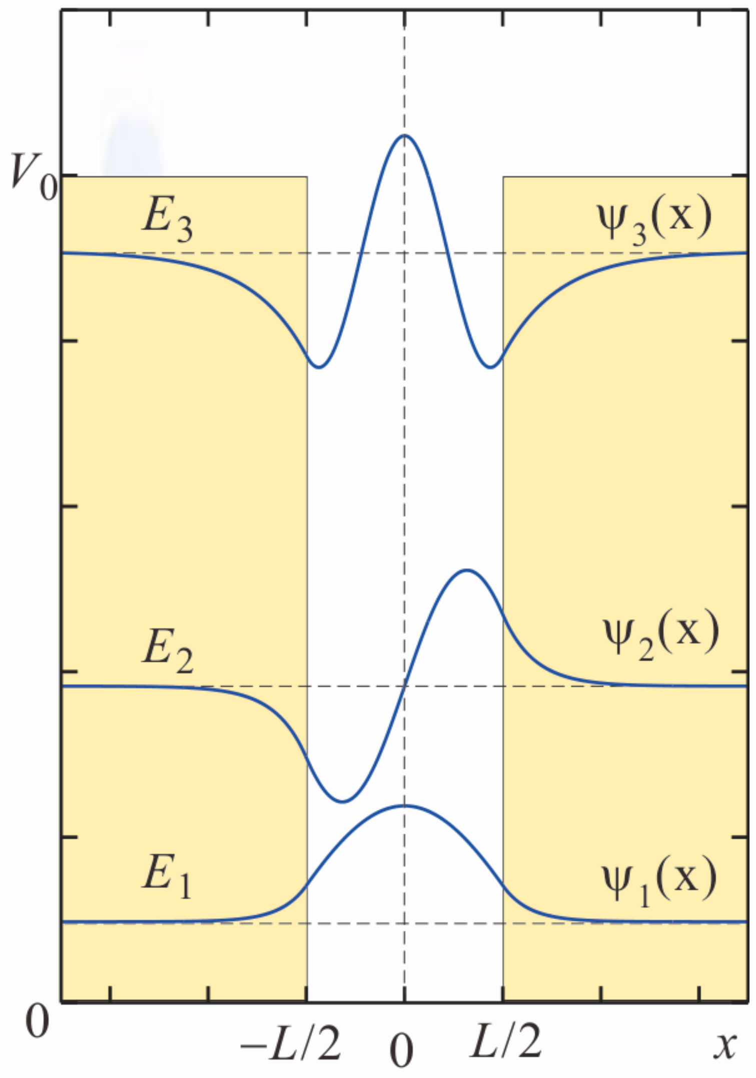
Envelope function connection

Continuity
$$\begin{cases} C_1 \exp(ikL/2) + C_2 \exp(-ikL/2) = D_2^+ \exp(-\kappa L/2), \\ C_1 \exp(-ikL/2) + C_2 \exp(ikL/2) = D_1^- \exp(-\kappa L/2), \end{cases}$$

Differentiability
$$\begin{cases} ikC_1 \exp(ikL/2) - ikC_2 \exp(-ikL/2) = -\kappa D_2^+ \exp(-\kappa L/2), \\ ikC_1 \exp(-ikL/2) - ikC_2 \exp(ikL/2) = \kappa D_1^- \exp(-\kappa L/2), \end{cases}$$

Quantum well

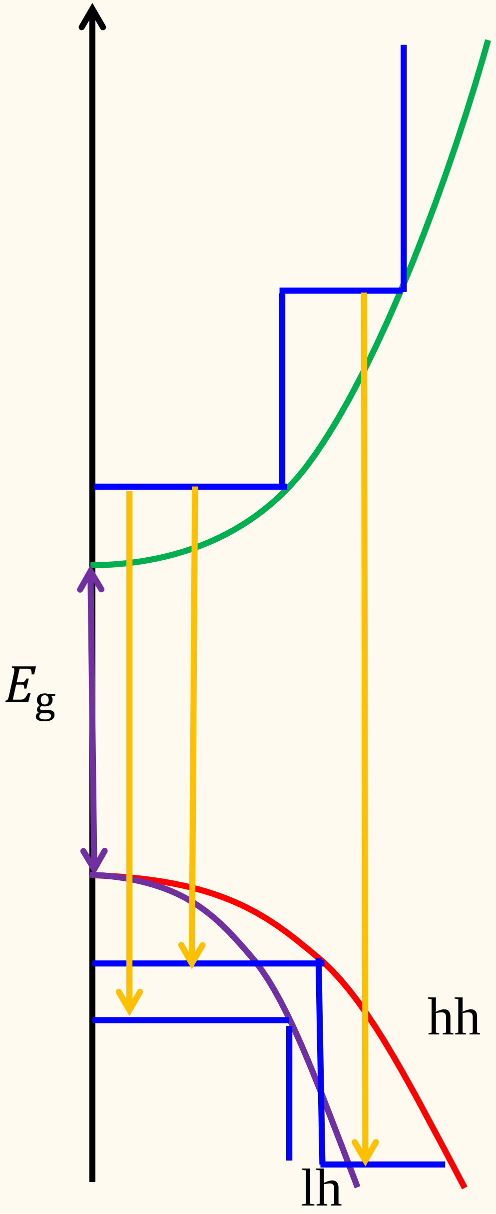




$$kL = -2\arctan\frac{k}{\sqrt{\kappa_0^2 - k^2}} + n\pi$$

$$\kappa_0^2 \equiv \frac{2mV_0}{\hbar^2}, \quad n = 1, 2, \cdots$$

Optical absorption of quantum wells



$$\left.\begin{aligned} \psi_e(\boldsymbol{r}) &= \boxed{\phi_e(z)}\exp(i\boldsymbol{k}_{xy}\cdot\boldsymbol{r}_{xy})\boxed{u_c(\boldsymbol{r})}, \\ \psi_h(\boldsymbol{r}) &= \boxed{\phi_h(z)}\exp(i\boldsymbol{k}_{xy}\cdot\boldsymbol{r}_{xy})\boxed{u_v(\boldsymbol{r})}. \end{aligned}\right\}$$

Envelope functions

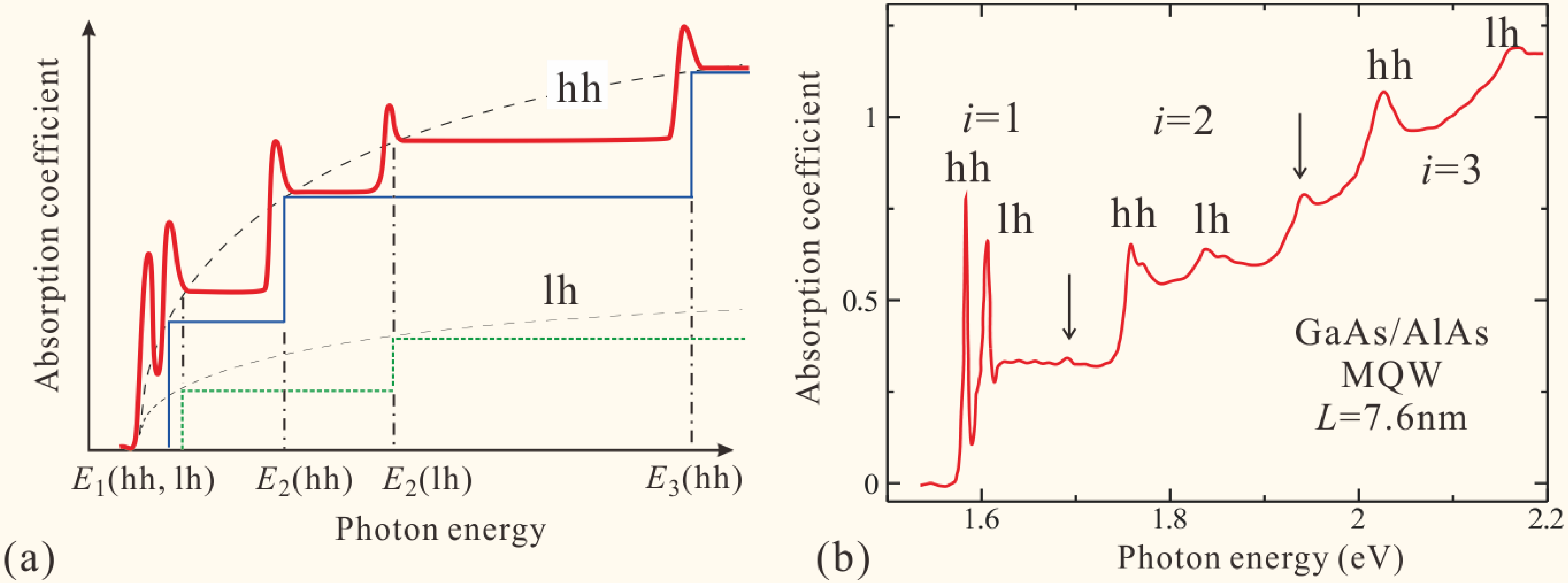
Lattice periodic functions

Direct transition rate: $P_{cv} \propto \langle u_c(\boldsymbol{r})|\boldsymbol{\nabla}|u_v(\boldsymbol{r})\rangle \int_{-\infty}^{\infty} dz\phi_e(z)^*\phi_h(z)$

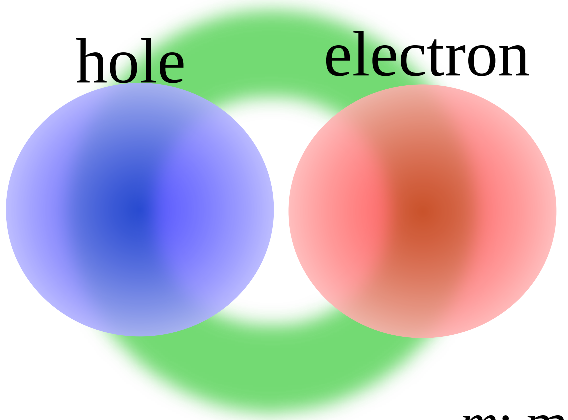
Transition energy: $E = E_g + \Delta E_n^{(eh)} + \dfrac{\hbar^2}{2\mu}k_{xy}^2$

Two dimensional density of states: $\dfrac{dn}{dE} = \dfrac{m^*}{2\pi\hbar^2}H(E) \quad (H(x)$: Heaviside function$)$

Optical absorption of quantum wells



Excitons in quantum well



Schrödinger equation

$$\left(-\frac{\hbar^2}{2m_\mathrm{r}^*}\nabla^2 - \frac{e^2}{4\pi\epsilon\epsilon_0|\boldsymbol{r}|}\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

