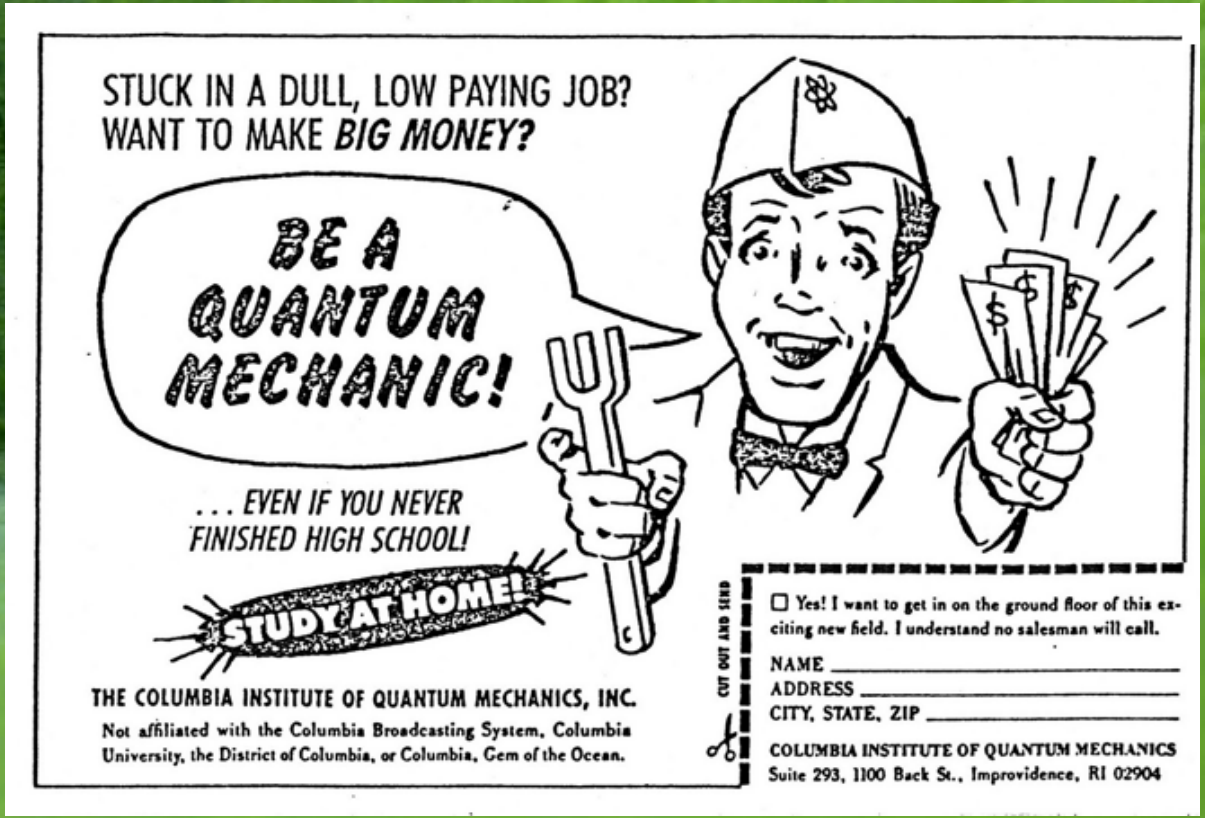
Semiconductor heterostructures – quantum wells



Faculty of Physics UW

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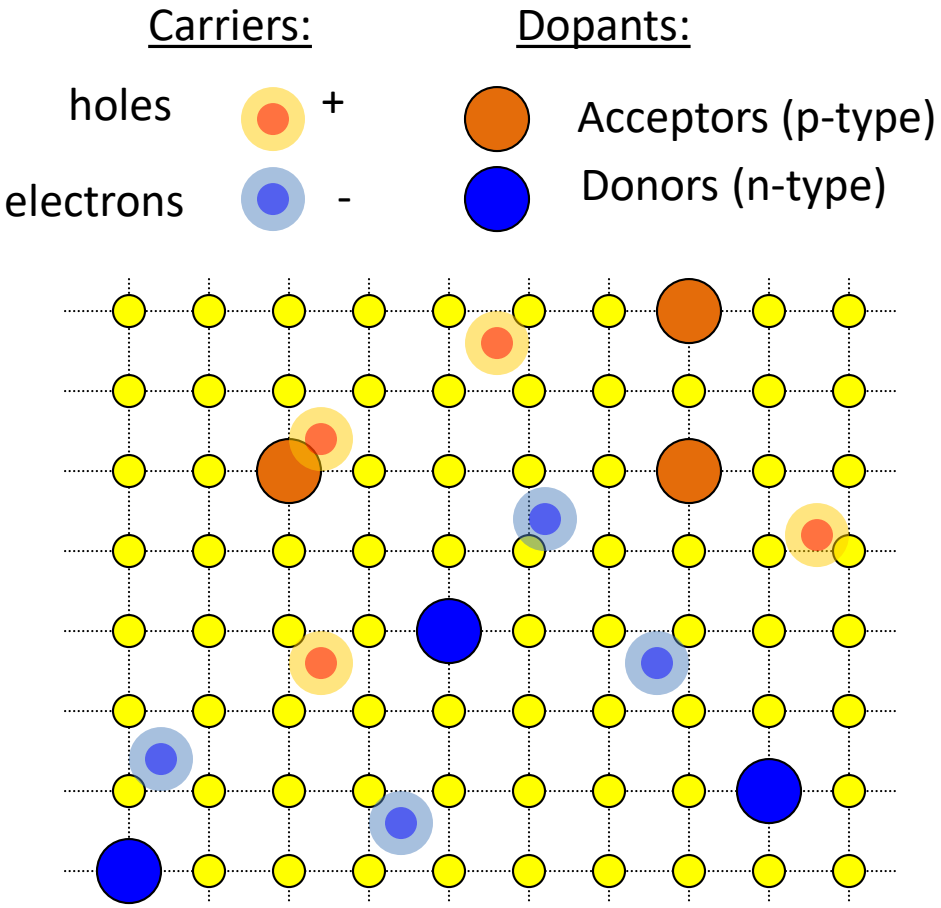
inżynieria nanostruktur

Domieszkowanie półprzewodników



Semiconductors

II	III	IV	V	VI
Be	B	C	N	O
Mg	Al	Si	P	S
Zn	Ga	Ge	As	Se
Cd	In	Sn	Sb	Te

Group IV: diamond, Si, Ge
Group III-V: GaAs, AlAs, InSb, InAs...
Group II-VI: ZnSe, CdTe, ZnO, SdS...

Semiconductor heterostructures

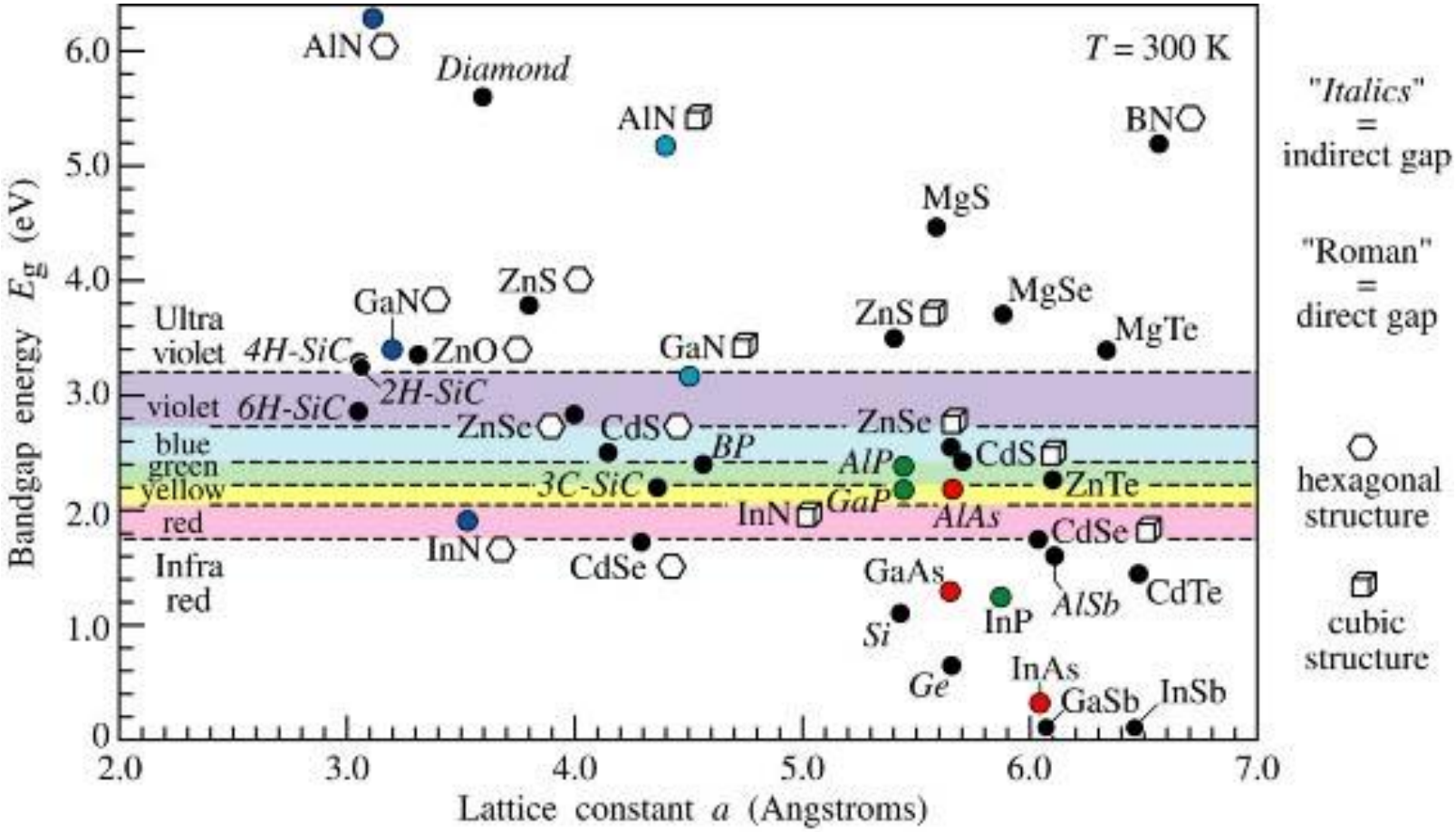


Fig. 11.4. Room-temperature bandgap energy versus lattice constant of common elemental and binary compound semiconductors.

Density of states

Density of states Number of states per unit energy $\rho^{nD}(E)$ depends on the dimension

If our crystal has a finite size the set of k –vectors is finite (though enormous!).
For example: we can assume periodic boundary conditions and then:

Born- von Karman boundary conditions

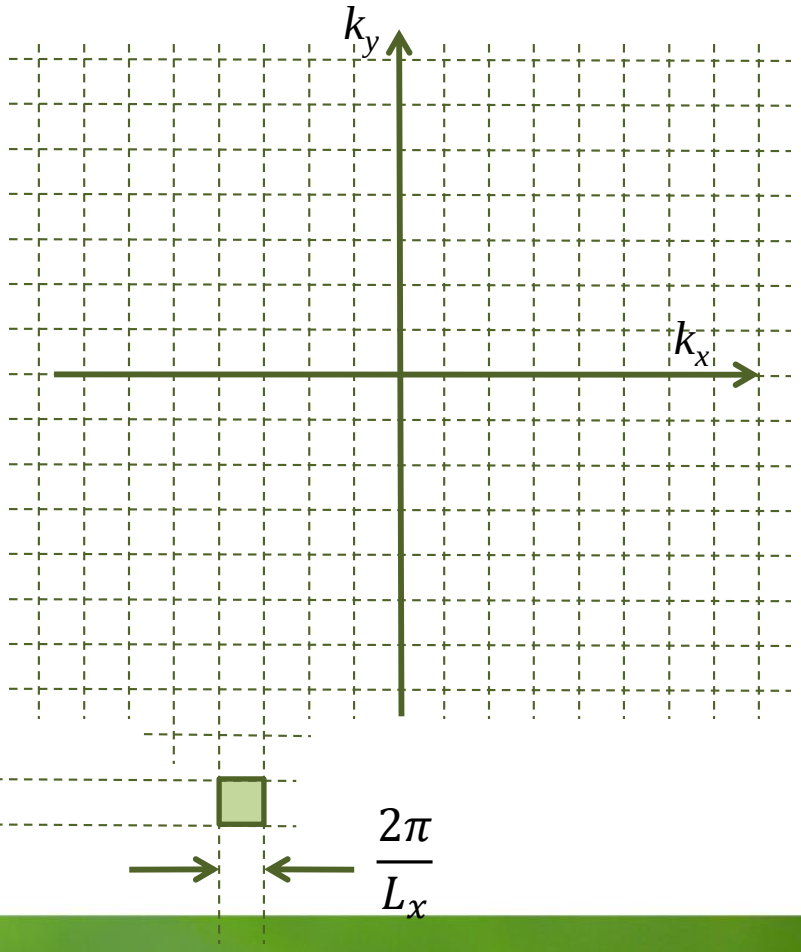
Finite size of the crystal L_x, L_y, L_z

Ψ – the Bloch function

$$\Psi(x + L_x, y, z) = \Psi(x, y + L_y, z) = \Psi(x, y, z + L_z)$$

$$e^{ik_x L_x} = 1$$
$$e^{ik_y L_y} = 1$$
$$e^{ik_z L_z} = 1$$

$$\vec{k}_i = 0, \pm\frac{2\pi}{L_i}, \pm\frac{4\pi}{L_i}, \ldots, \pm\frac{2\pi n_i}{L_i}$$



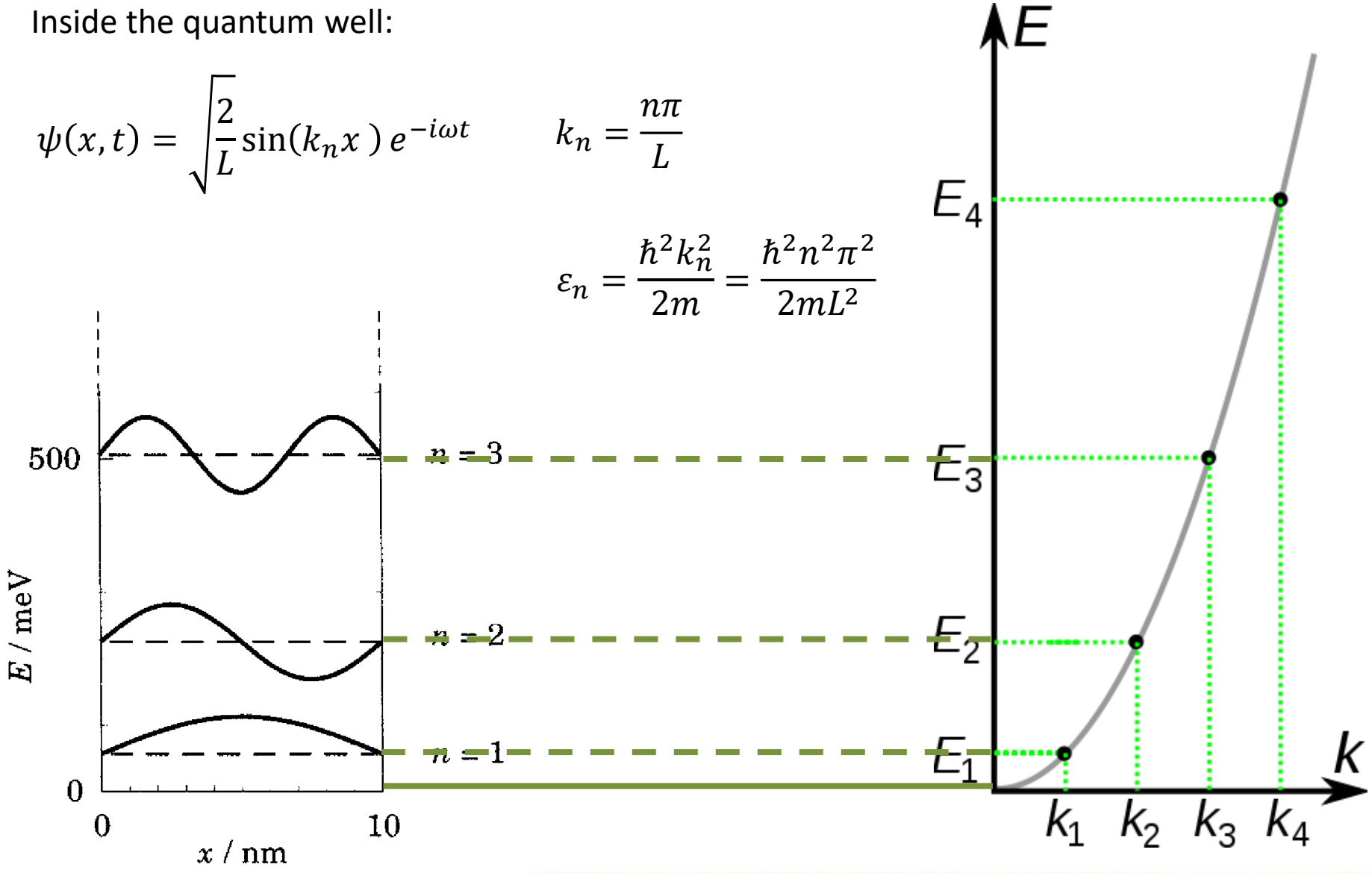
Number of states in the volume V $= \dfrac{2}{\frac{2\pi}{L_x} \times \frac{2\pi}{L_y} \times \frac{2\pi}{L_z}} = \dfrac{2V}{(2\pi)^3}$

Infinite square quantum well

Inside the quantum well:

$$\psi(x,t) = \sqrt{\frac{2}{L}}\sin(k_n x)\, e^{-i\omega t} \qquad k_n = \frac{n\pi}{L}$$

$$\varepsilon_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

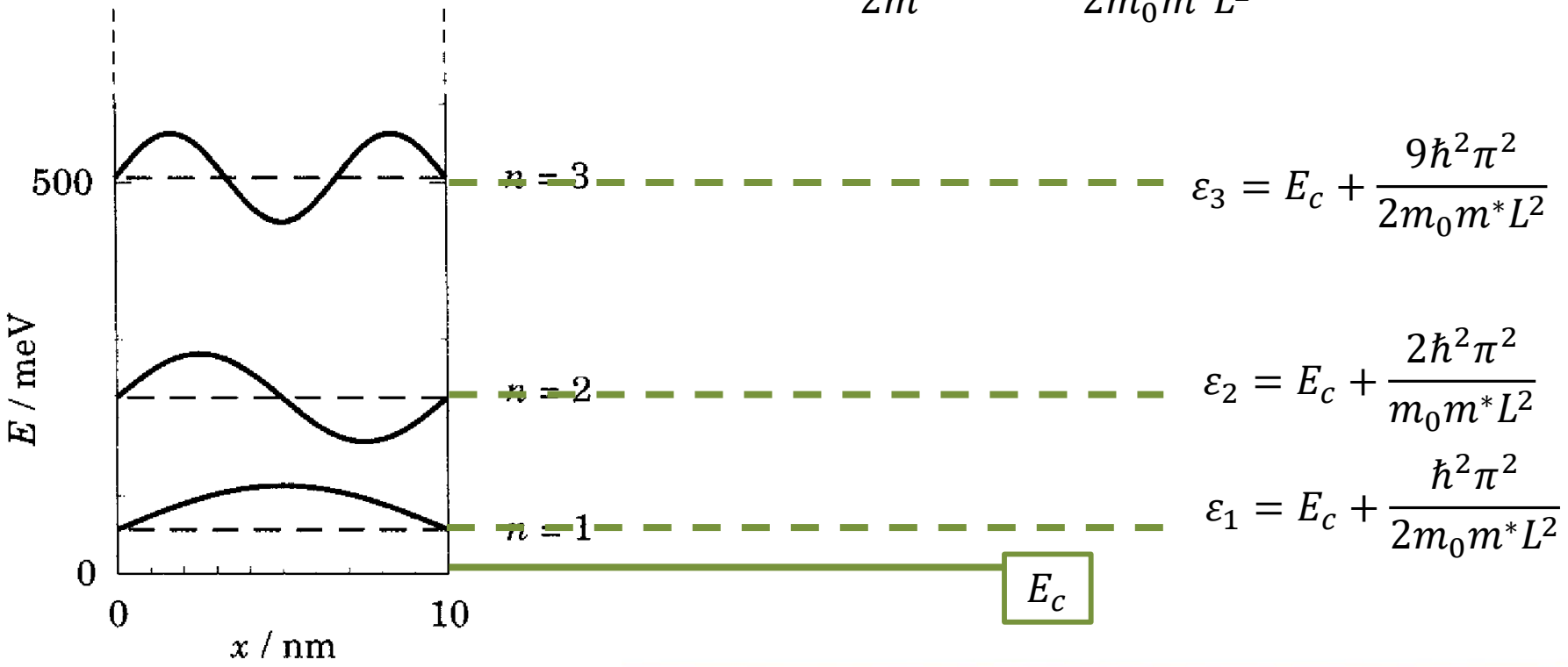


Infinite square quantum well

Inside the quantum well:

$$\psi(x,t) = \sqrt{\frac{2}{L}}\sin(k_n x)\, e^{-i\omega t} \qquad k_n = \frac{n\pi}{L}$$

$$\varepsilon_n = E_c + \frac{\hbar^2 k_n^2}{2m} = E_c + \frac{\hbar^2 n^2 \pi^2}{2m_0 m^* L^2}$$

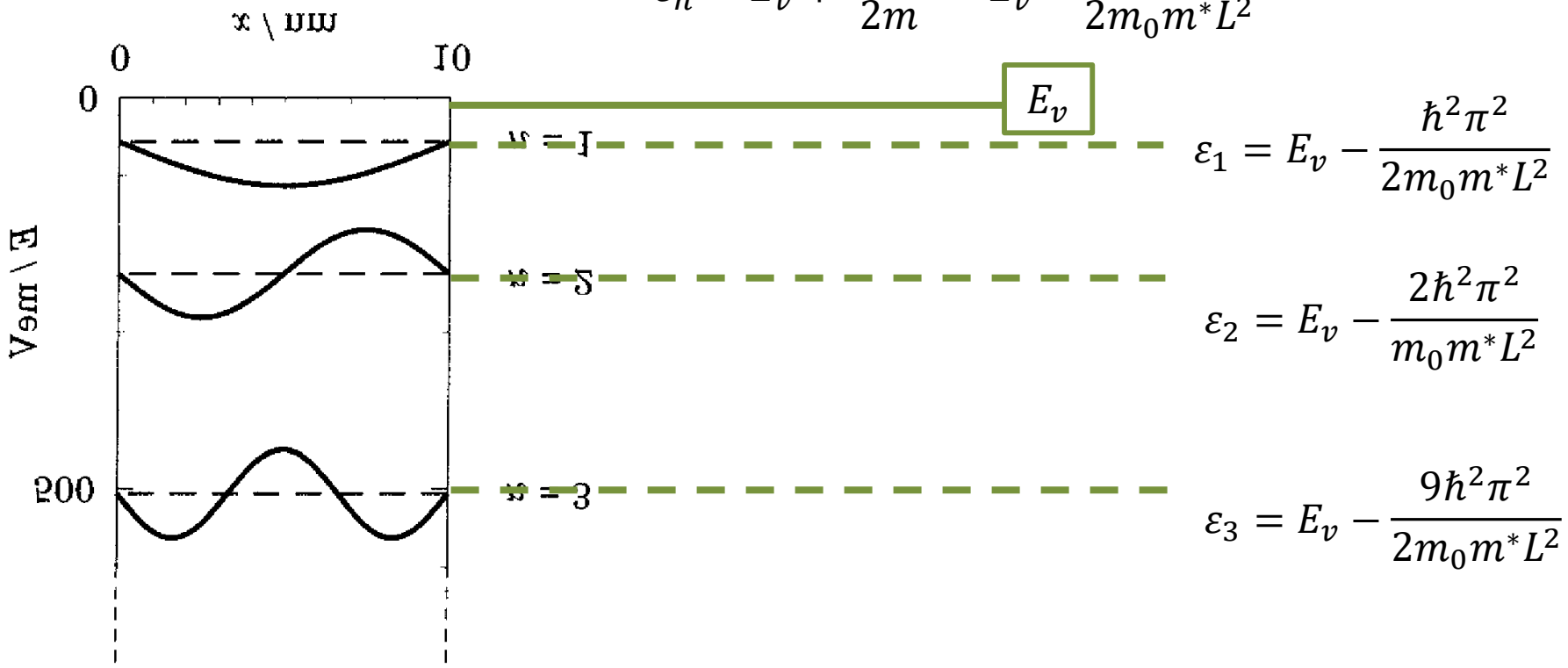


Infinite square quantum well

Inside the quantum well:

$$\psi(x,t) = \sqrt{\frac{2}{L}}\sin(k_n x)\, e^{-i\omega t} \qquad k_n = \frac{n\pi}{L}$$

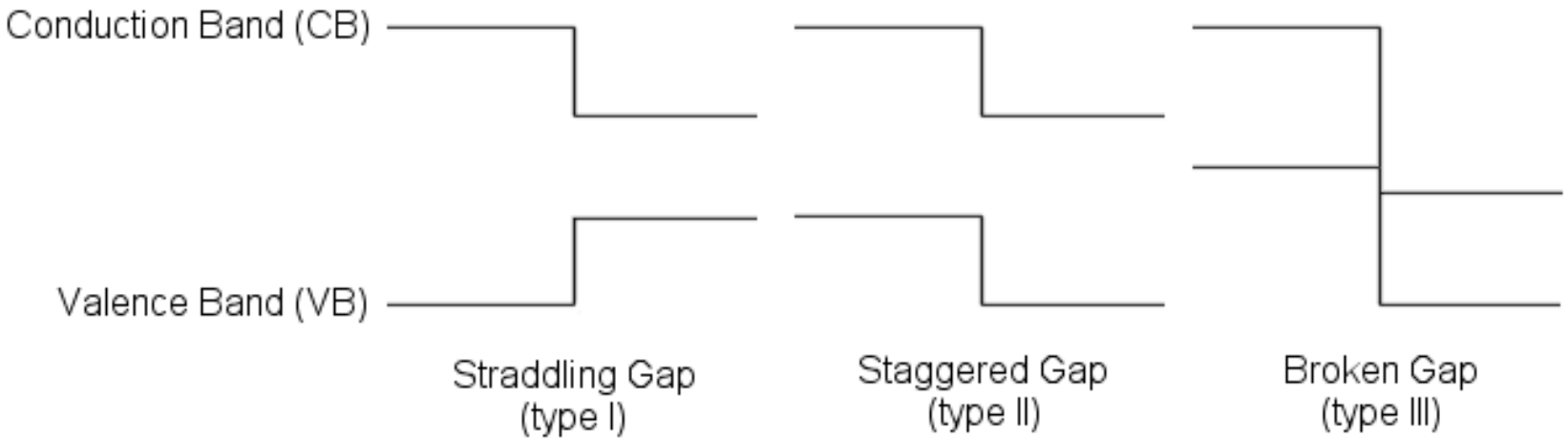
$$\varepsilon_n = E_v + \frac{\hbar^2 k_n^2}{2m} = E_v - \frac{\hbar^2 n^2 \pi^2}{2m_0 m^* L^2}$$



Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress



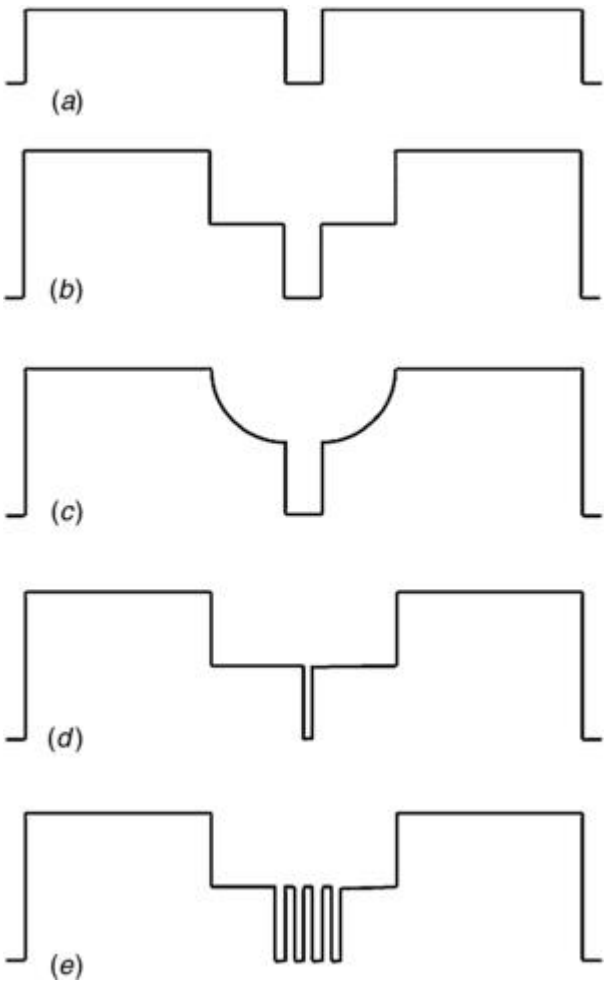


Figure 5. Schematic diagrams depicting the evolution of the conduction band structure in the transverse direction: (*a*) double heterostructure, (*b*) separate confinement heterostructure (SCH), (*c*) graded-index separate confinement heterostructure (GRIN-SCH), (*d*) single quantum well heterostructure (QWH), and (*e*) multiple quantum well (MQW).