Variable separation

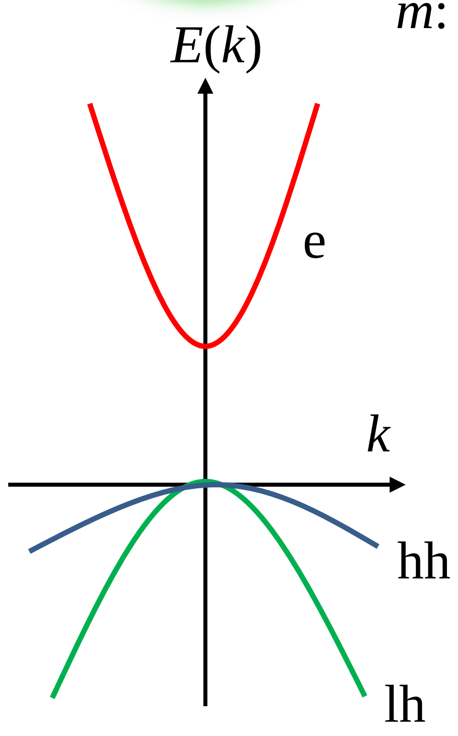
$$\psi^{2\mathrm{d}} = \rho^{|m|}e^{-\rho/2}R(\rho)e^{im\varphi} \qquad \rho = \frac{\sqrt{-8m_\mathrm{r}^*E}}{\hbar}r$$

Radial wavefunction

$$\left[\rho\frac{\partial^2}{\partial\rho^2} + (2|m|+1-\rho)\frac{\partial}{\partial\rho} + \lambda - |m| + \frac{1}{2}\right]R(\rho) = 0$$

m: magnetic quantum number

$$\lambda \equiv \frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{-\frac{m_\mathrm{r}^*}{2E}}$$



Power series expansion

$$R(\rho) = \sum_\nu \beta_\nu\rho^\nu, \qquad \beta_{\nu+1} = \beta_\nu\frac{\nu-\lambda+|m|+1/2}{(\nu+1)(\nu+p+1)}$$

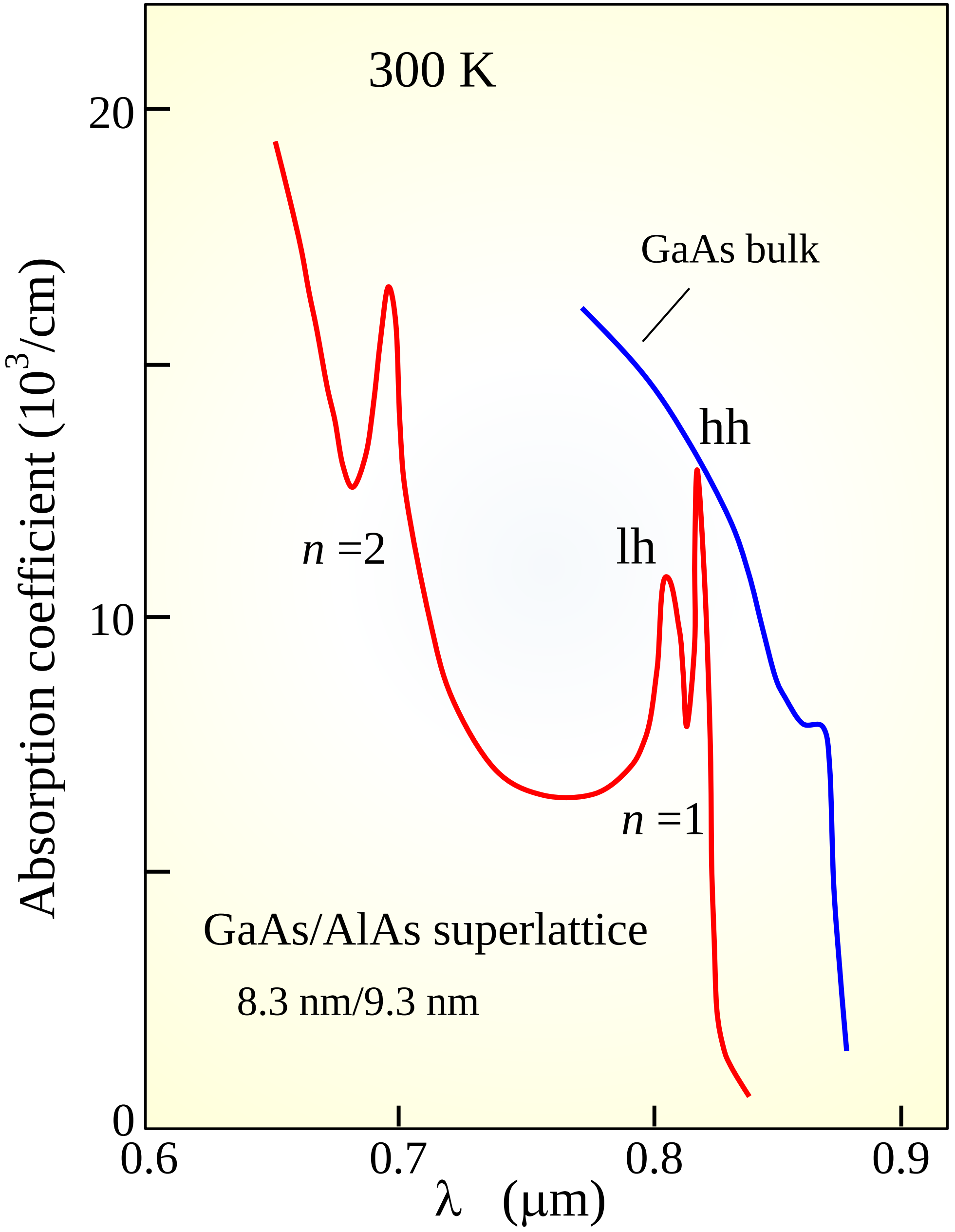
The series to be stopped at a finite length

$$E_{\mathrm{b}n}^{2\mathrm{d}} = -\frac{E_0}{(n+1/2)^2} \qquad n = 0, 1, \cdots$$

$$E_0 = \frac{e^2}{8\pi\epsilon\epsilon_0 a_0^*}, \qquad a_0^* = \frac{4\pi\epsilon\epsilon_0\hbar^2}{m_\mathrm{r}^* e^2}$$

$$E_\mathrm{ground}^{2\mathrm{d}} = 4E_0, \qquad a_0^{2\mathrm{d}} = a_0^*/2$$

Excitons in quantum well



$$\left(-\frac{\hbar^2}{2m_{\mathrm{r}}^*}\nabla^2 - \frac{e^2}{4\pi\epsilon\epsilon_0|\boldsymbol{r}|}\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

$$\psi^{2\mathrm{d}} = \rho^{|m|}e^{-\rho/2}R(\rho)e^{im\varphi} \qquad \rho = \frac{\sqrt{-8m_{\mathrm{r}}^*E}}{\hbar}r$$

$$\left[\rho\frac{\partial^2}{\partial\rho^2} + (2|m|+1-\rho)\frac{\partial}{\partial\rho} + \lambda - |m| + \frac{1}{2}\right]R(\rho) = 0$$

$$\lambda \equiv \frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{-\frac{m_{\mathrm{r}}^*}{2E}}$$

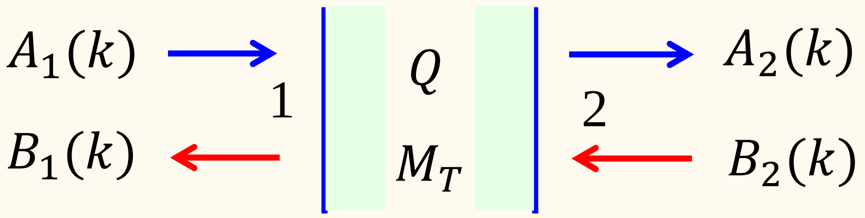
$$R(\rho) = \sum_\nu \beta_\nu\rho^\nu, \qquad \beta_{\nu+1} = \beta_\nu\frac{\nu - q}{(\nu+1)(\nu+p+1)}$$

$$E_{\mathrm{b}n}^{2\mathrm{d}} = -\frac{E_0}{(n+1/2)^2} \qquad n = 0, 1, \cdots$$

$$E_0 = \frac{e^2}{8\pi\epsilon\epsilon_0 a_0^*}, \qquad a_0^* = \frac{4\pi\epsilon\epsilon_0\hbar^2}{m_{\mathrm{r}}^* e^2}$$

$$E_{\mathrm{ground}}^{2\mathrm{d}} = 4E_0, \qquad a_0^{2\mathrm{d}} = a_0^*/2$$

Quantum barrier



momentum conservation

$\to$ relation between wavefunctions

Simpler way to consider tunneling through energy barriers

Generally $\sqrt{v_g}\psi$

- Transfer matrix: T-matrix
- Scattering matrix: S-matrix

Transfer matrix: M_T $\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \equiv M_T \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$

M_T for a barrier width L height V_0 $\quad \kappa \equiv \sqrt{2m(V_0 - E(k))}/\hbar$

Inside the barrier $\quad V_2 = V_1 e^{-\kappa L}, \quad W_2 = W_1 e^{\kappa L}$

Boundary condition: value $\quad A_1 + B_1 = V_1 + W_1, \qquad A_2 + B_2 = e^{-\kappa L} V_1 + e^{\kappa L} W_1,$

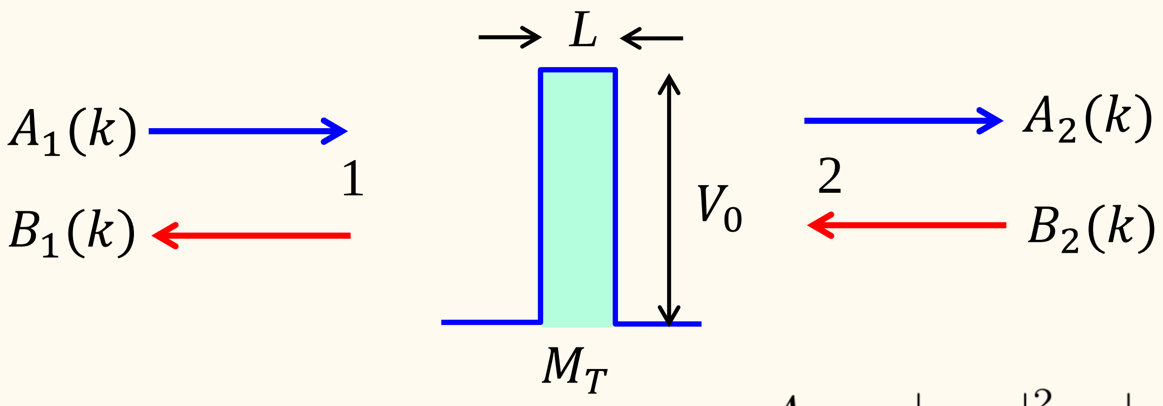
derivative $\quad ik(A_1 - B_1) = \kappa(-V_1 - W_1), \qquad ik(A_2 - B_2) = \kappa(-e^{-\kappa L} V_1 + e^{\kappa L} W_1)$

Then $M_T = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$

is obtained as

$$\begin{cases} m_{11} = \left[\cosh(\kappa L) + i\dfrac{k^2 - \kappa^2}{2k\kappa}\sinh(\kappa L)\right], \\ m_{12} = -i\dfrac{k^2 + \kappa^2}{2k\kappa}\sinh(\kappa L), \\ m_{21} = m_{12}^*, \qquad m_{22} = m_{11}^*, \end{cases}$$