The development of the semiconductor laser diode after the first demonstration in 1962 J J Coleman Semicond. Sci. Technol. 27 (2012) 090207

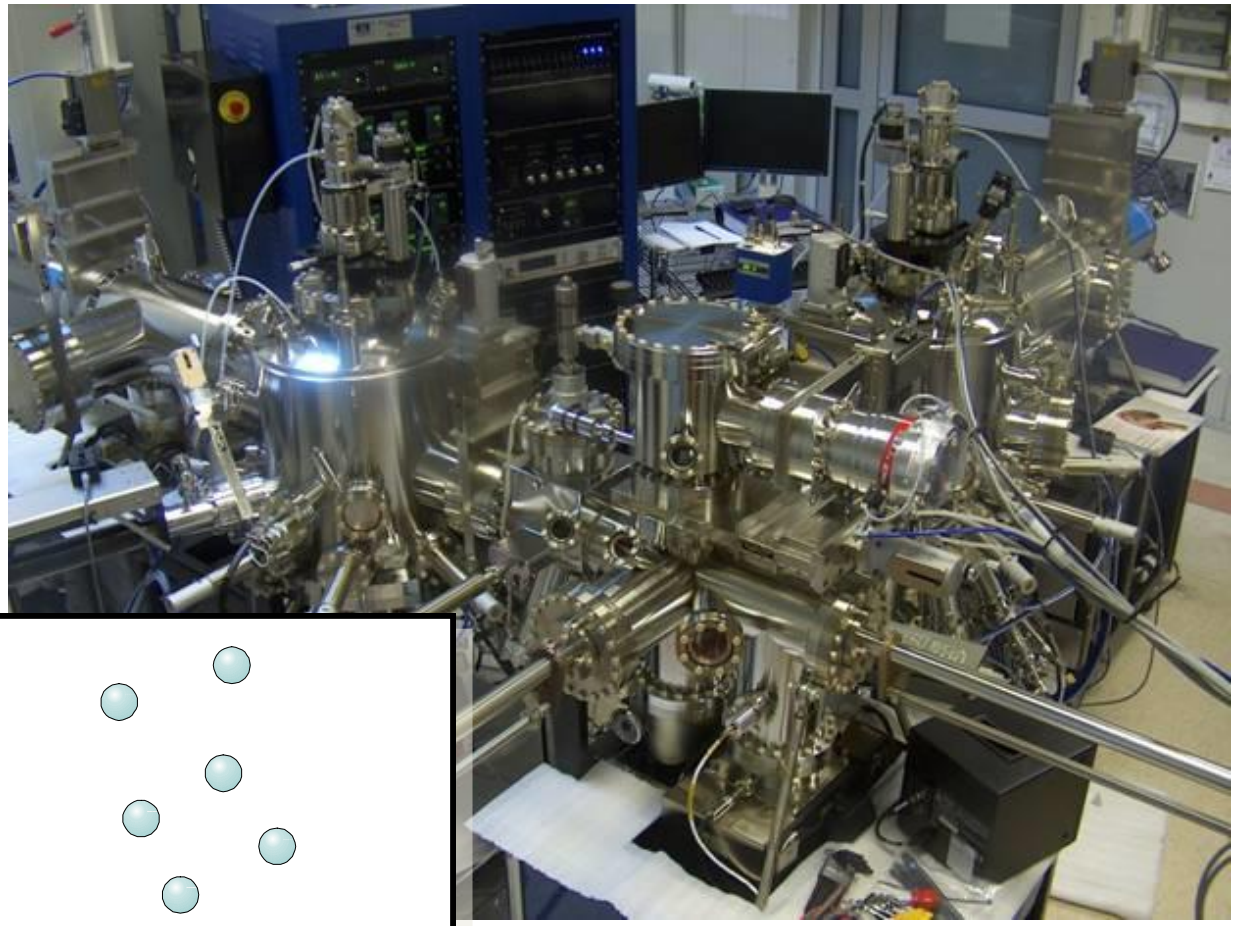
Jak się robi heterostruktury?

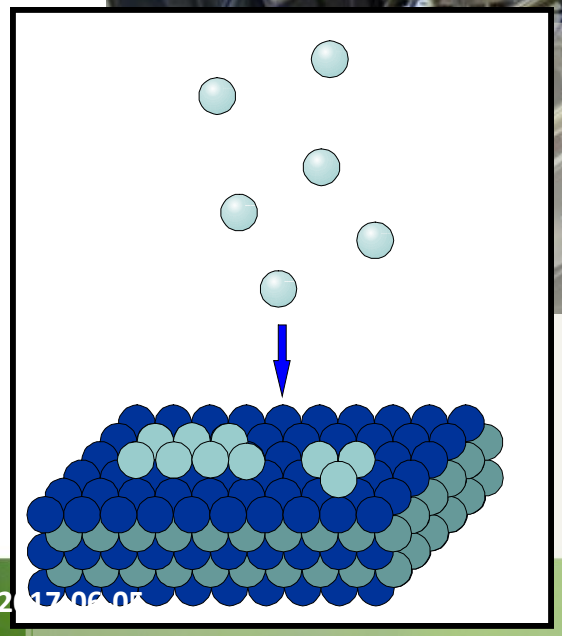
Liquid-phase (LPE)
wzrost z fazy ciekłej na podłożu w temperaturach niższych od temperatury topnienia hodowanego materiału. Półprzewodnik jest rozpuszczony w cieczy innego materiału, wzrost w warunkach bliskich równowagi roztworu i depozycji; prędkości wzrostu 0.1 to 1 μm/min.

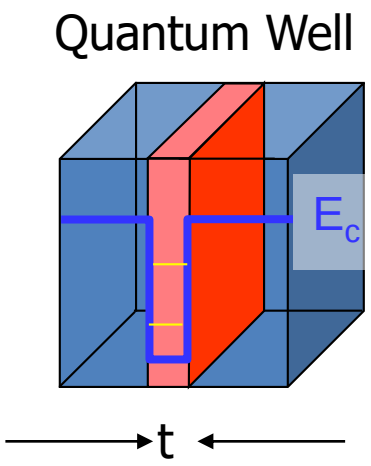
Vapor-phase (VPE, CVD)
wzrost z fazy gazowej dzięki reakcjom chemicznym prekursorów na powierzchni, często dzielony ze względu na źródłowe gazy na wodorkową VPE i metalorganiczną VPE (MOCVD); prędkości wzrostu >10 -20 nm/min.

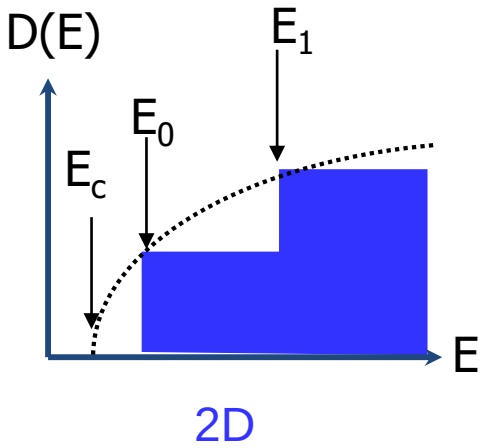
Molecular-beam (MBE)
Materiał źródłowy podgrzewany w komórkach produkuje strumień cząsteczek. W wysokiej próżni (10^{-8} Pa) cząsteczki docierają do podłoża i osadzają się na nim; prędkości wzrostu < 1 monowarstwa/s (1 μm/h).

Jak się robi heterostruktury?









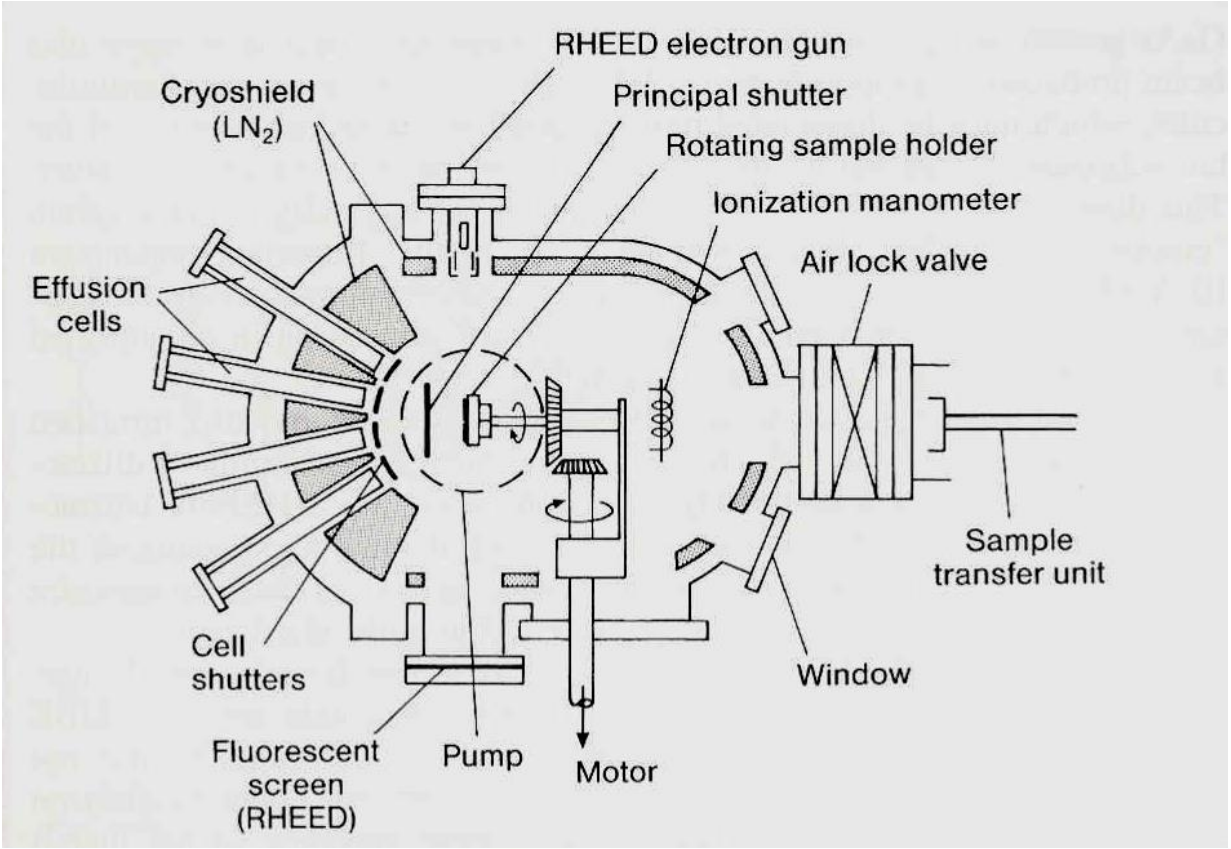
MBE→ Osadzanie z atomową precyzją warstw o różnym składzie lub domieszkowaniu

Hubert J. Krenner

Jak się robi heterostruktury?

Wzrost warstw **MBE** jest monitorowany przez Reflection High Energy Electron Diffraction (REED). Komputer steruje przesłonami (shutterami) na froncie podgrzewanych komórek efuzyjnych, co pozwala na precyzyjną kontrolę wzrostu do poziomu pojedynczej warstwy atomowej.

Wzrost warstw z jamami kwantowymi (quantum wells), kropek kwantowych (quantum dots) – struktury LD, LED.



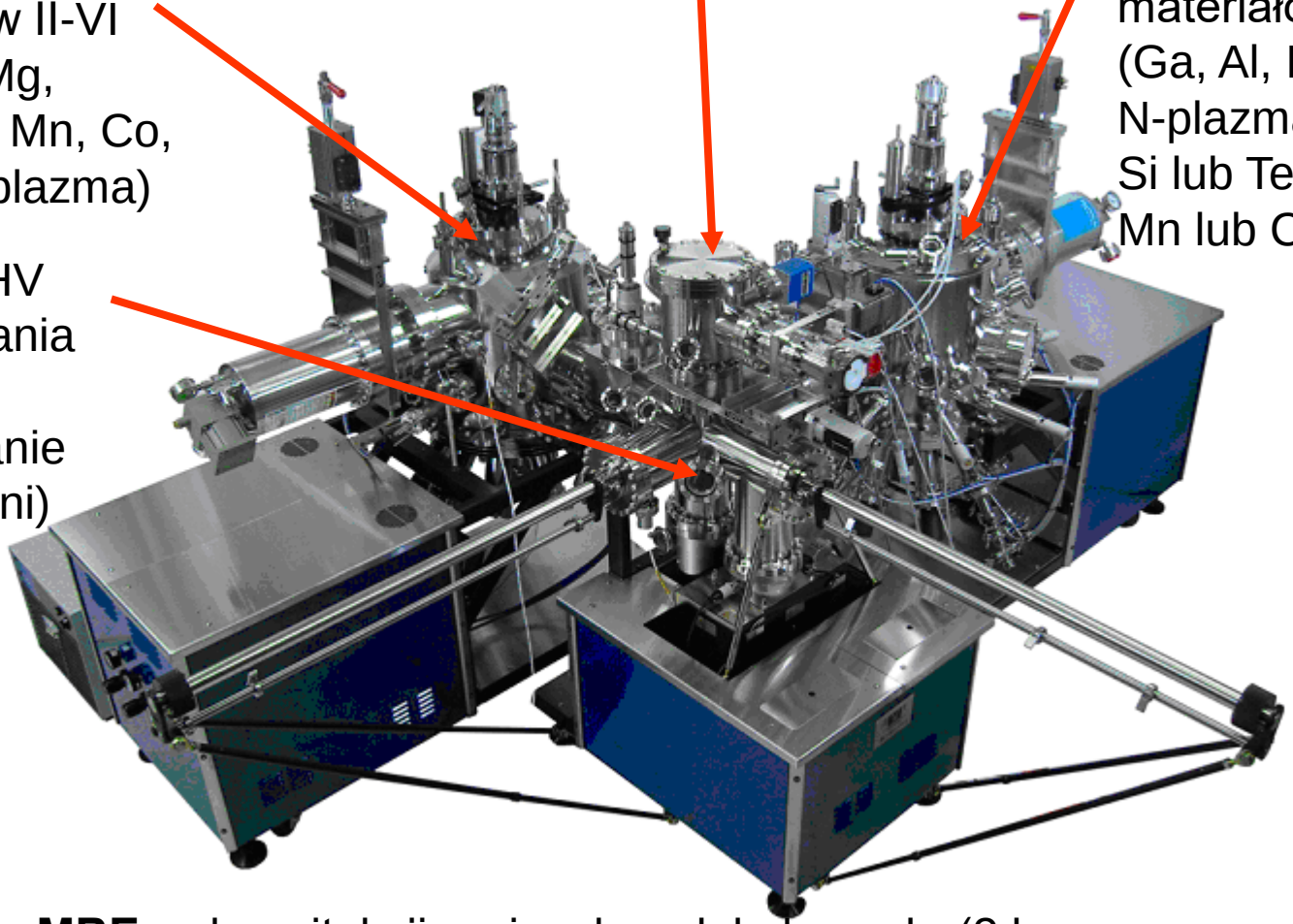
Jak się robi heterostruktury?

komora UHV wzrostu materiałów II-VI (Zn, Cd, Mg, S, Se, Te, Mn, Co, $ZnCl_2$, N-plazma)

komora załadunkowa

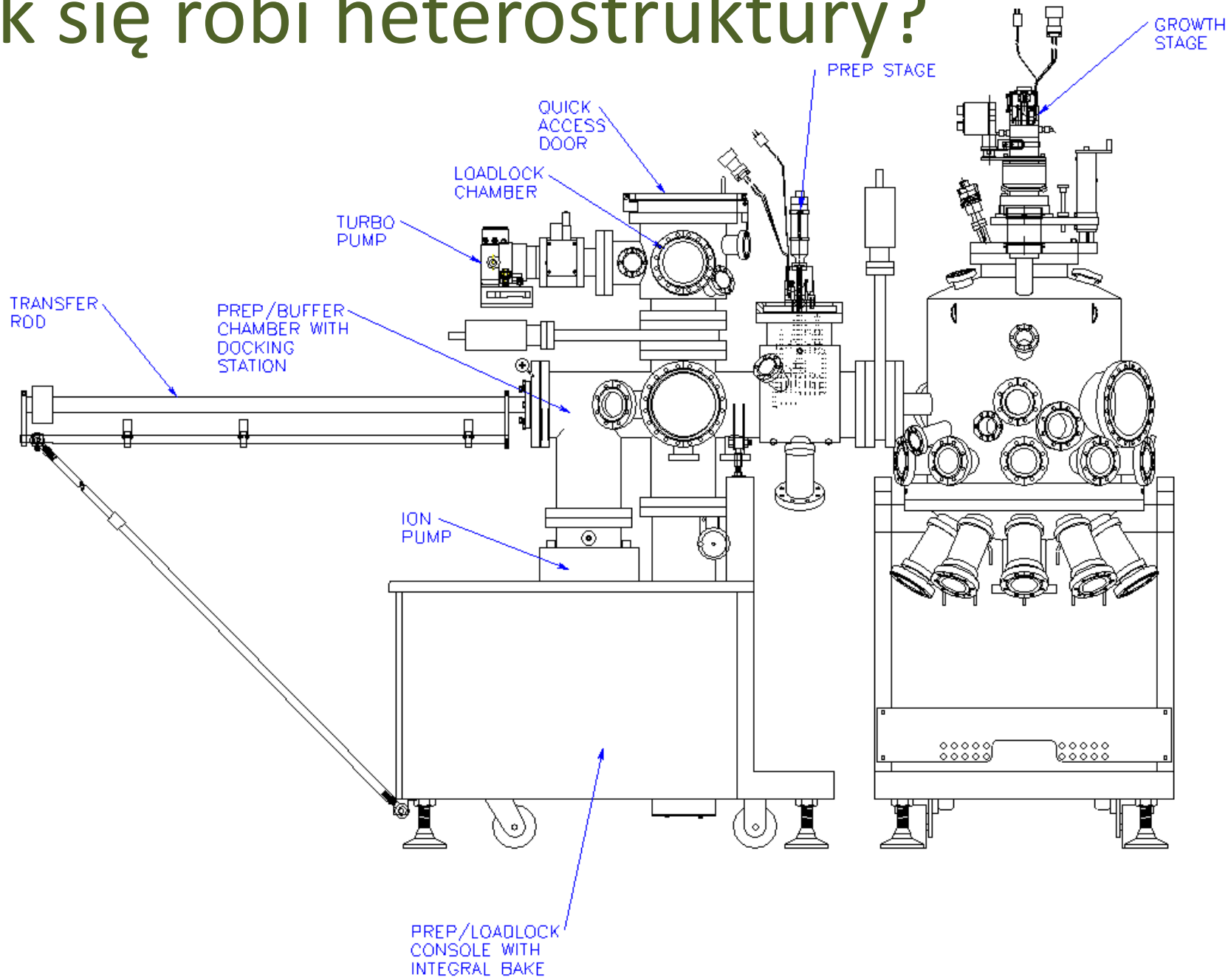
komora UHV wzrostu materiałów III-V (Ga, Al, In, As, Sb, N-plazma, Si lub Te, Be lub Zn, Mn lub Cr lub Co)

komora UHV przygotowania podłoży (odgazowanie powierzchni)