Transfer matrix for rectangular barrier



$$\begin{cases} m_{11} = \left[\cosh(\kappa L) + i\dfrac{k^2-\kappa^2}{2k\kappa}\sinh(\kappa L)\right], \\ m_{12} = -i\dfrac{k^2+\kappa^2}{2k\kappa}\sinh(\kappa L), \\ m_{21} = m_{12}^*, \qquad m_{22} = m_{11}^*, \end{cases}$$

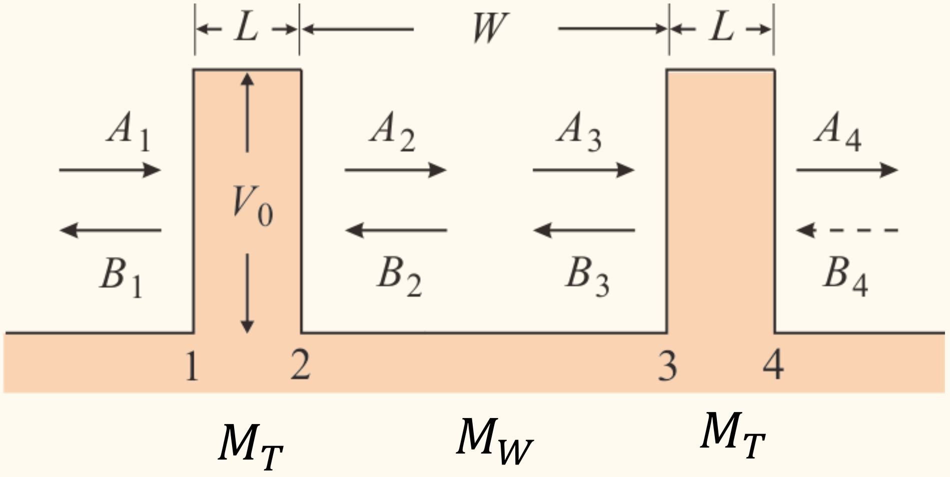
$$\begin{cases} t \equiv \dfrac{A_2}{A_1} = \dfrac{|m_{11}|^2 - |m_{12}|^2}{m_{11}^*} = \dfrac{1}{m_{11}^*} \\ \quad = \dfrac{2ik\kappa}{(k^2-\kappa^2)\sinh(\kappa L) + 2ik\kappa\cosh(\kappa L)} \\ r \equiv \dfrac{B_1}{A_1} = -\dfrac{m_{21}}{m_{22}} = \dfrac{(k^2+\kappa^2)\sinh(\kappa L)}{(k^2-\kappa^2)\sinh(\kappa L) - 2ik\kappa\cosh(\kappa L)} \end{cases}$$

t, r : complex transmission and reflection coefficients

Transmission coefficient $T = |t|^2$, reflection coefficient $R = |r|^2$

Then the transfer matrix is expressed as $M_T = \begin{pmatrix} 1/t^* & -r^*/t^* \\ -r/t & 1/t \end{pmatrix}$

Application of transfer matrix: double barrier transmission



T-matrix for well

$$M_W = \begin{pmatrix} \exp(ikW) & 0 \\ 0 & \exp(-ikW) \end{pmatrix}$$

$$M_{DB} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} e^{ikW} & 0 \\ 0 & e^{-ikW} \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

$$\equiv \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}$$

Calculation of transmission coefficient

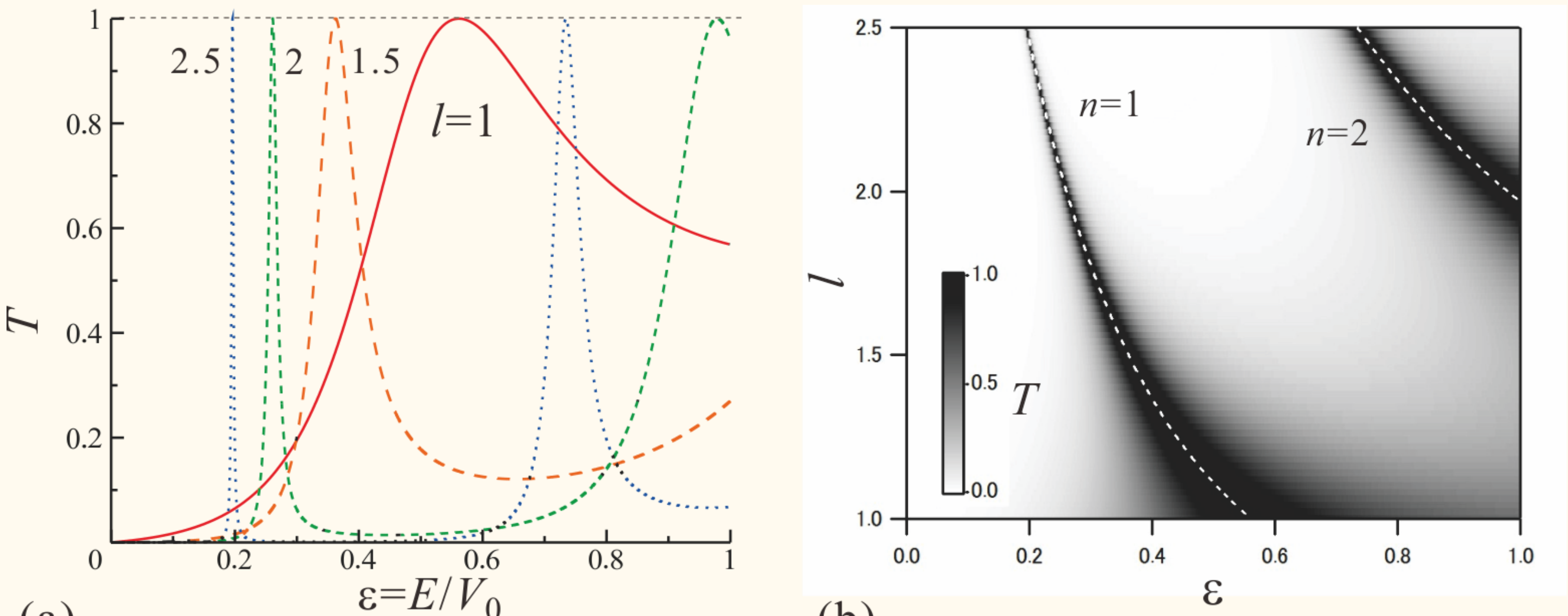
$$\begin{cases} m_{11} = \left[\cosh(\kappa L) + i\dfrac{k^2 - \kappa^2}{2k\kappa}\sinh(\kappa L)\right], \\ m_{12} = -i\dfrac{k^2 + \kappa^2}{2k\kappa}\sinh(\kappa L), \\ m_{21} = m_{12}^*, \qquad m_{22} = m_{11}^*, \end{cases}$$

$$T_{11} = m_{11}^2 \exp(ikW) + |m_{12}|^2 \exp(-ikW) \quad (\because m_{12} = m_{21}^*)$$

$$\begin{aligned} T_{11}T_{11}^* &= ((|m_{11}|^2 e^{2i\varphi} e^{ikW} + |m_{12}|^2 e^{-ikW})(|m_{11}|^2 e^{-2i\varphi} e^{-ikW} + |m_{12}|^2 e^{ikW}) \\ &= (|m_{11}^2 - |m_{12}|^2)^2 + 2|m_{11}|^2|m_{12}|^2\,(1 + \cos(2(\varphi + kW))) \\ &= 1 + 4|m_{11}|^2|m_{12}|^2\cos^2(\varphi + kW) \end{aligned}$$

$$T = \frac{1}{|T_{11}|^2} = \frac{1}{1 + 4|m_{11}|^2|m_{12}|^2\cos^2(\varphi + kW)}$$

Double barrier transmission



(a) (b)

$$T = \frac{1}{|T_{11}|^2} = \frac{1}{1 + 4|m_{11}|^2|m_{12}|^2 \cos^2(\varphi + kW)}$$

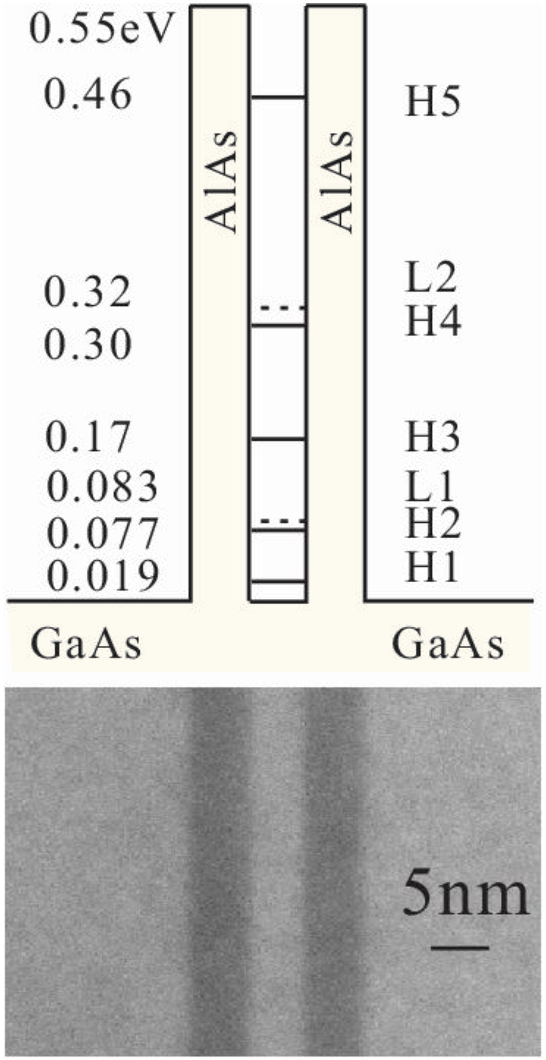
Resonant transmission condition: zero points of cosine term

$$\varphi + kW = \left(n - \frac{1}{2}\right)\pi \quad (n = 1, 2, \cdots)$$

$$\varphi = \arctan\left[\frac{k^2 - \kappa^2}{2k\kappa}\tanh(\kappa L)\right]$$

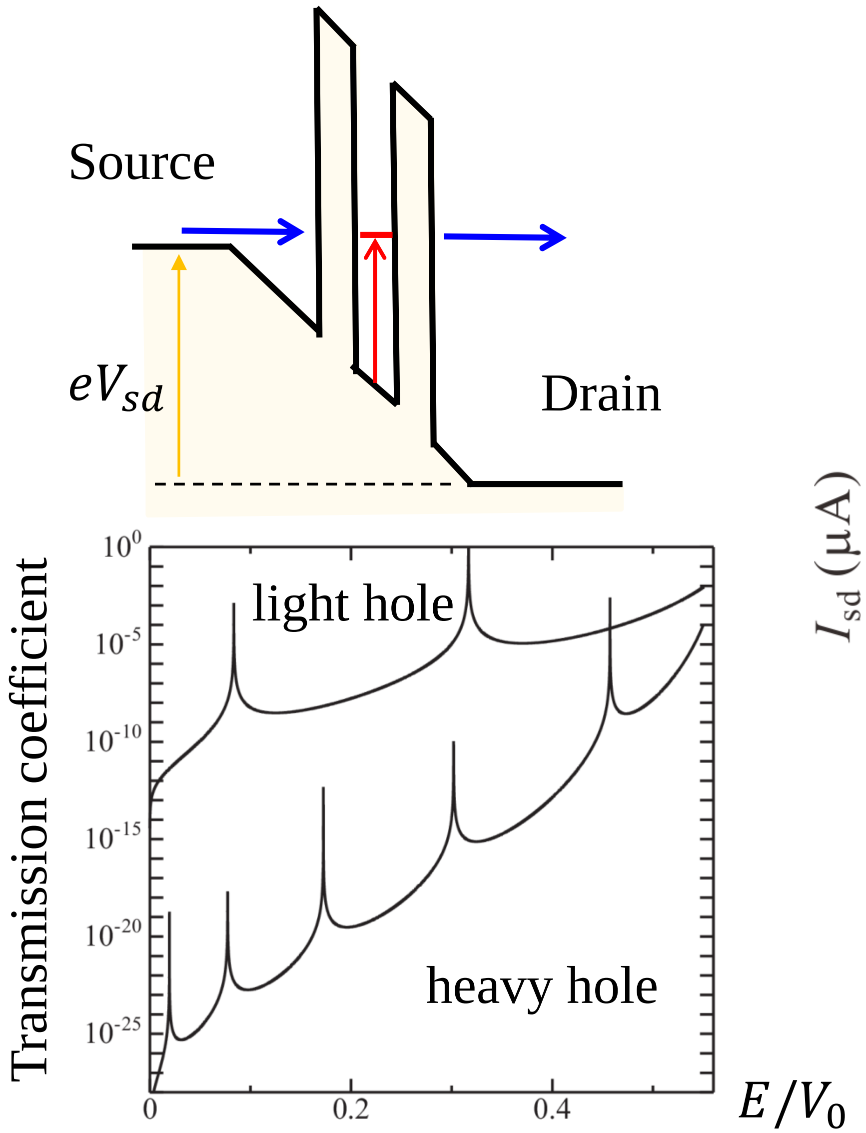
Transport experiment of double barrier conduction

Sample structure



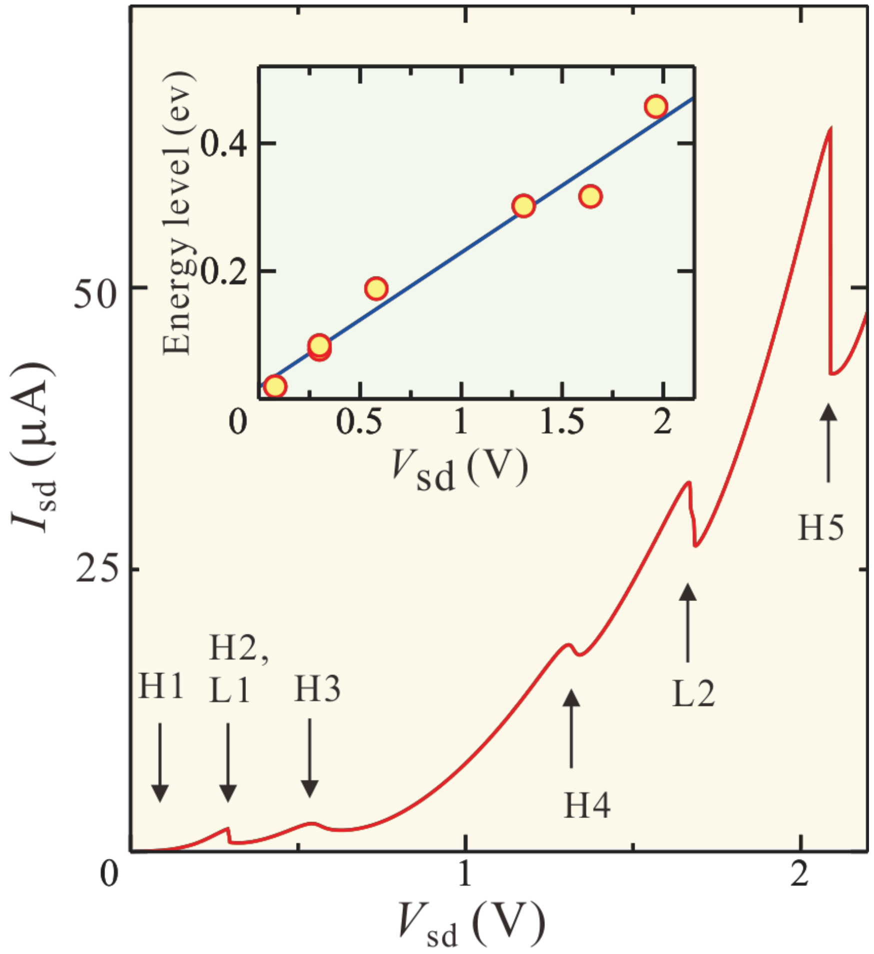
STEM image

Measurement scheme

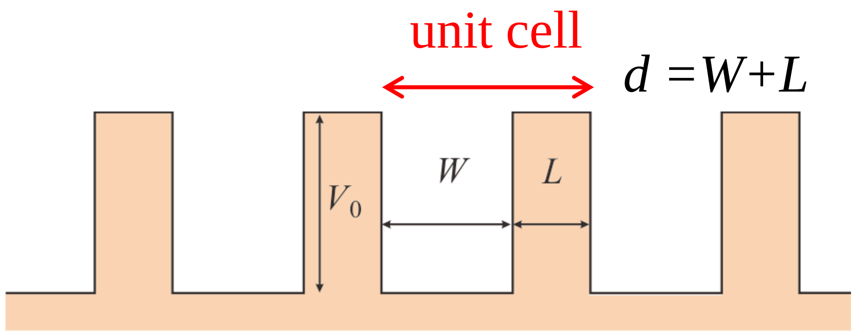


Calculated transmission coefficient

Result at 4.2 K



Application of T-matrix (2): Semiconductor superlattice



Kronig-Penny potential: $V_{KP}(x)$

Schrödinger equation

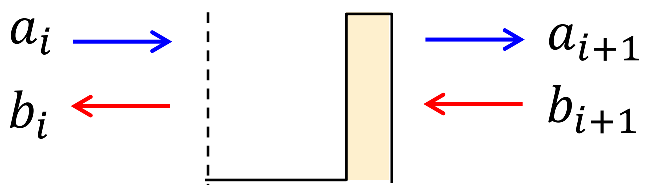
$$\left[-\frac{\hbar^2 d^2}{2m dx^2} + V_{\mathrm{KP}}(x)\right]\psi(x) = E\psi(x), \qquad V_{\mathrm{KP}}(x) = V_{\mathrm{KP}}(x+d)$$

Bloch theorem

$$\psi_K(x) = u_K(x) e^{iKx}, \quad u_K(x+d) = u_K(x), \quad K \equiv \frac{\pi s}{Nd}$$

$$s = -N+1, \cdots, N-1$$

Unit cell transfer matrix



$$M_d(k) = \begin{pmatrix} e^{ikW} & 0 \\ 0 & e^{-ikW} \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} = \begin{pmatrix} m_{11} e^{ikW} & m_{12} e^{ikW} \\ m_{21} e^{-ikW} & m_{22} e^{-ikW} \end{pmatrix}$$

$$\begin{pmatrix} a_{i+1} \\ b_{i+1} \end{pmatrix} = M_d \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \underline{e^{iKd}} \begin{pmatrix} a_i \\ b_i \end{pmatrix}$$

Eigenvalues $e^{\pm Kd}$ (M_d: unitary)

Theorem: $\mathrm{Tr}(A) = \sum(\text{eigenvalue})$ $\longrightarrow$ $e^{iKd} + e^{-iKd} = 2\cos Kd = \mathrm{Tr} M_d = 2\mathrm{Re}(e^{-ikW} m_{11}^*)$

$$\cos\left[K(L+W)\right] = \cosh(\kappa L)\cos(kW) - \frac{k^2 - \kappa^2}{2k\kappa}\sinh(\kappa L)\sin(kW)$$

The relation between k (free electron wavenumber) and K (crystal wavenumber)

Semiconductor superlattice

$$\cos\left[K(L+W)\right] = \cosh(\kappa L)\cos(kW) - \frac{k^2-\kappa^2}{2k\kappa}\sinh(\kappa L)\sin(kW)$$

$$L \to 0\ (W \to d),\ V_0 \to +\infty \text{ with } V_0 L = C(\text{constant})$$

δ-function series with the coefficient C.

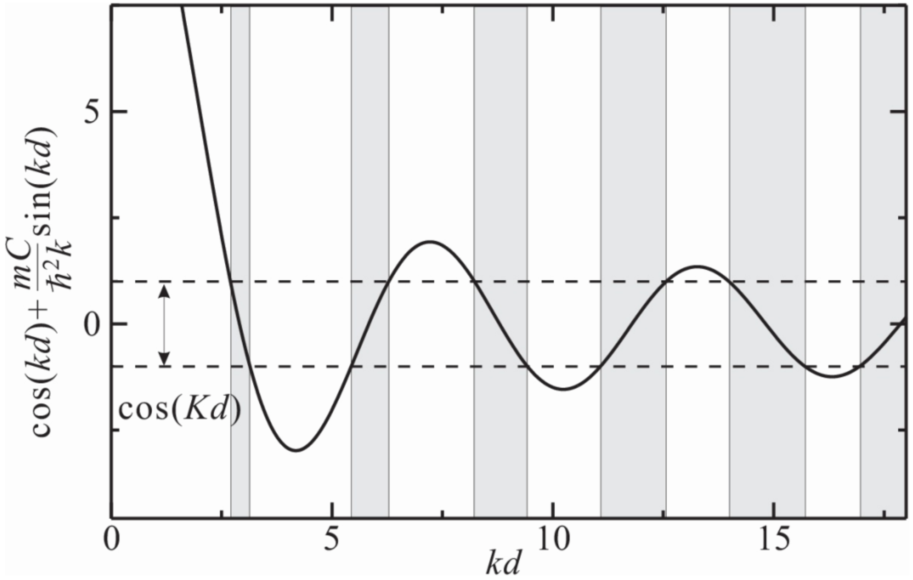
$$\cos(Kd) = \cos(kd) + \underline{\frac{mC}{\hbar^2 k}\sin(kd)}$$

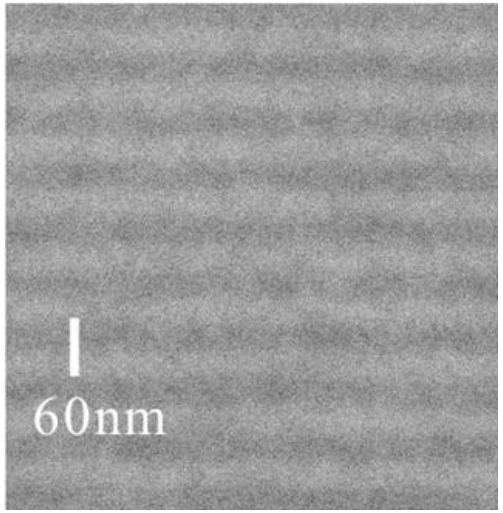
effect of superlattice potential

Raphael Tsu and Leo Esaki, 1975

$$\left|\cos(kd) + \frac{mC}{\hbar^2 k}\sin(kd)\right| > 1$$:no solution → band gap