Urządzenie MBE - do epitaksji z wiązek molekularnych (2 komory wzrostu) producent SVTA (USA). Zakup przez Wydział Fizyki w r. 2010, program CePT

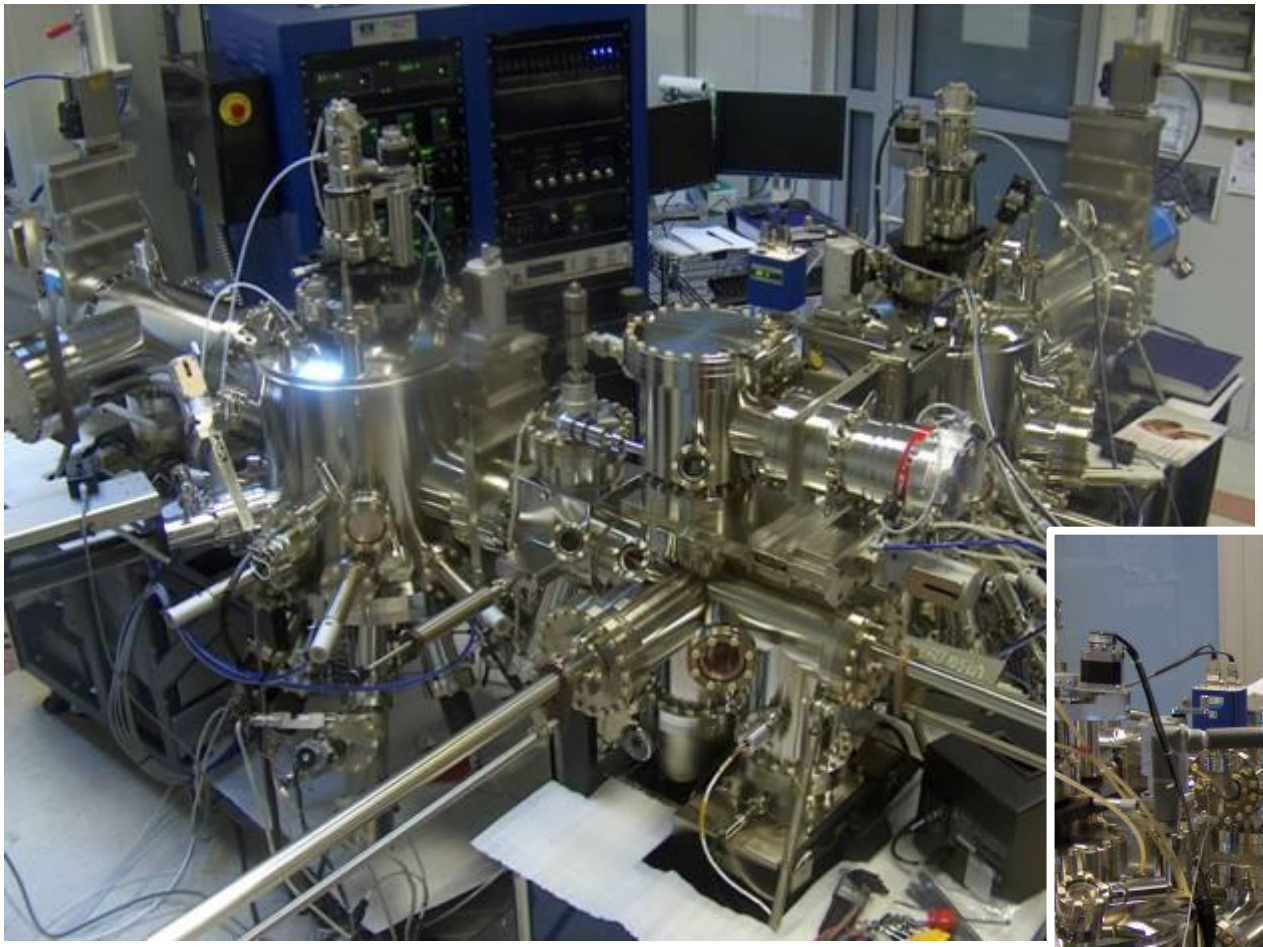
Jak się robi heterostruktury?



Jak się robi heterostruktury?

MBE na Wydziale Fizyki UW

Jak się robi heterostruktury?



MBE na Wydziale Fizyki UW

Jak się robi heterostruktury?

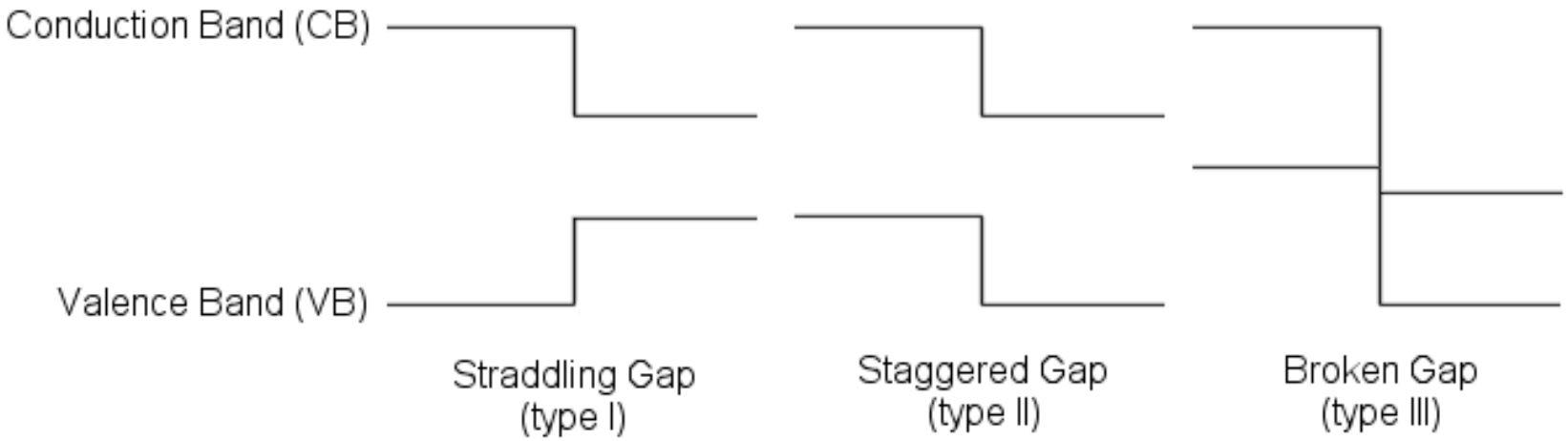
Reaktor Metal-Organic Chemical Vapour Epitaxy (MOCVD) w Zakładzie Fizyki Ciała Stałego

Heterostruktury GaInSb, AlGaInAs and AlGaN.

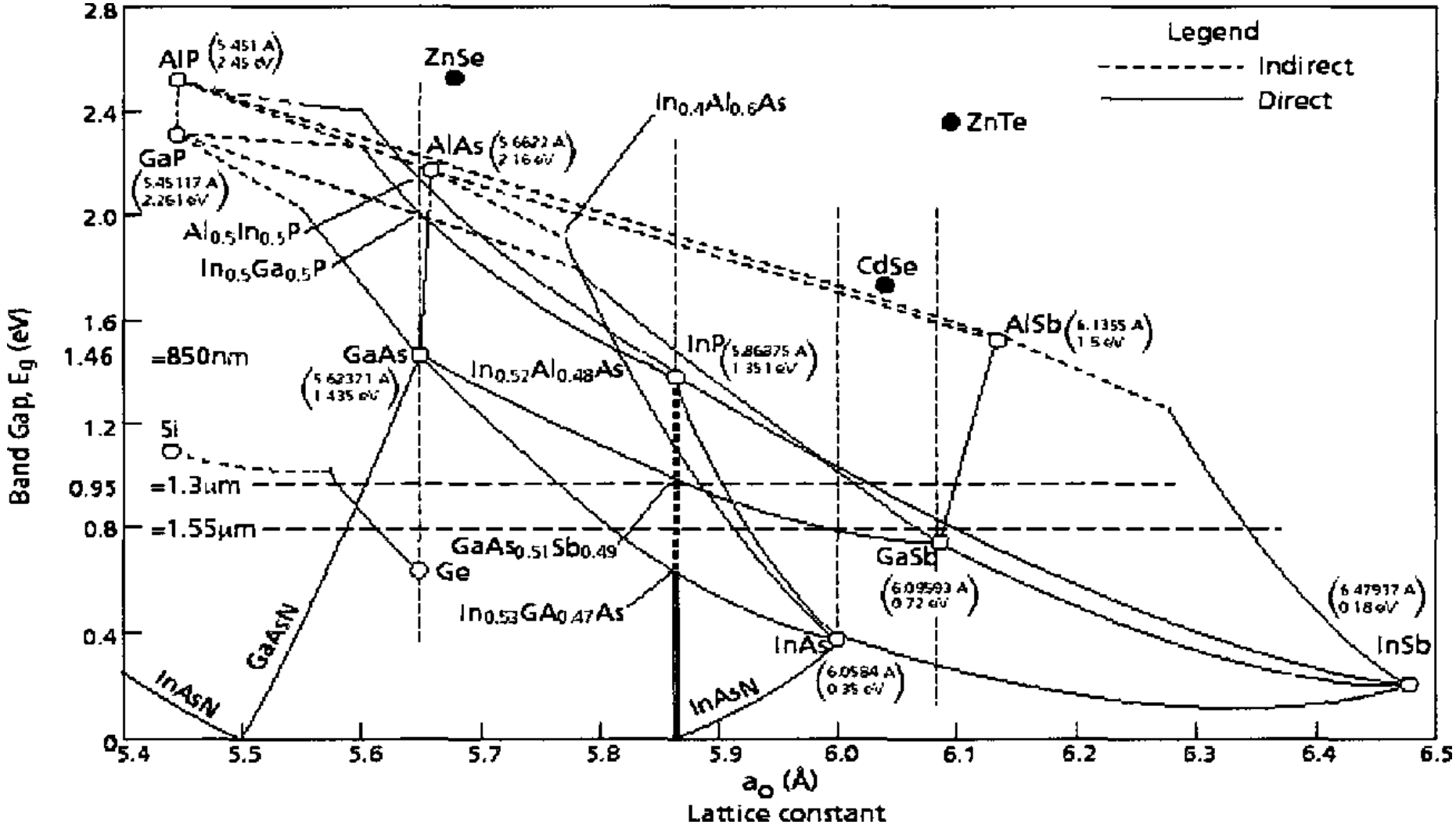
Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress



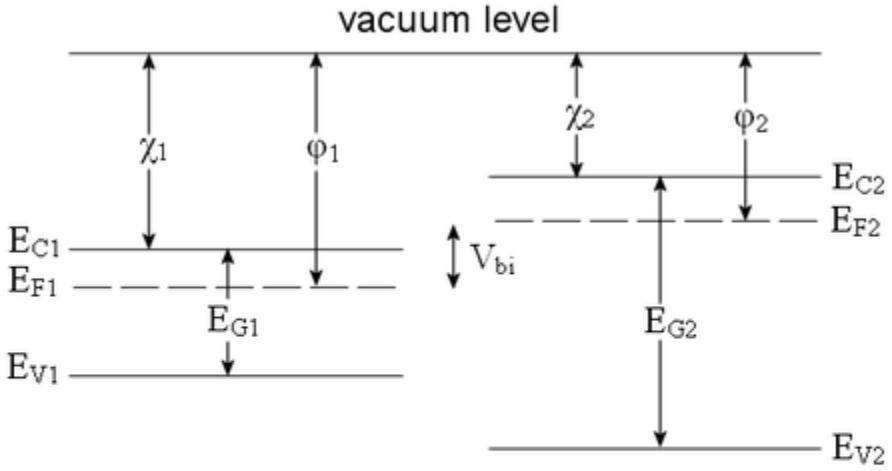
Semiconductor heterostructures



Investigation of high antimony-content gallium arsenic nitride-gallium arsenic antimonide heterostructures for long wavelength application

Bandgap engineering

Valence band offset (Anderson's rule)

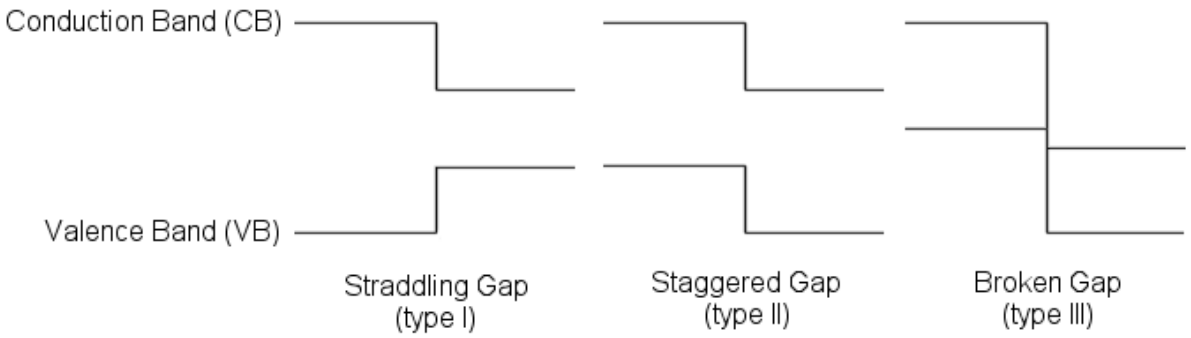


φ = work function
χ = electron affinity (powinowactwo)
E_G = band gap
E_C = conduction band
E_V = valence band

$$\Delta E_C = \chi_1 - \chi_2 = \Delta\chi$$
$$\Delta E_G = E_{G2} - E_{G1}$$

Valence band offset: $\Delta E_V = \Delta E_G - \Delta\chi$

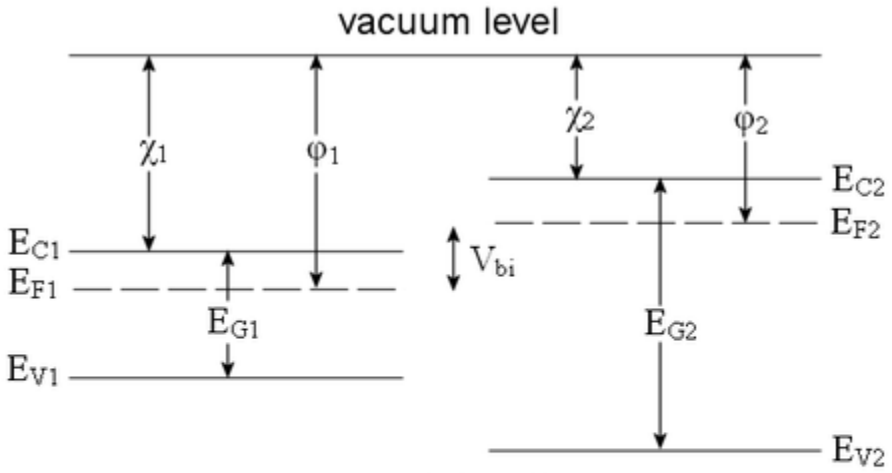
$$\Delta E_G = \Delta E_C + \Delta E_V$$



http://en.wikipedia.org/wiki/Heterojunction

Bandgap engineering

Valence band offset (Anderson's rule)