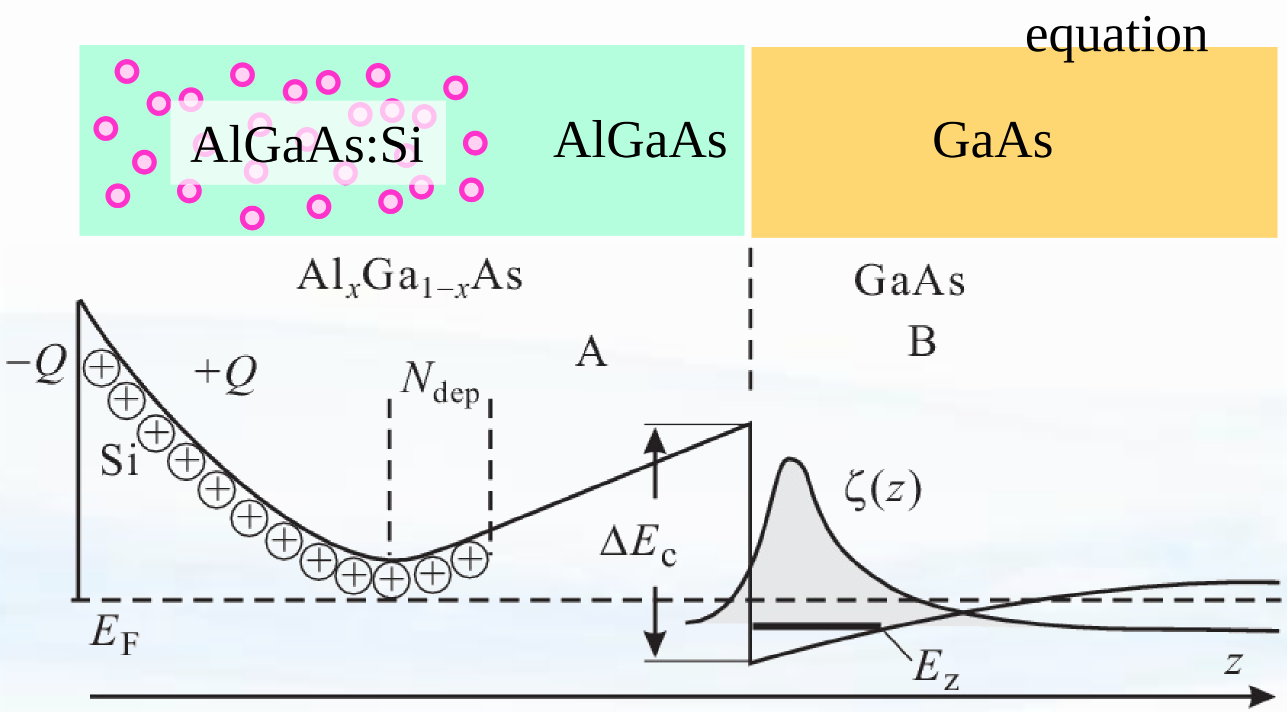
Around $kd = n\pi\ (n = 1,2,\cdots)$





STEM image of
AlAs (30 nm)/GaAs (30nm)
superlattice

Modulation doping and 2-dimensional electrons



Donor potential $V_D(z) = \frac{4\pi e^2}{\epsilon\epsilon_0} N_{\rm dep} z \quad z > 0$

$$\Psi(\boldsymbol{r}) = \psi(x, y)\zeta(z)$$

Electric field of sheet charge at z' $-\frac{4\pi e^2}{\epsilon\epsilon_0} n_{2d} |\zeta(z')|^2 |z - z'|$

$$V_{2d}(z) = -\frac{4\pi e^2}{\epsilon\epsilon_0} n_{2d}(E_z) \int_{-\xi}^{\infty} |\zeta(z')|^2 |z - z'| dz'$$

Heterointerface potential $V_h(z) = \Delta E_{\rm c}[1 - H(z)]$

Poisson-Schrödinger scheme

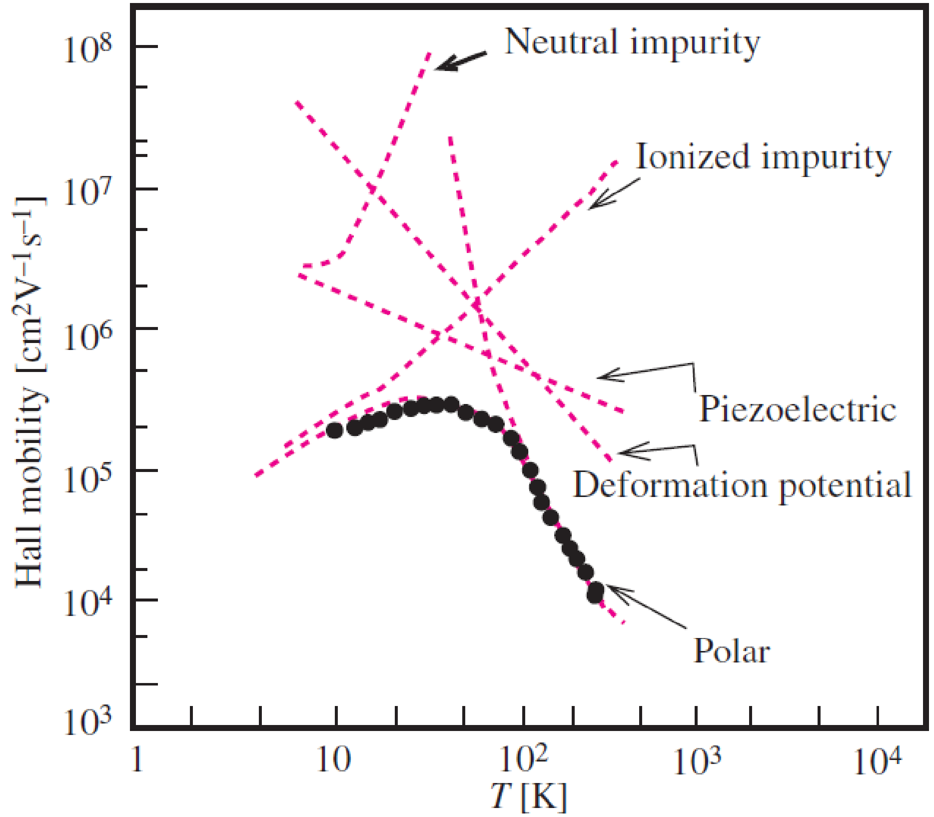
potential
$$V(z) = V_h(z) + \frac{4\pi e^2}{\epsilon\epsilon_0} \left[N_{\rm dep} z - n_{2d}(E_z) \int_{-\xi}^{\infty} |z - z'| |\zeta(z')|^2 dz' \right]$$

Schrödinger equation
$$\left[-\frac{\hbar^2}{2m^*(z)} \frac{\partial^2}{\partial z^2} + V(z) \right] \zeta(z) = E_z \zeta(z)$$

Boundary condition
$$\zeta(0)^{(\rm A)} = \zeta(0)^{(\rm B)}, \quad \frac{1}{m_{\rm A}^*} \frac{d\zeta^{(\rm A)}}{dz} \bigg| = \frac{1}{m_{\rm B}^*} \frac{d\zeta^{(\rm B)}}{dz} \bigg|$$

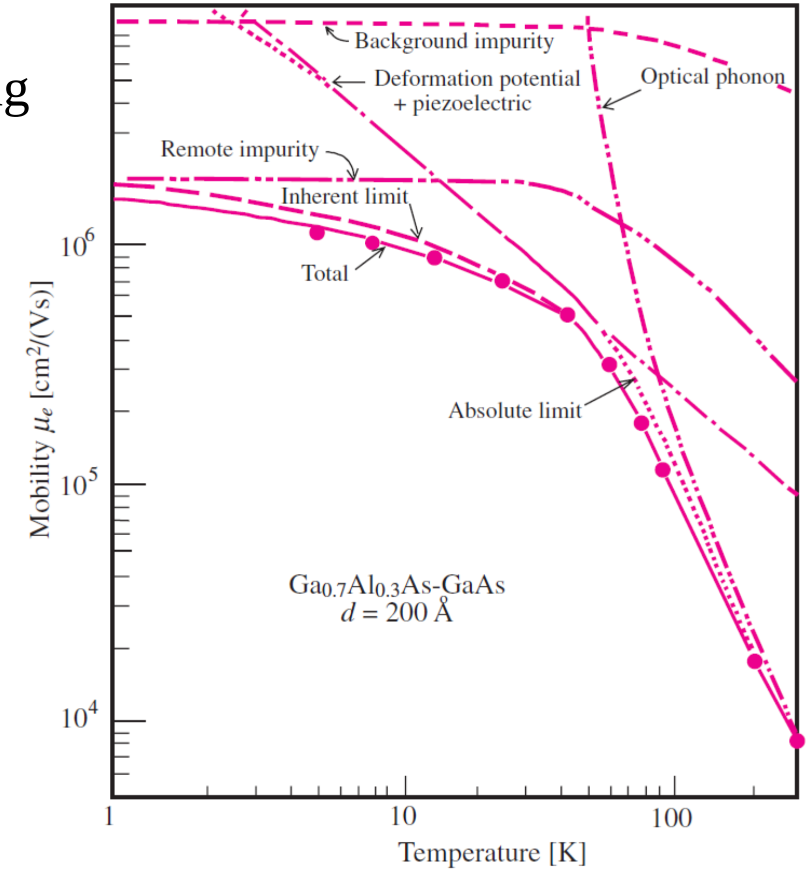
Matthiessen's rule (series connection of scattering)

$$\frac{1}{\tau_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\tau_{\beta}} = \frac{1}{\tau_{\mathrm{defects}}} + \frac{1}{\tau_{\mathrm{cattier}}} + \frac{1}{\tau_{\mathrm{lattice}}} + \cdots \qquad \frac{1}{\mu_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\mu_{\beta}} = \frac{1}{\mu_{\mathrm{defects}}} + \frac{1}{\mu_{\mathrm{cattier}}} + \frac{1}{\mu_{\mathrm{lattice}}} + \cdots$$