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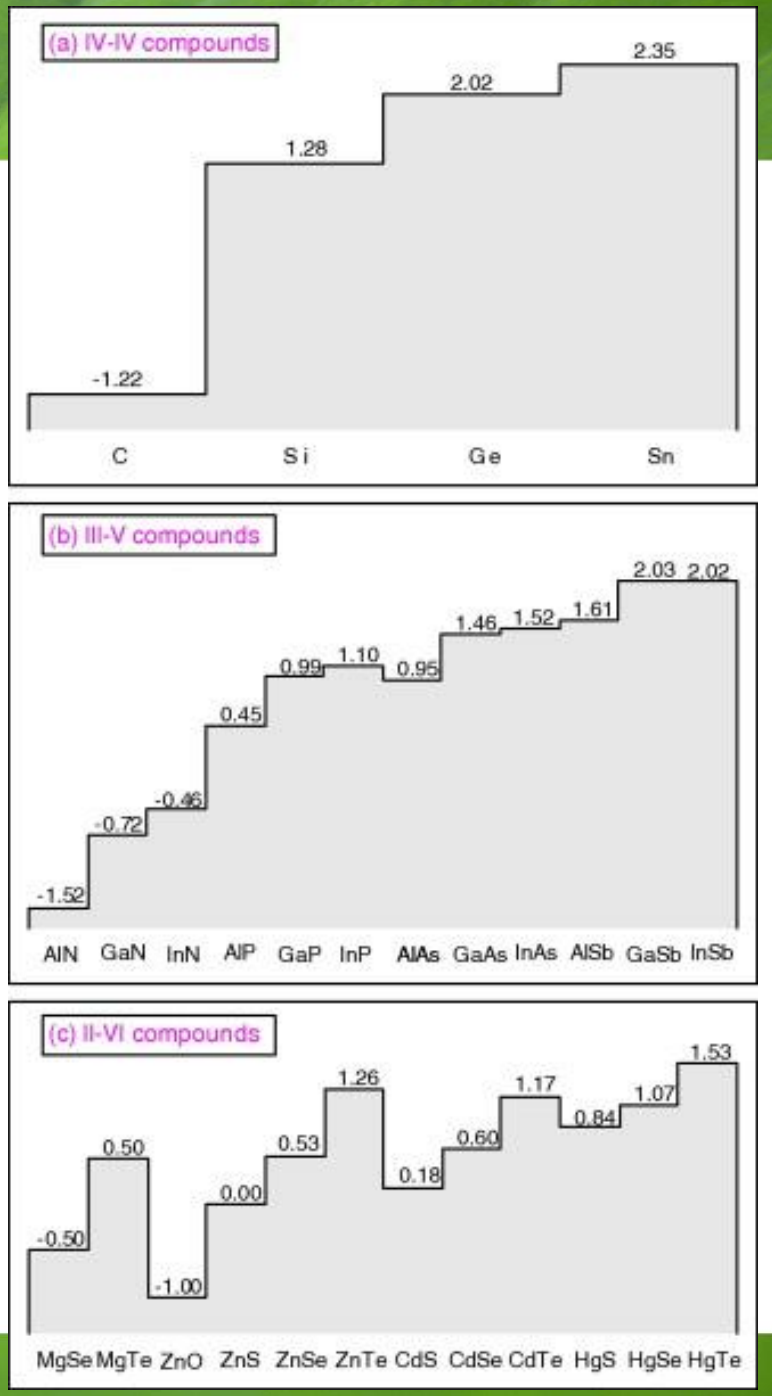
$$\Delta E_G = \Delta E_C + \Delta E_V$$



Su-Huai Wei, Computational Materials Science, 30, 337–348 (2004)

Bandgap enginee

Valence band offset

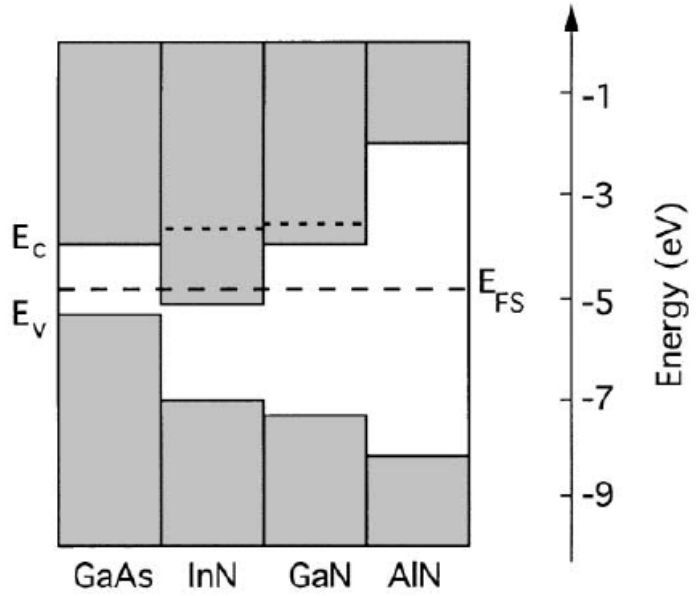


Fig. 4. Band offsets for group III-Nitrides. The dashed lines represent the Fermi energy for the maximum achievable free electron concentration in GaN and InN.

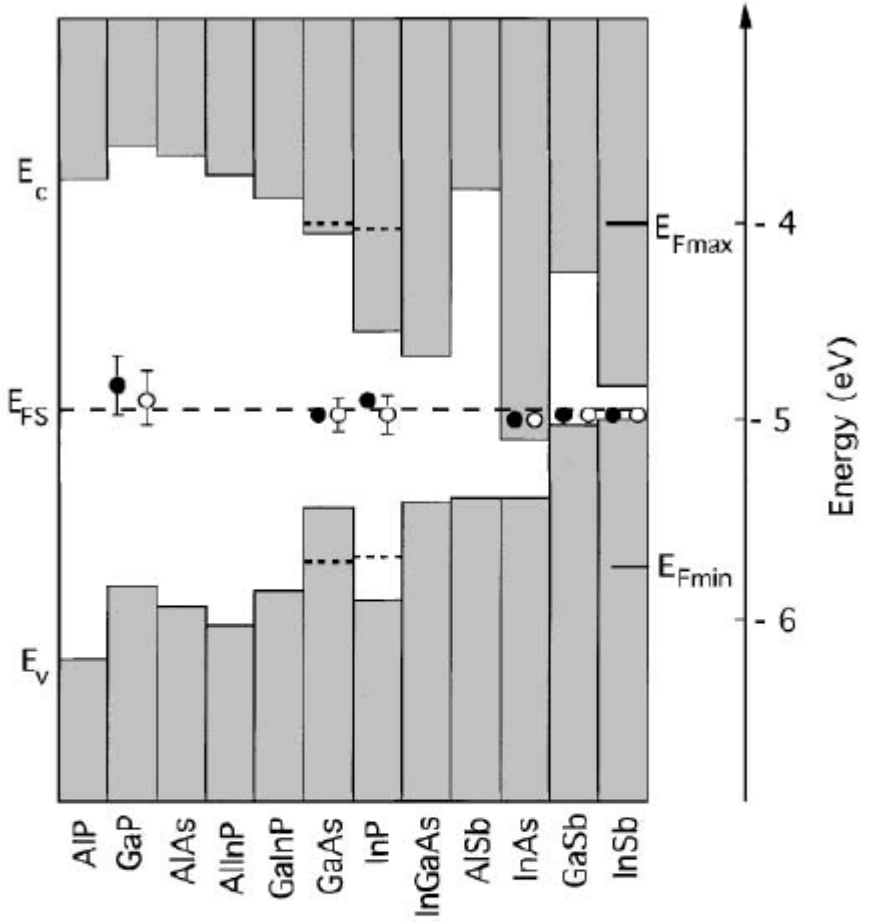


Fig. 1. Band offsets and the Fermi level stabilization energy (E_{FS}) in III–V compounds. The energy is measured relative to the vacuum level. The filled circles represent stabilized Fermi energies in heavily damaged materials, exposed to high energy radiation. The open circles correspond to the location of the Fermi energy on pinned semiconductor surfaces and at metal/semiconductor interfaces. The dashed lines show the location of the Fermi energy for a maximum equilibrium n- and p-type doping in GaAs and InP.

Walukiewicz Physica B 302–303 (2001) 123–134

Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress

Vegard's law:
the **empirical heuristic** that the lattice parameter of a solid solution of two constituents is approximately equal to a rule of mixtures of the two constituents' (A and B) lattice parameters at the same temperature:

$$a = a_A(1 - x) + a_B x$$

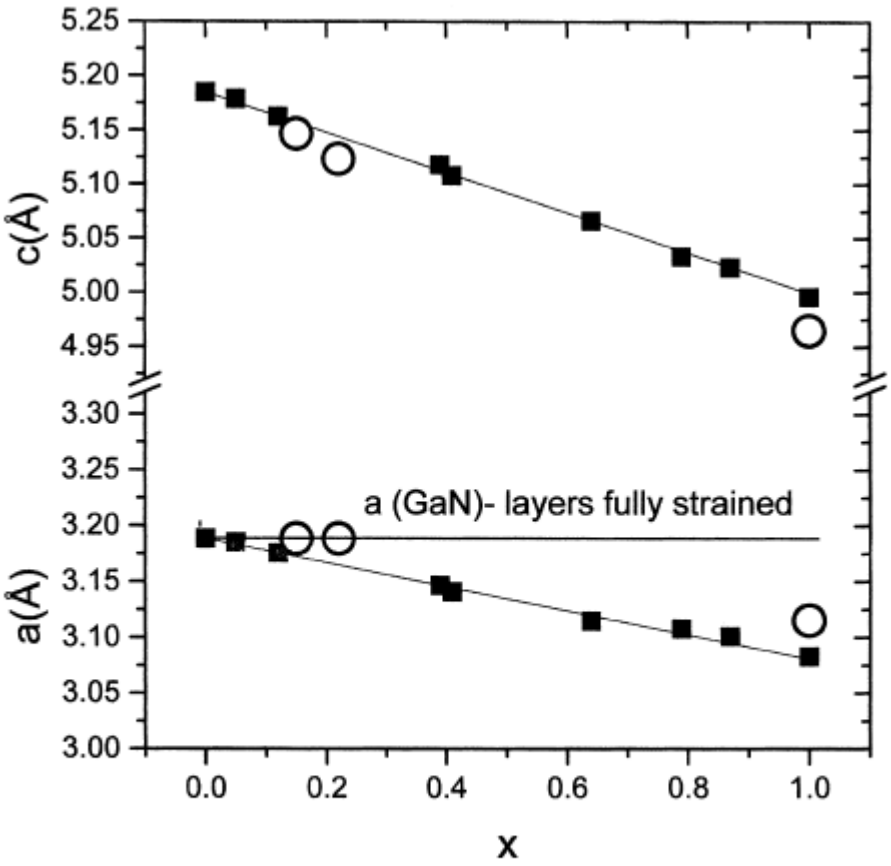


Fig. 5. Lattice parameters of 0.15–0.20 μm $Al_xGa_{1-x}N$ layers. Lines– Vegard's law between values for the AlN and GaN single crystals, Solid squares– layers on SiC, Open circles– layers on bulk GaN.

Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
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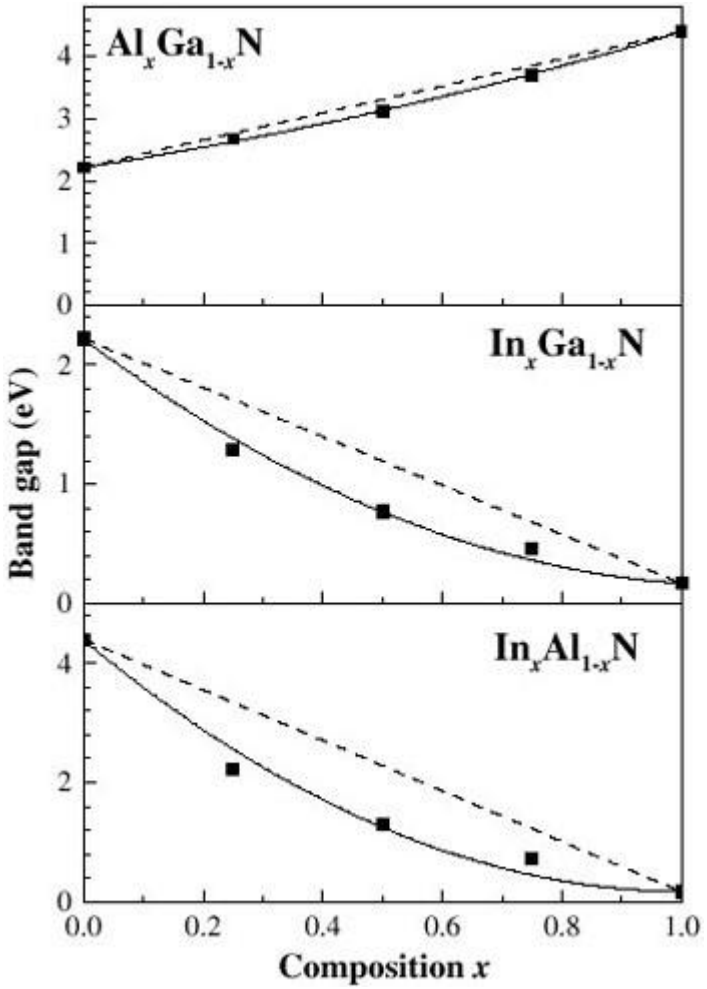
Vegard's law:
Relationship to band gaps of „binary compound":