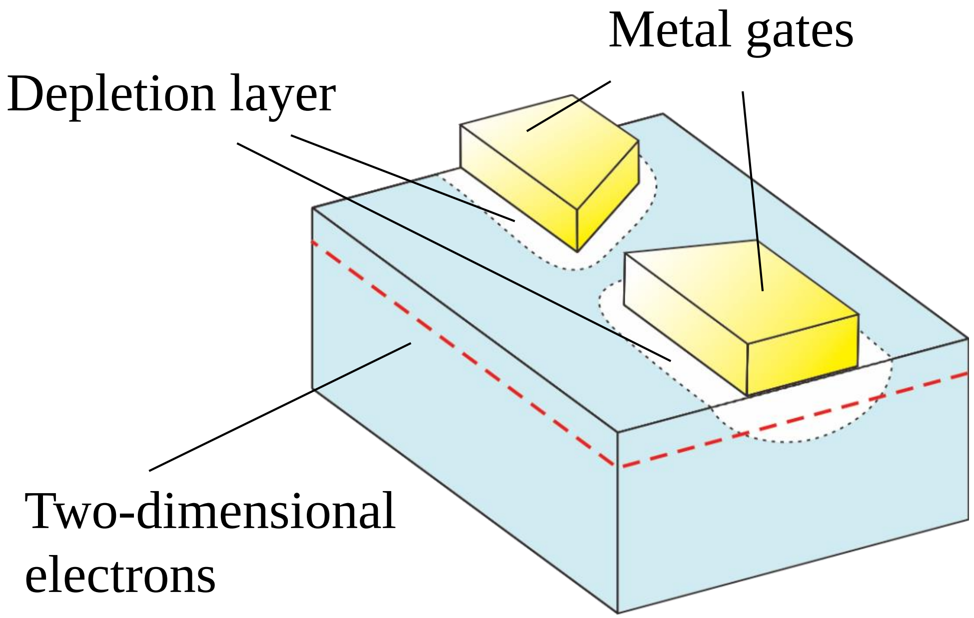
Fletcher *et al.*, J. Phys. C **5**, 212 (1972)

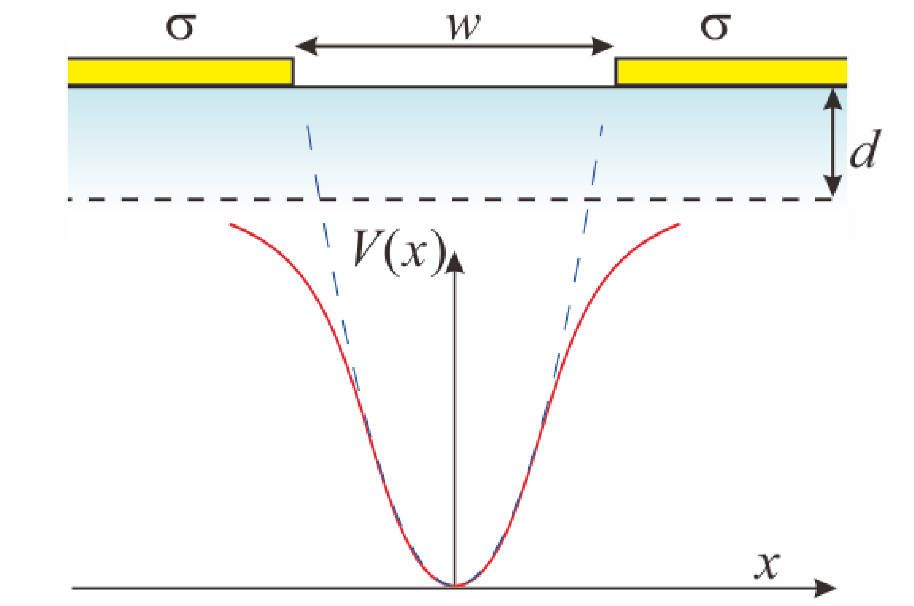
Reduction of impurity scattering by modulation doping structure



Walukiewicz *et al.* Phys. Rev. B **30**, 4571 (1984).

Formation of quantum wires: split gate



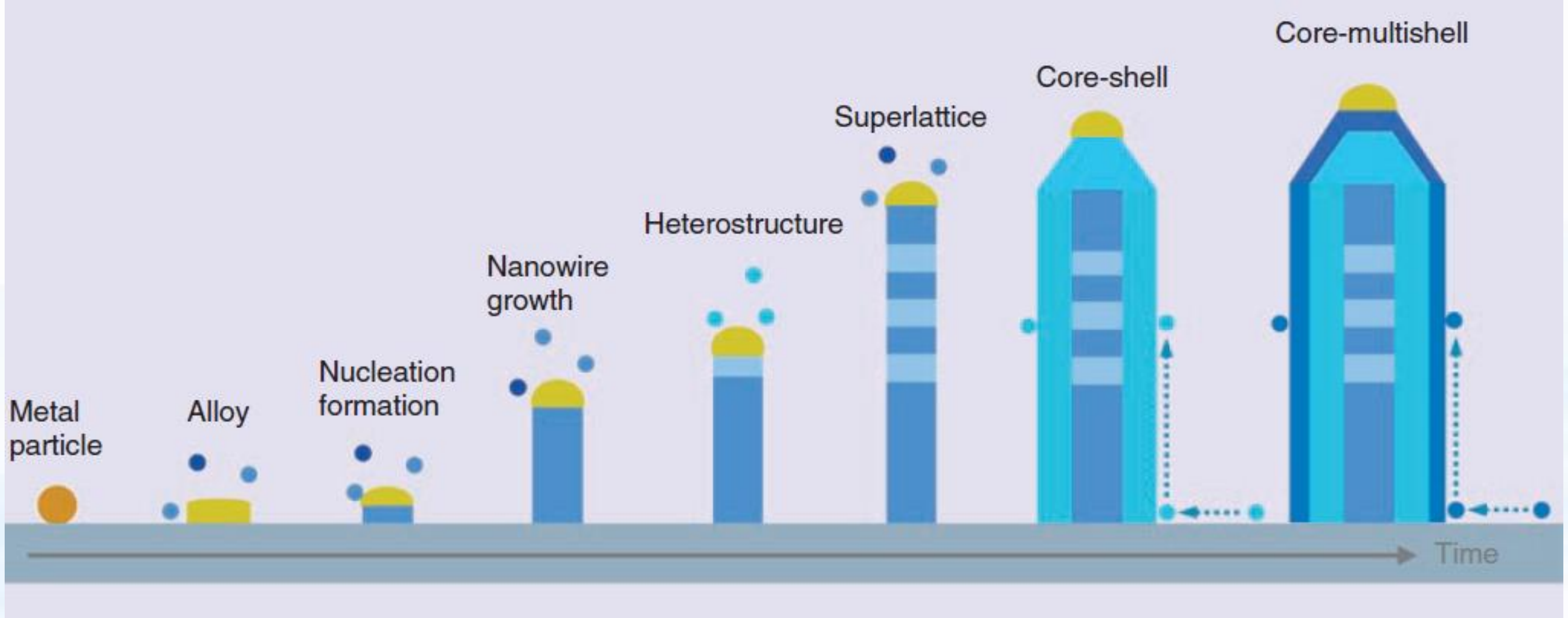


Two-dimensional electrons are pinched with depletion layers from Schottky gates to a one-dimensional system.

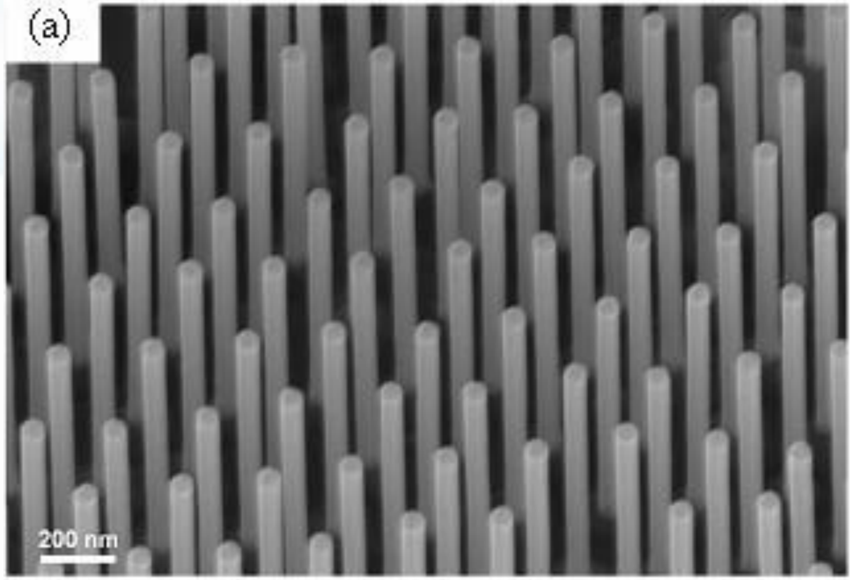
Electric field along z-axis can be approximated as $$\mathcal{E}_z(d) = \frac{-\sigma}{2\pi\epsilon\epsilon_0}\left[\pi + \arctan\frac{x - w/2}{d} - \arctan\frac{x + w/2}{d}\right]$$

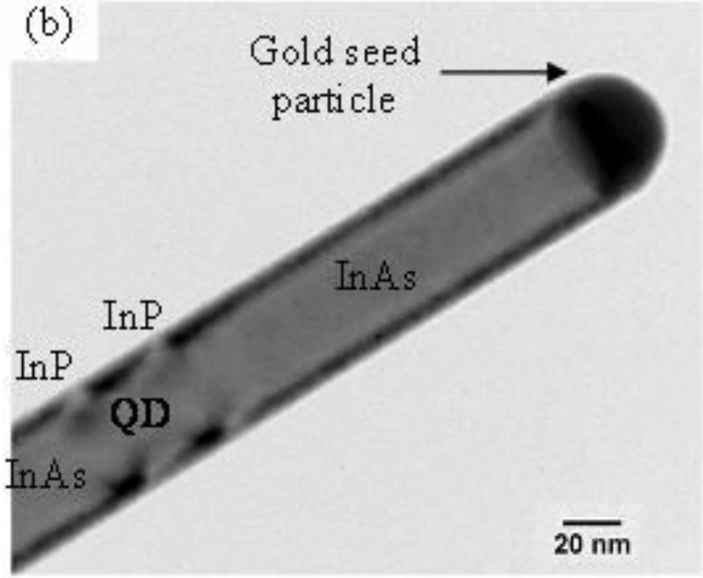
The bottom part of the confinement potential can be approximated by harmonic potential.