$$E = E_A(1-x) + E_B x - bx(1-x)$$

b – so-called „bowing" (curvature) of the energy gap



Z Dridi et al. Semicond. Sci. Technol. **18** No 9 (September 2003) 850-856

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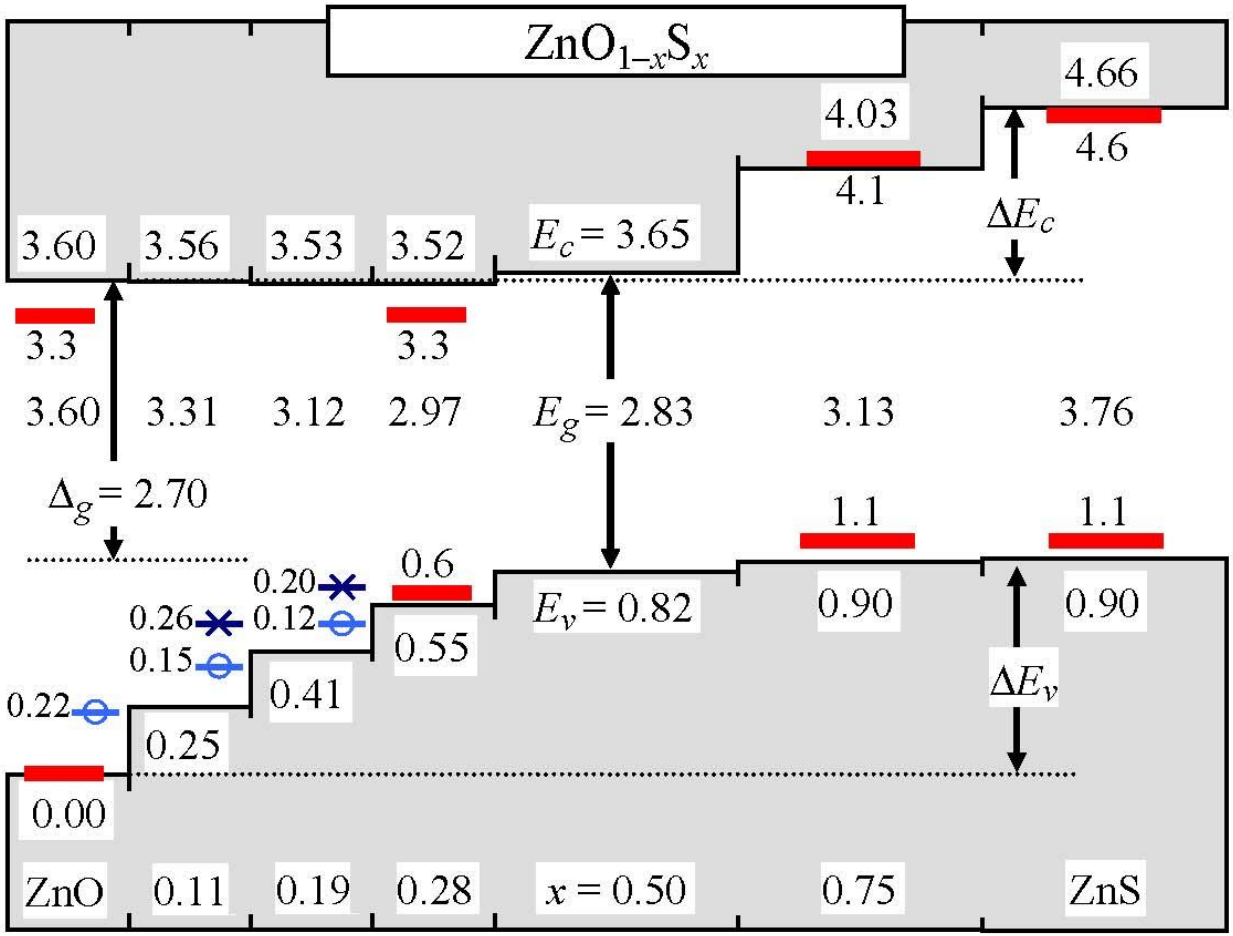
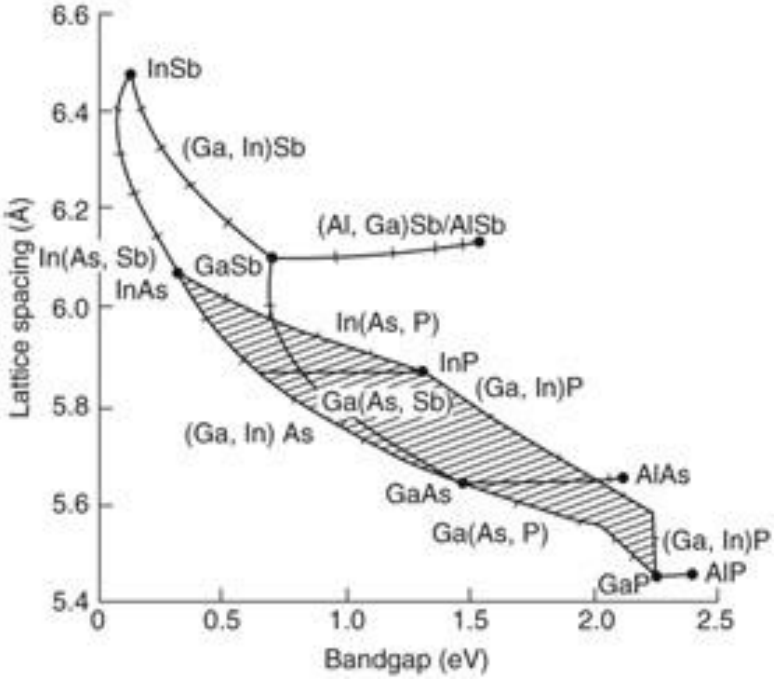
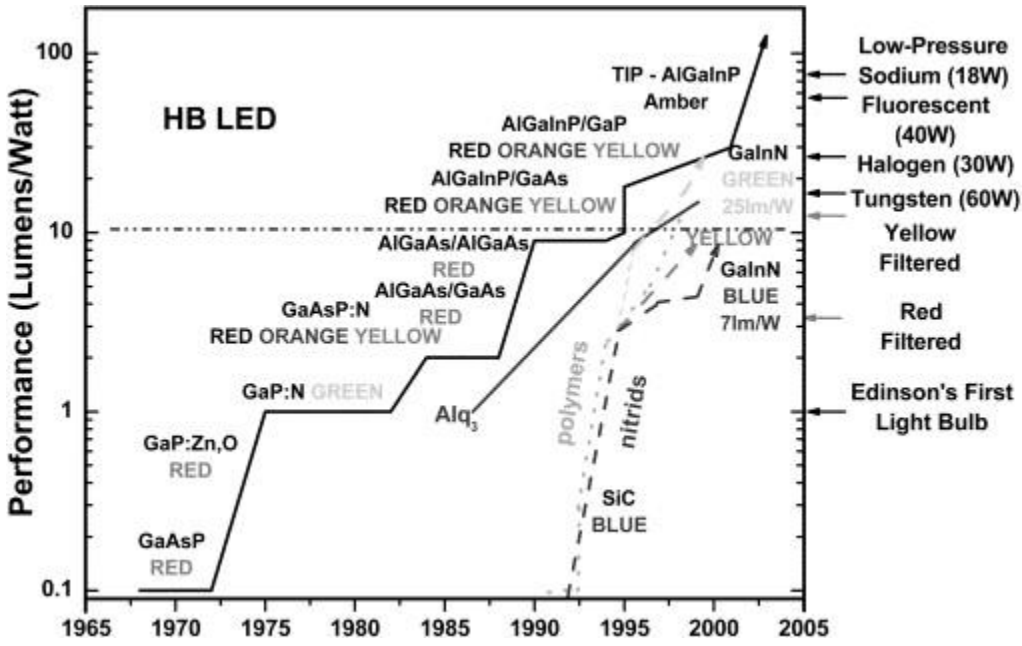


Semiconductor heterostructures

Quaternary compounds

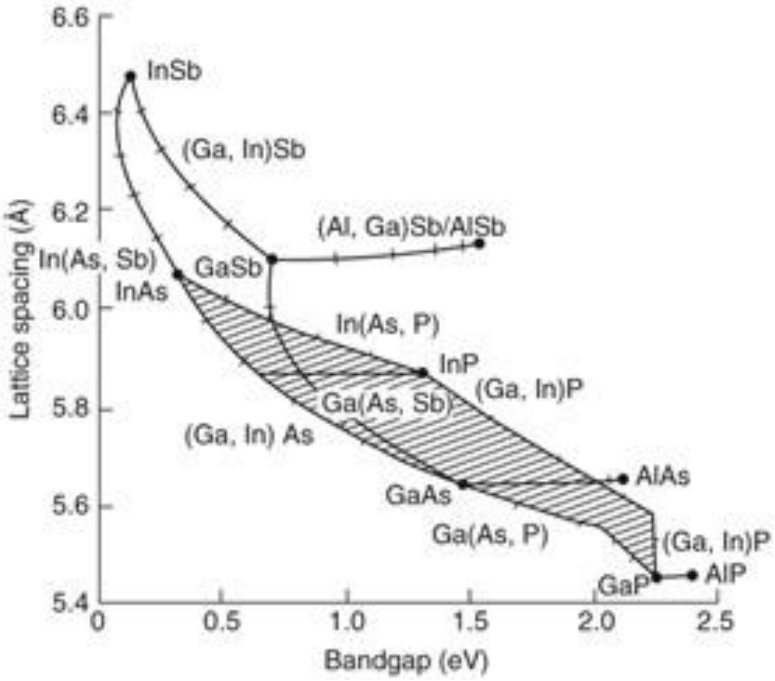




http://beta.globalspec.com/reference/45139/203279/chapter-iii-optical-properties

Thin Solid Films 433 (2003) 22–26

Semiconductor heterostructures



http://beta.globalspec.com/reference/45139/203279/chapter-iii-optical-properties

Quinternary compounds

50 nm p^+ -GaSb contact	Be: $1x10^{19}$ cm^{-3}
20 nm *p*-AlSb/GaSb grading	Be: $1x10^{18}$ cm^{-3}
2 µm *p*-$Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92}$ cladding	Be: $1x10^{18}$ cm^{-3}
1 µm *p*-$Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92}$ cladding	Be: $1x10^{17}$ cm^{-3}
300 nm $Al_{0.3}Ga_{0.2}In_{0.5}As_{0.44}Sb_{0.56}$ waveguide	
10 nm $Ga_{0.28}In_{0.72}As_{0.44}Sb_{0.56}$ QW	x 5
10 nm $Al_{0.3}Ga_{0.2}In_{0.5}As_{0.44}Sb_{0.56}$ barrier	
290 nm $Al_{0.3}Ga_{0.2}In_{0.5}As_{0.44}Sb_{0.56}$ waveguide	
1 µm *n*-$Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92}$ cladding	Te: $1x10^{17}$ cm^{-3}
2 µm *n*-$Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92}$ cladding	Te: $2x10^{17}$ cm^{-3}
20 nm *n*-AlSb/GaSb grading	Te: $1x10^{18}$ cm^{-3}
n-GaSb buffer	Te: $5x10^{17}$ cm^{-3}
n-GaSb substrate	Te: $5x10^{17}$ cm^{-3}

Quinternary barriers push room-temperature operation of GaSb-based type-I lasers further into mid-infrared

Comments on the conduction band

Depending on the semiconductor the bottom of the conduction band may be constructd from a differnent valleys – the same heterostructure may be a well in a one band (eg. Γ) and a barrier in another (eg. X).

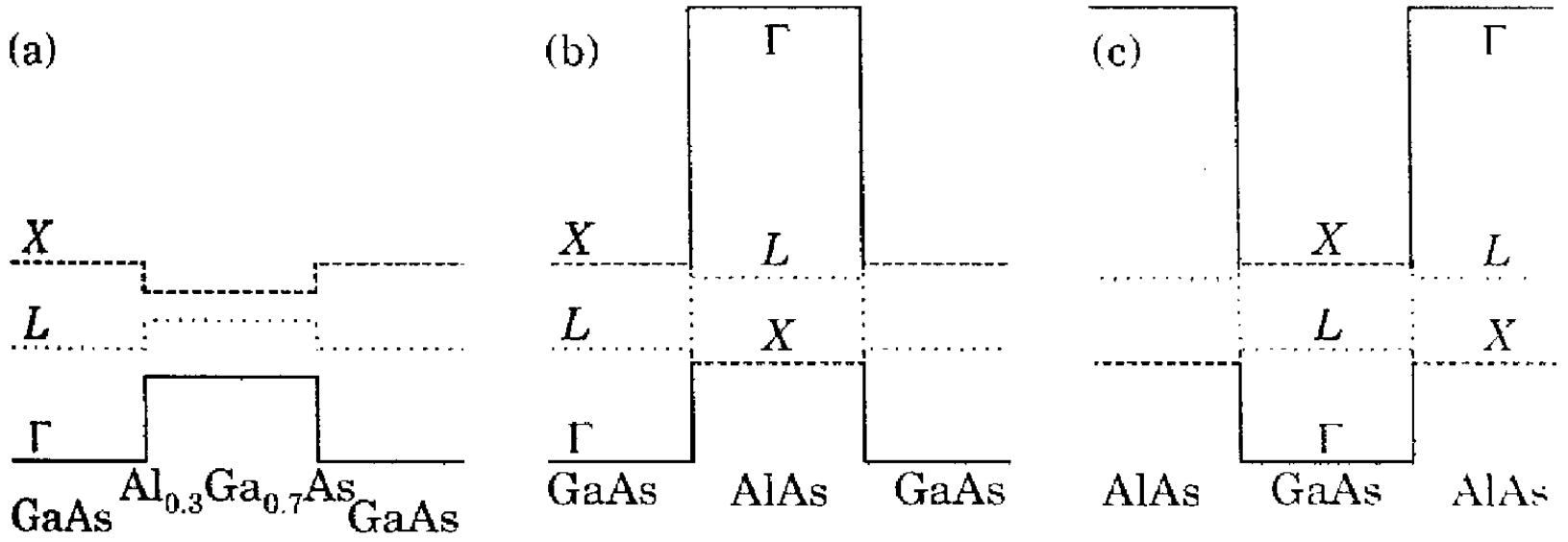


FIGURE 3.8. Barriers and wells in GaAs–$Al_xGa_{1-x}As$, showing the three lowest conduction bands. (a) Barrier of $Al_{0.3}Ga_{0.7}As$, where Γ is the lowest minimum throughout. (b) Barrier of AlAs, where X is the lowest minimum in the barrier. (c) Well of GaAs surrounded by AlAs.

Comments on the conduction band

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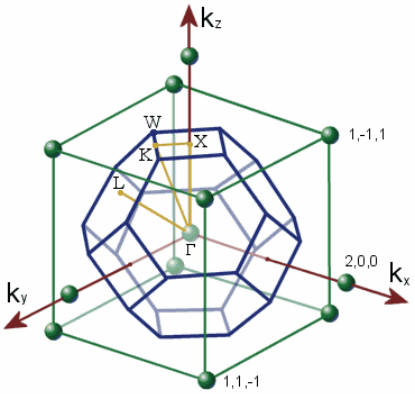
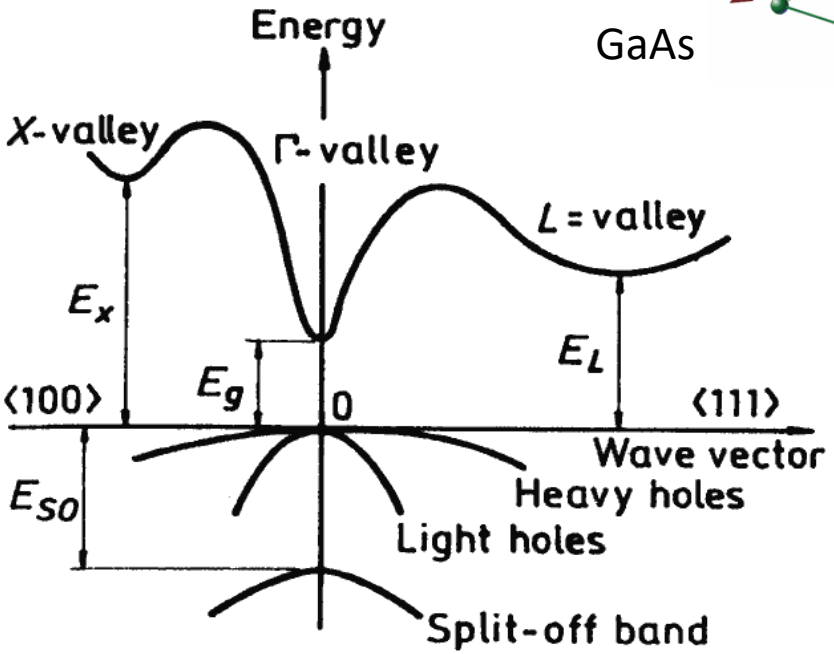
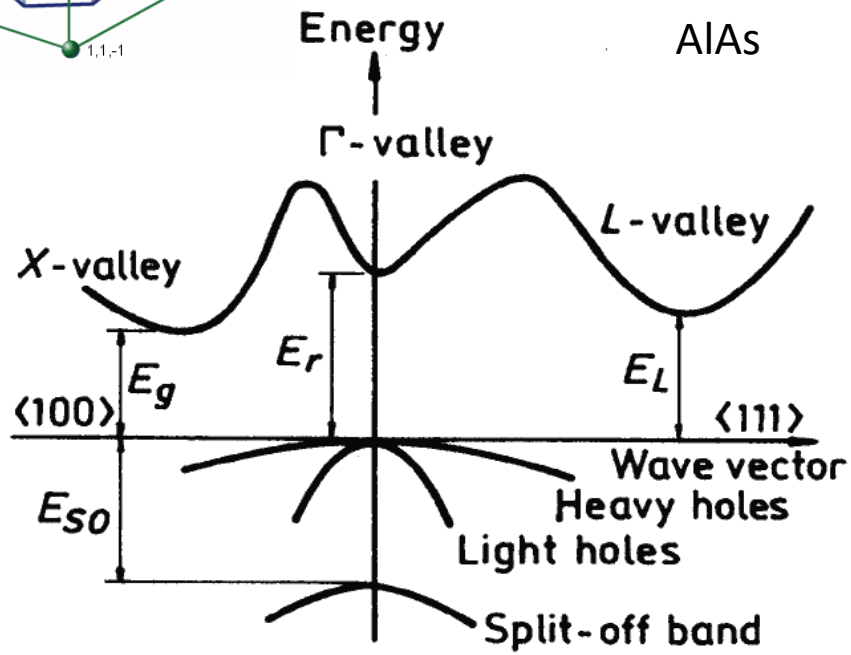


GaAs

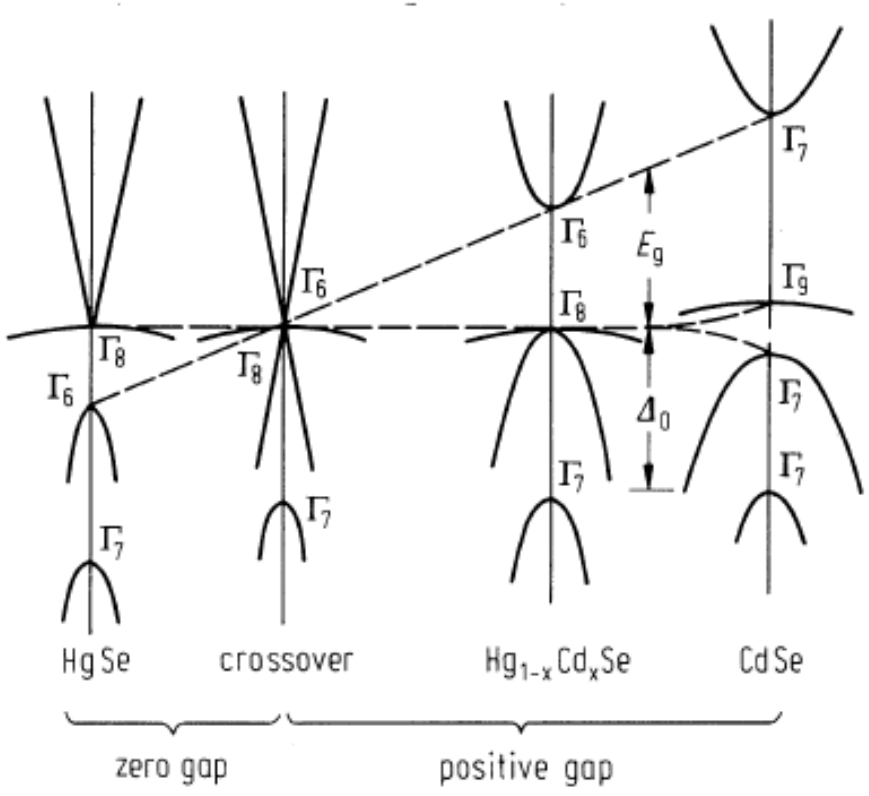


AlAs



Heterostruktury półprzewodnikowe

HgSe. Schematic band structure of the Hg–Cd–Se system near the Γ point

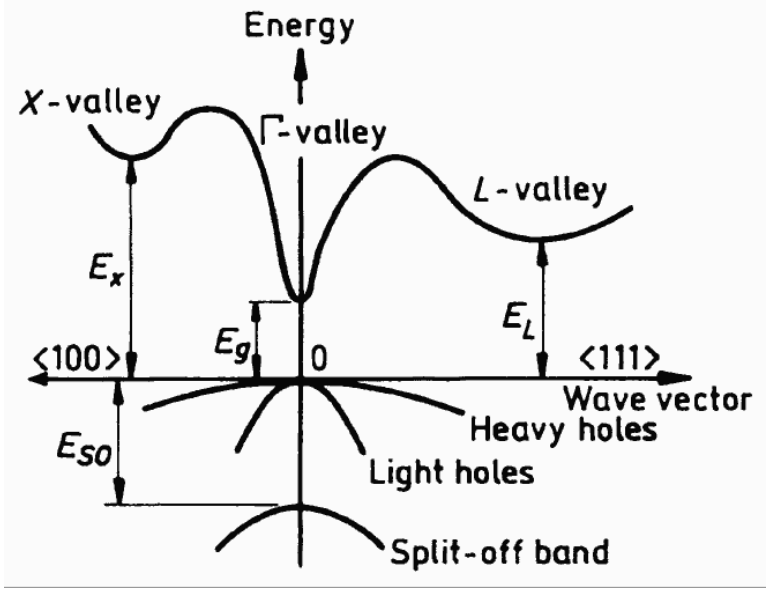


http://www.springermaterials.com/docs/pdf/10681719_656.html

Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress



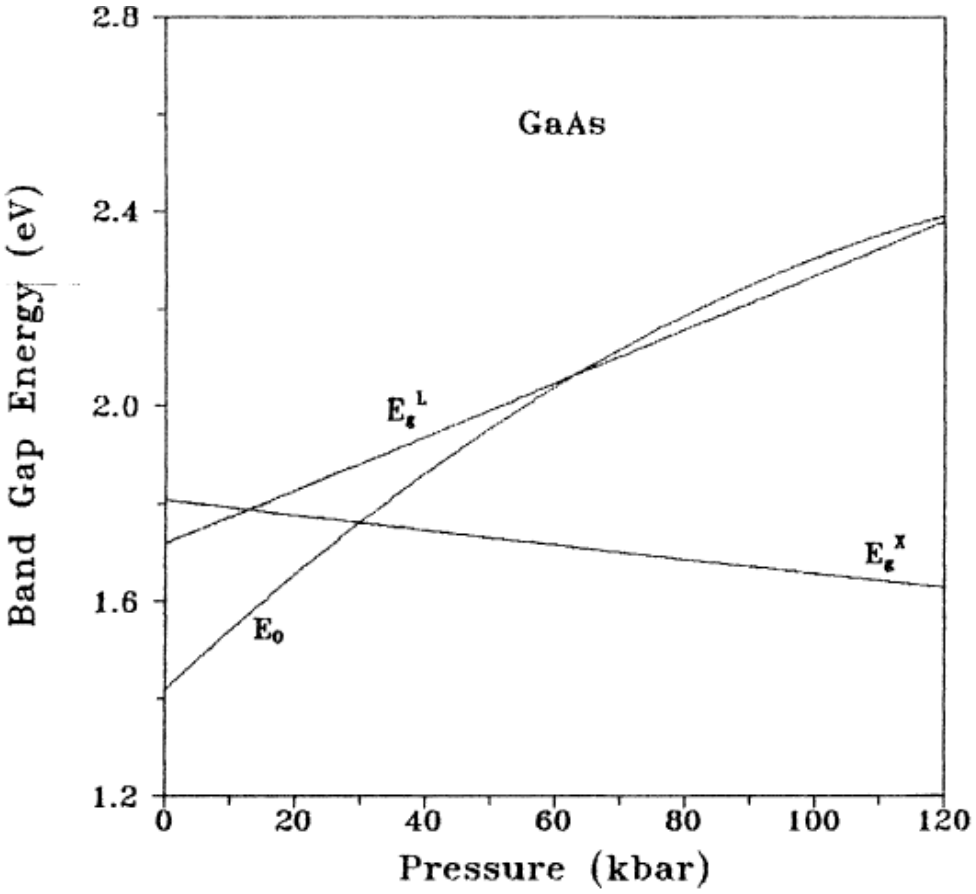


Fig. 2. Direct and indirect band gaps in GaAs as a function of pressure.

Bandgap engineering

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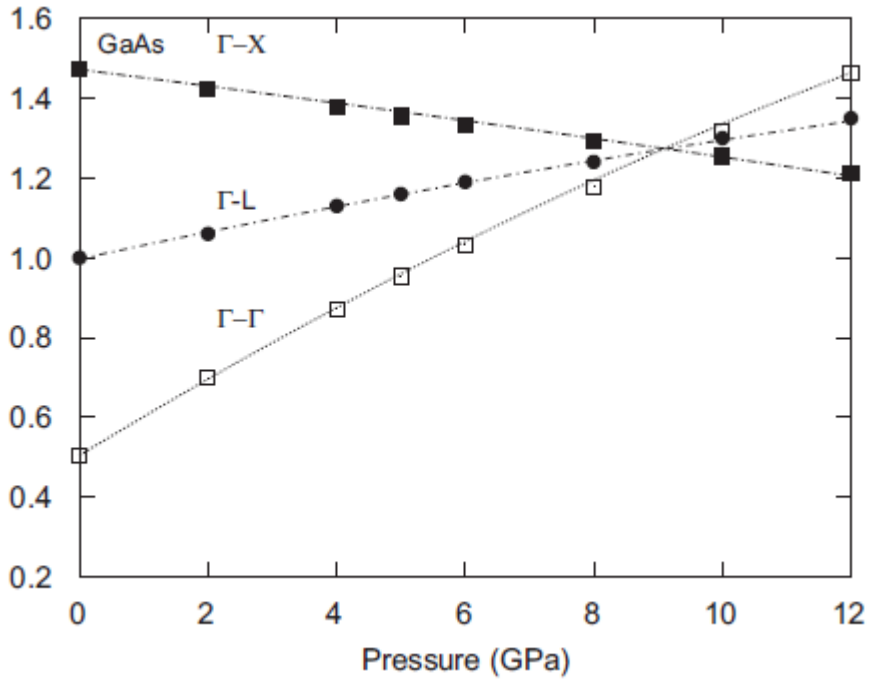

Satyam S. Parashari et al. Physica B 403 (2008) 3077–3088

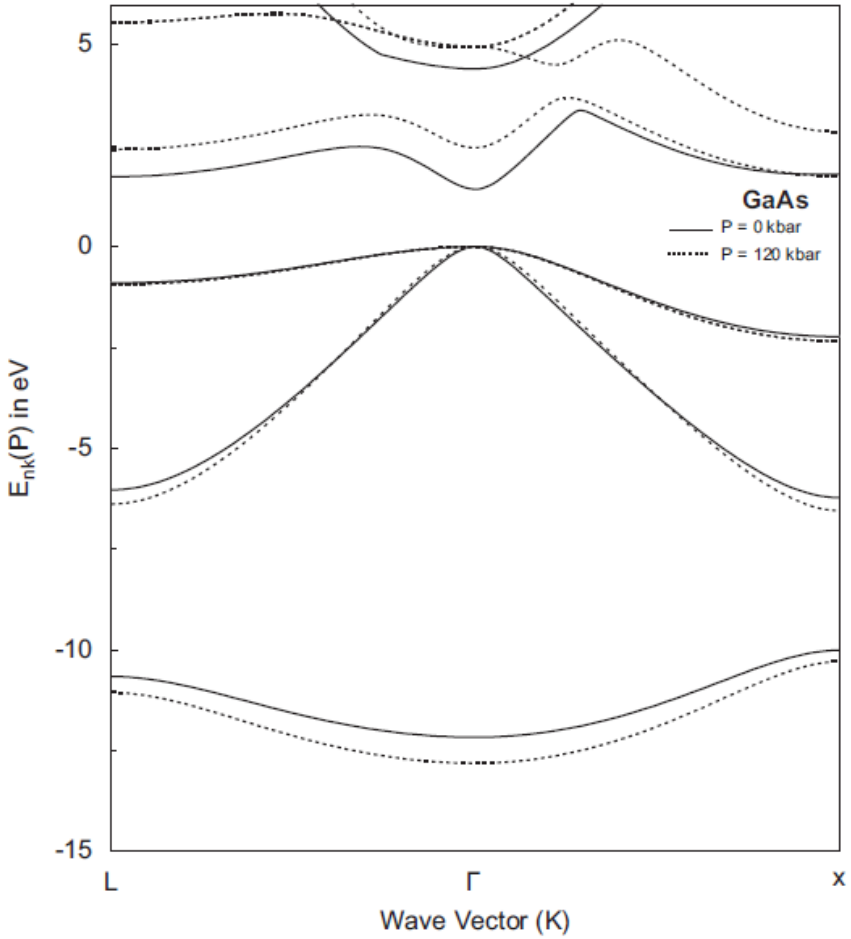

Fig. 3. Variation of the pressure dependent electronic energy band structure, $E_{nk}(P)$ for GaAs, at two different pressures, 0 kbar (solid line) and 120 kbar (dashed line).

Elabsy et al. Physica B 405 (2010) 3709–3713

Bandgap engineering

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- controlling the composition
- controlling the stress

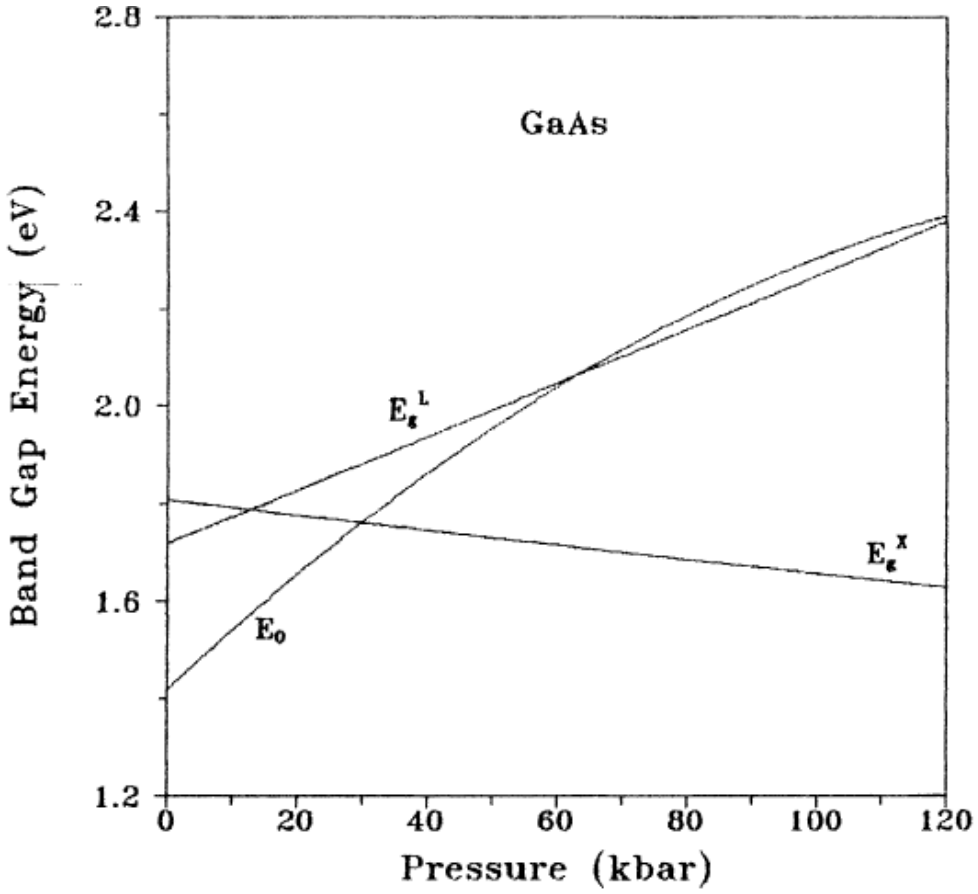

Fig. 2. Direct and indirect band gaps in GaAs as a function of pressure.