Self-assembled nano-wires



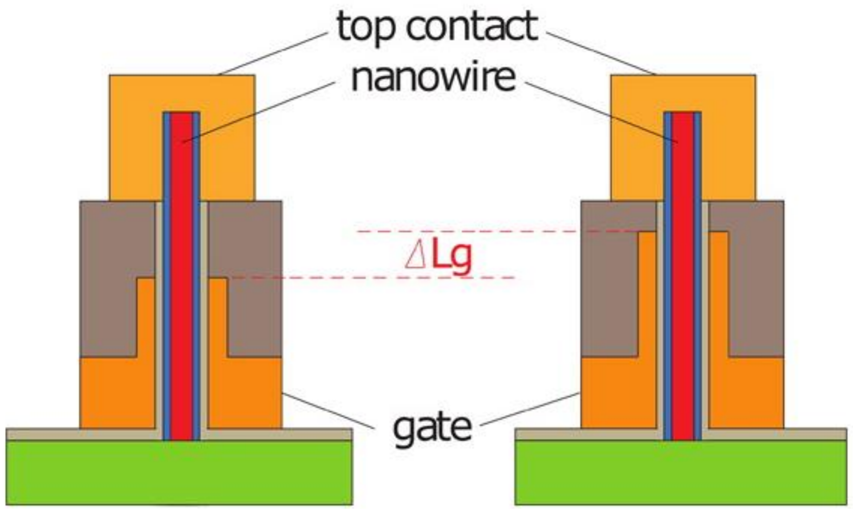
G. Zhang et al. NTT technical Review

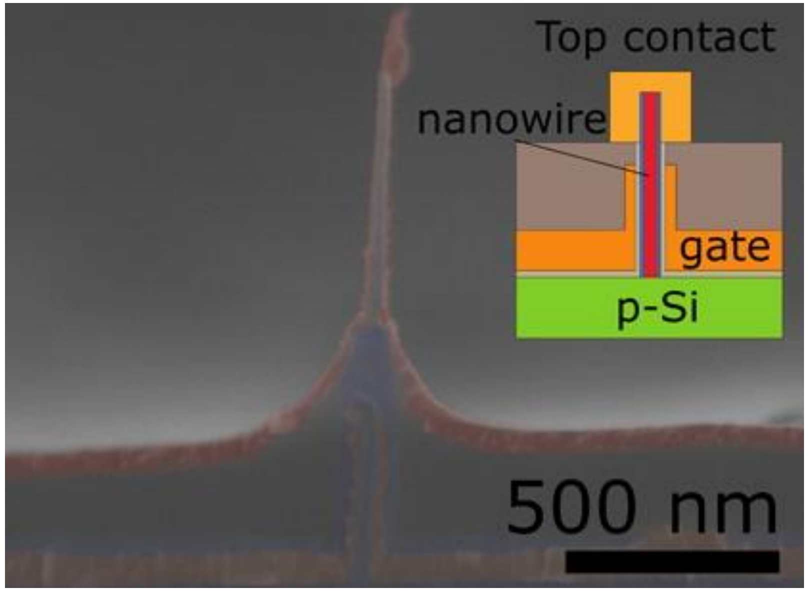


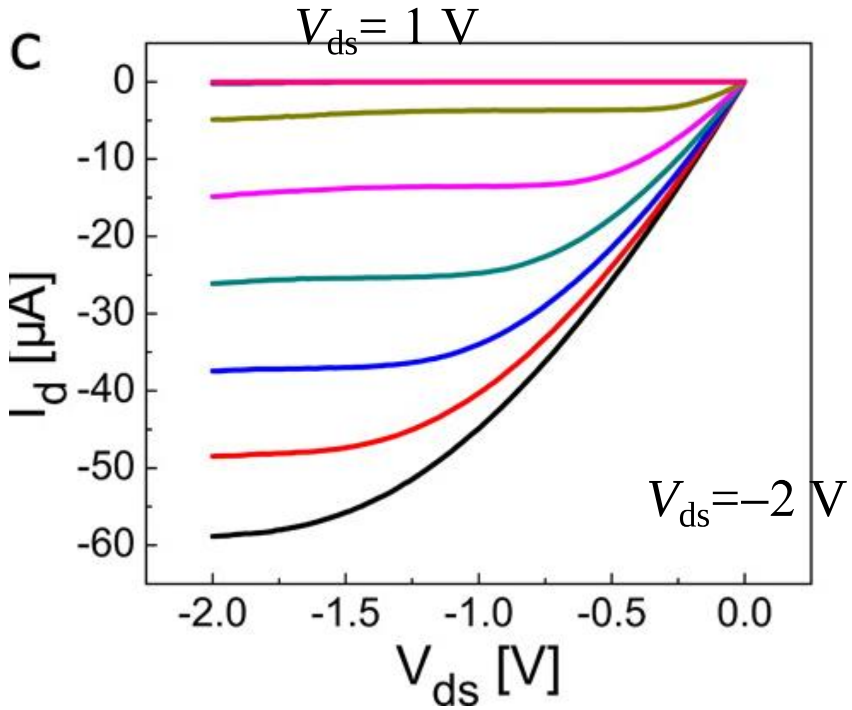


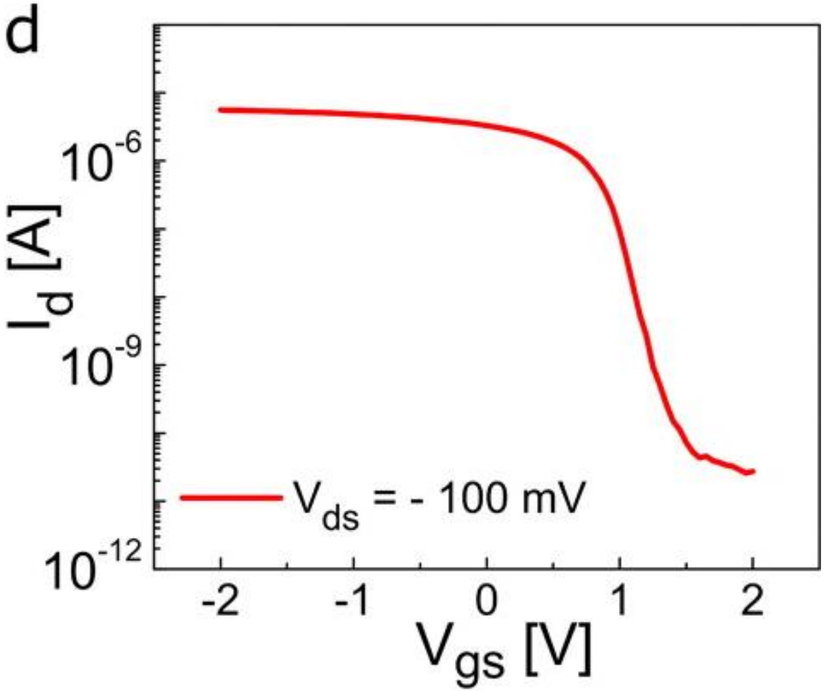
http://iemn.univ-lille1.fr/sites_perso/vignaud/english/35_nanowires.htm

Core-shell nanowire transistor



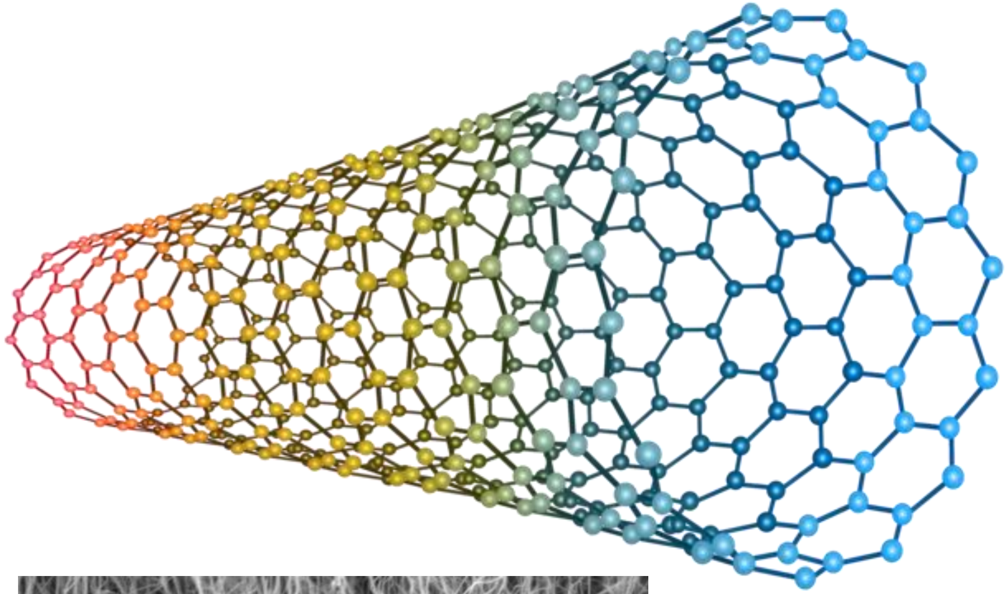


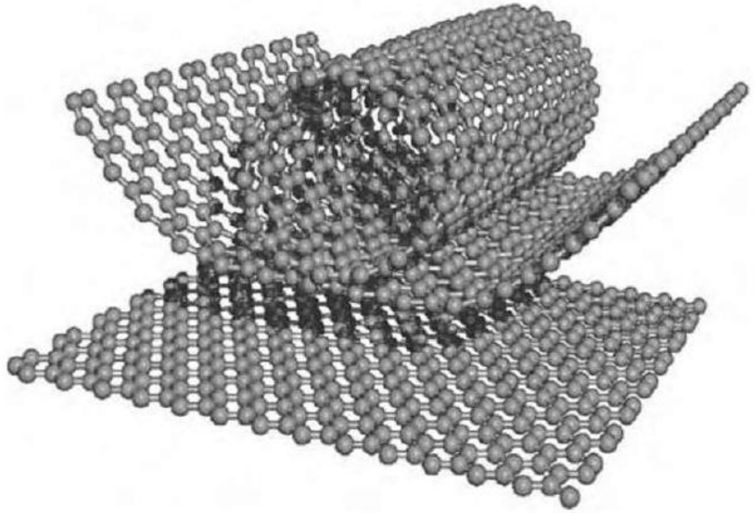


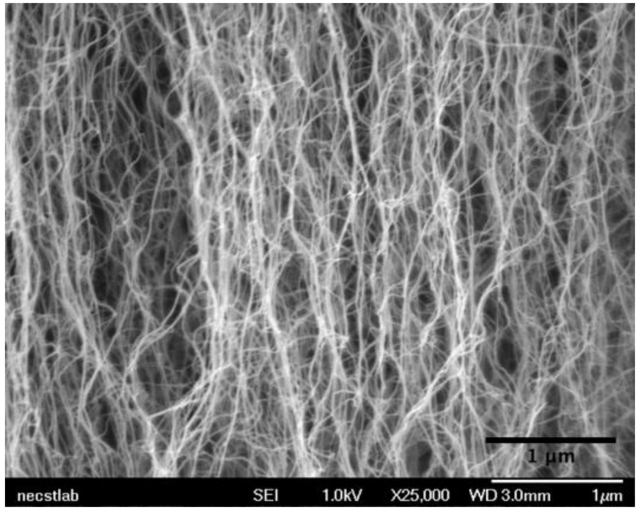


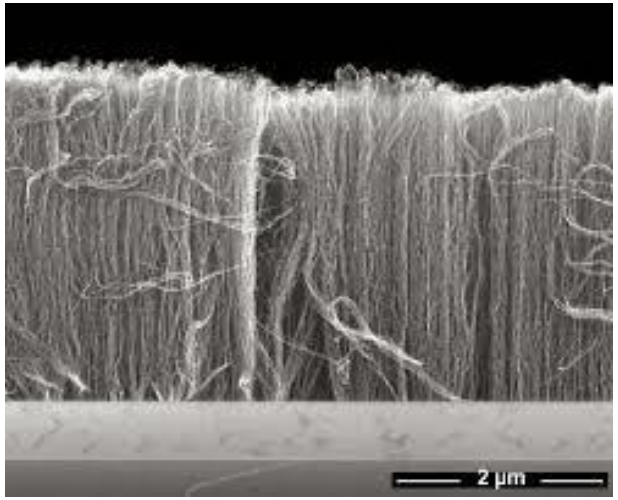
L. Chen *et al.*,
Nano Letters **16**, 420 (2016).

Carbon nanotube



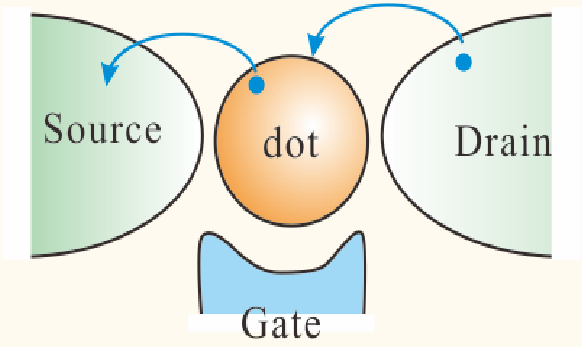






Quantum dots: zero-dimensional system

Quantum dots with nano-fabrication techniques



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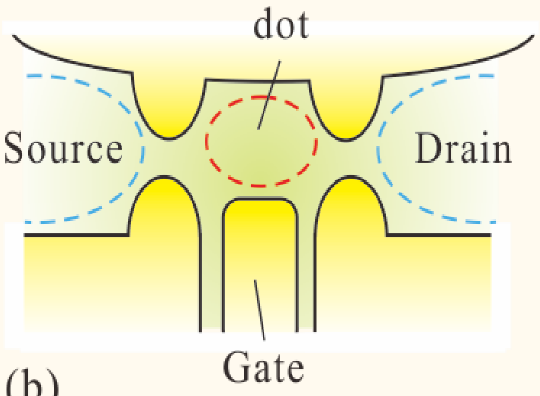

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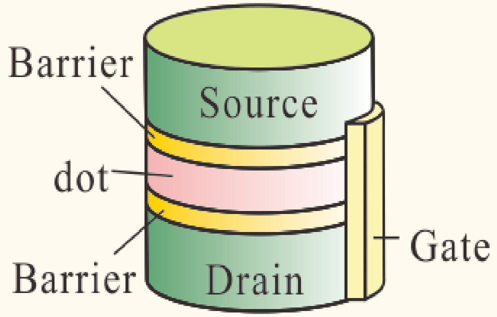

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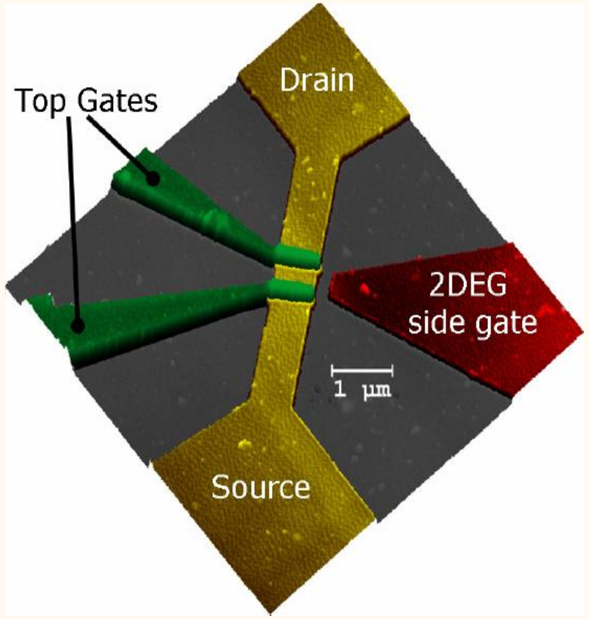
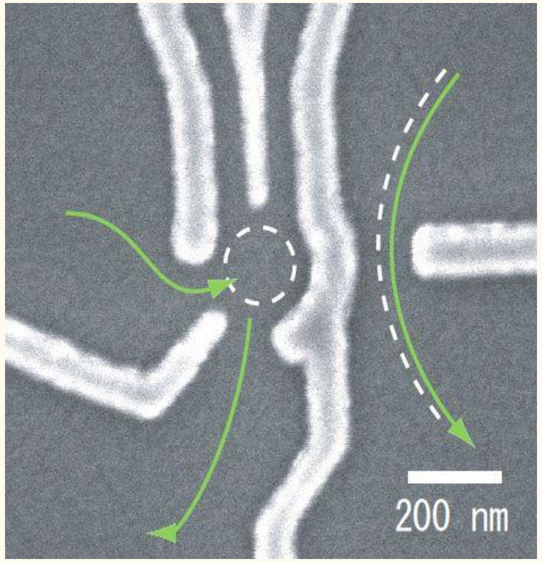
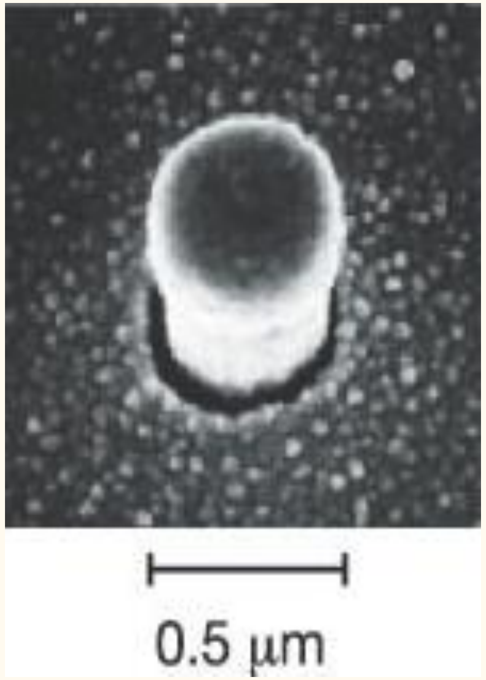


wrap gate



split gate

with charge detector

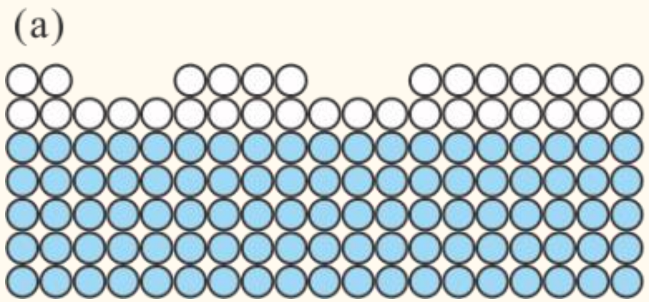


vertical type

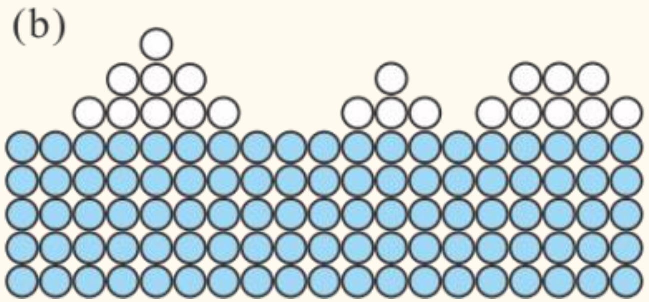
Formation of quantum dots: self assemble

MBE growth modes

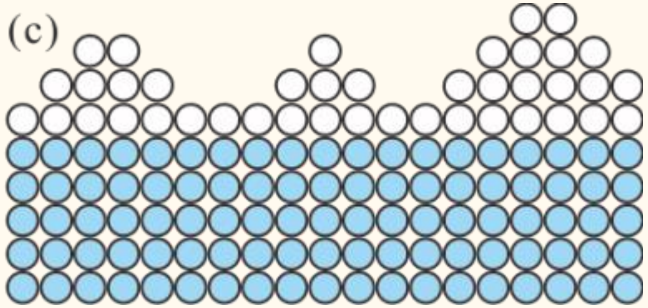
Frank-van der Merve

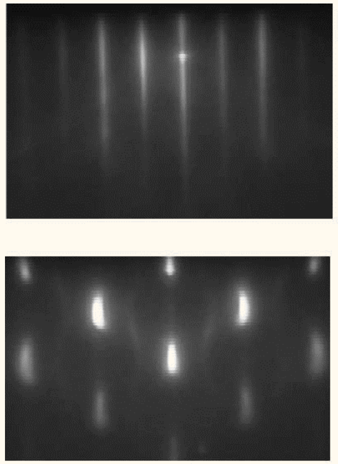


Volmer-Weber

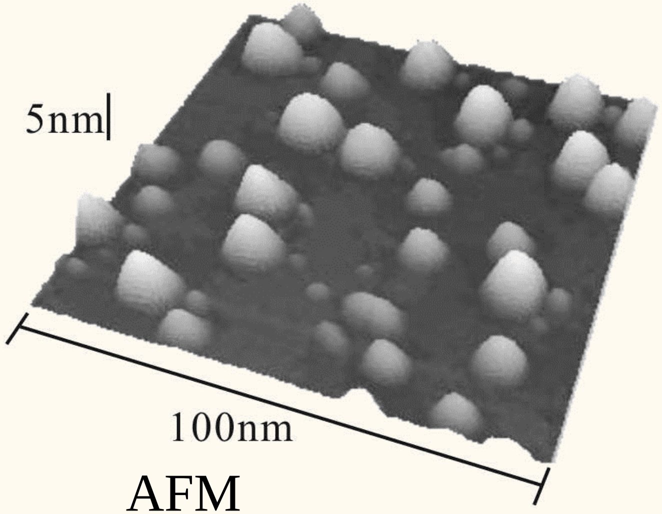


Stranski-Krastanow

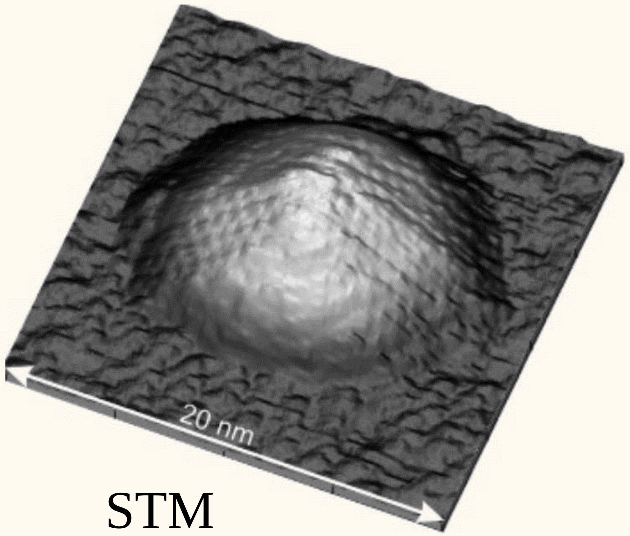




RHEED



AFM



STM

Formation of quantum dots: Colloidal nano-crystals