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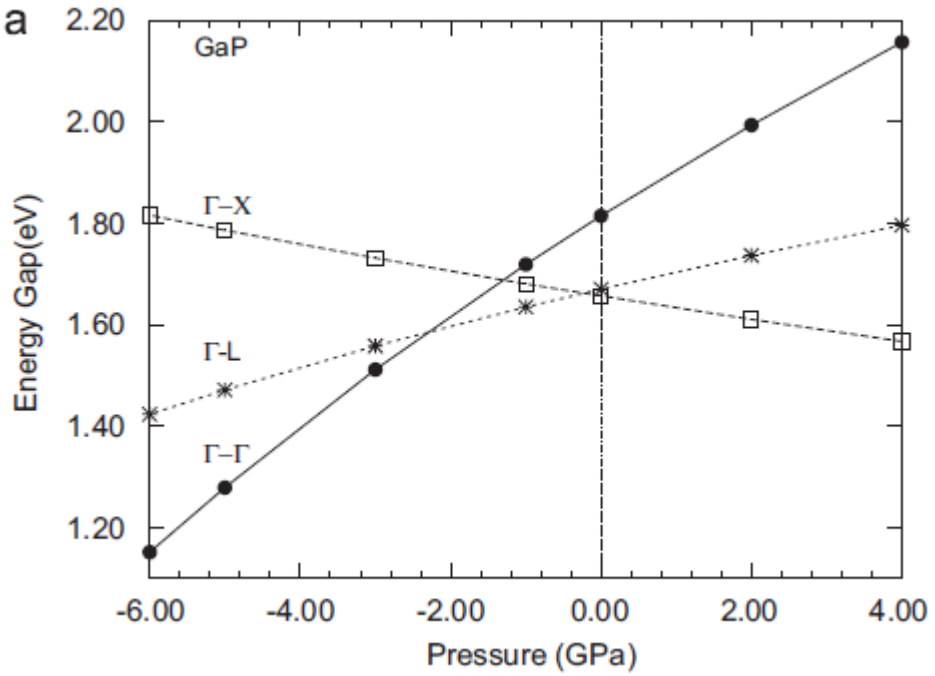

Satyam S. Parashari et al. Physica B 403 (2008) 3077–3088

Bandgap engineering

How can we change the heterostructure band structure:

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- controlling the composition
- controlling the stress

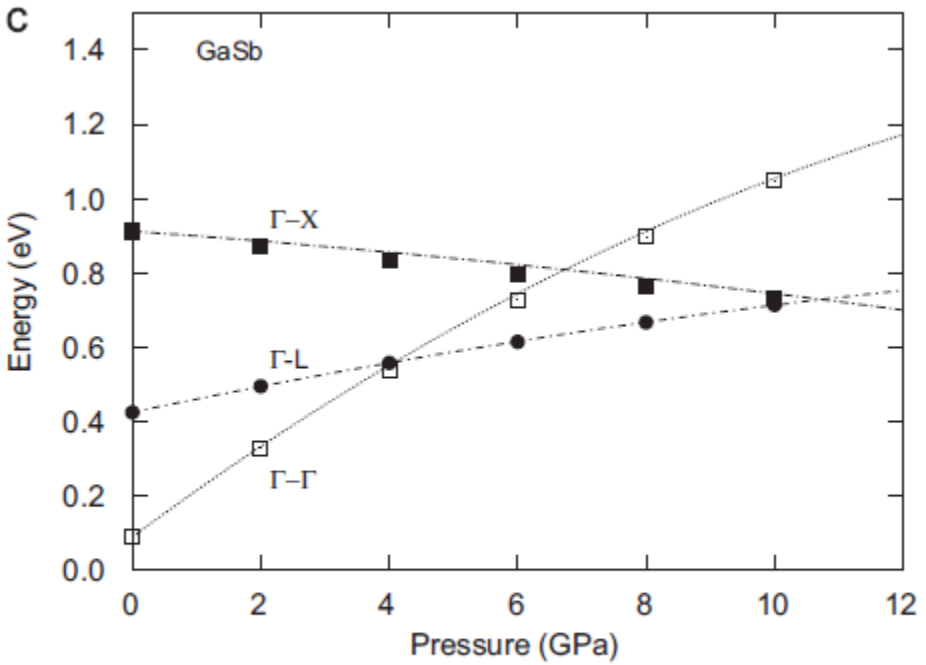

Fig. 5. Direct and indirect band gaps in GaP, GaAs and GaSb as a function of pressure.

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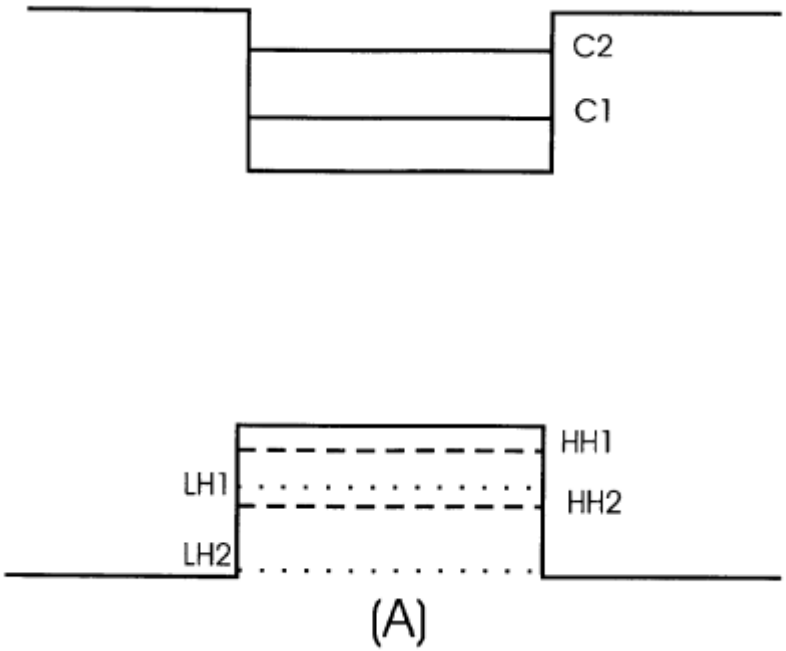
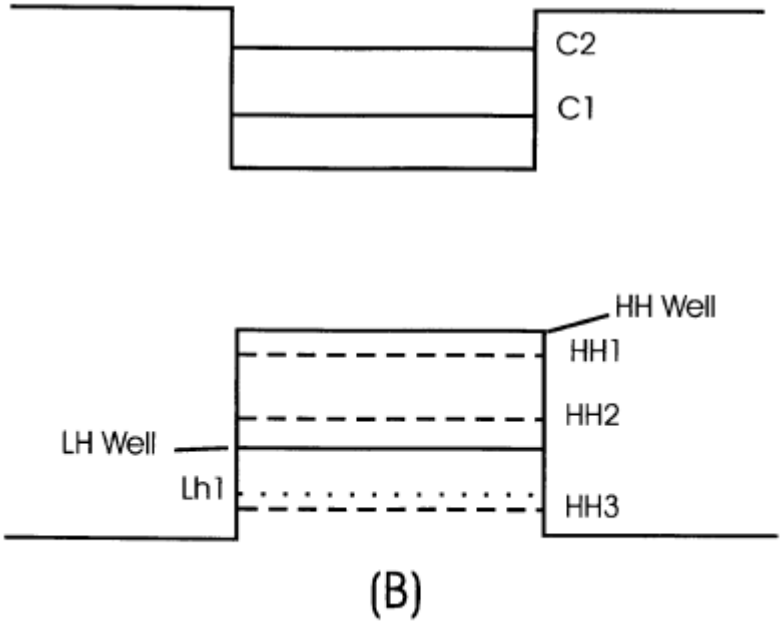
Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress

uniaxial





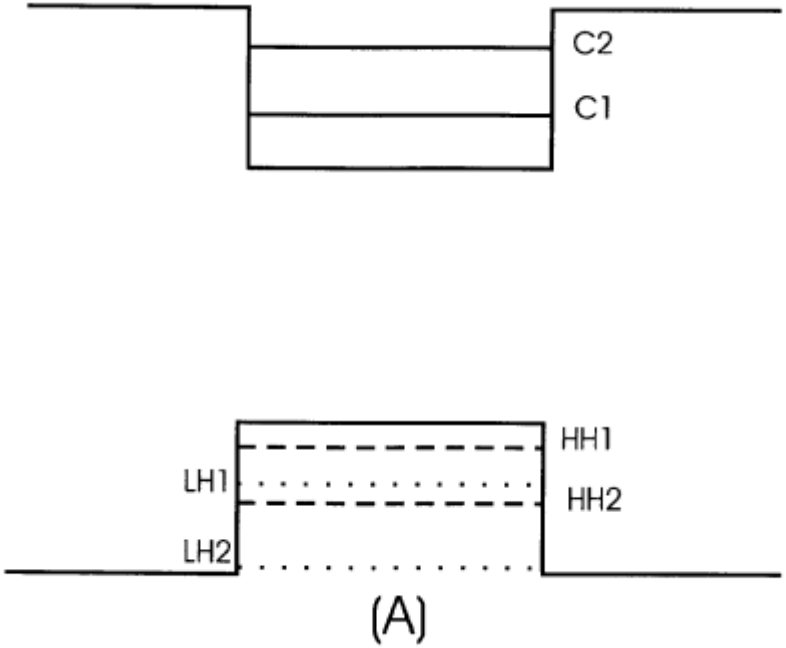
Prog. Quant. Electr. Vol. 21, No. 5, pp. 361±419, 1998

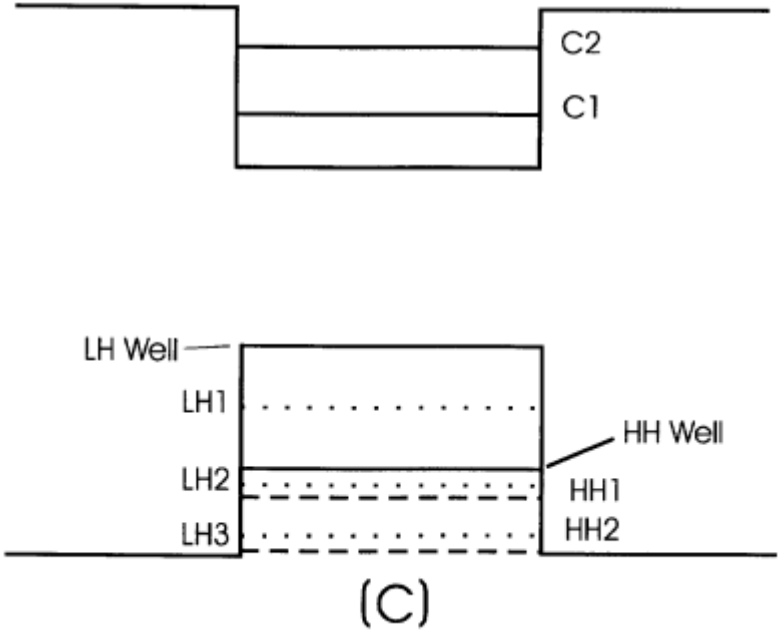
Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress

biaxial



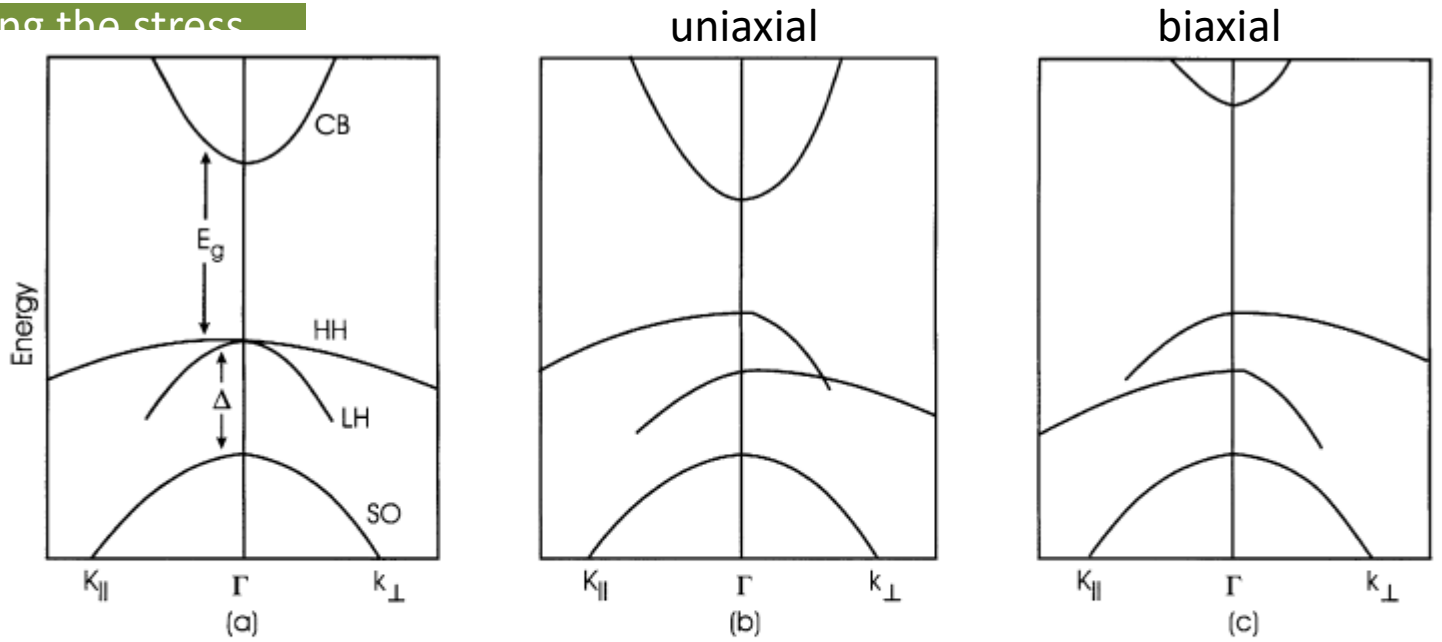


Prog. Quant. Electr. Vol. 21, No. 5, pp. 361±419, 1998

Bandgap engineering

How can we change the heterostructure band structure:

- selecting a material (eg., GaAs / AlAs)
- controlling the composition
- controlling the stress



⊥ allong the strain axis

FIG. 6. (a) Schematic representation of the band structure of an unstrained direct-gap tetrahedral semiconductor (as in Fig. 2). (b) Under bi-axial tension, the hydrostatic component of the tension reduces the mean band gap, while the axial component splits the degeneracy of the valence band maximum and introduces an anisotropic valence band structure, with the highest band being light along the strain axis ($k_\perp$) and comparatively heavy perpendicular to that axis. (c) Under bi-axial compression the mean band gap increases and the valence splitting is reversed so the highest band is now heavy along the strain axis ($k_\perp$) and comparatively light perpendicular to it (reprinted with permission of[167] ©1989 Institute of Physics).

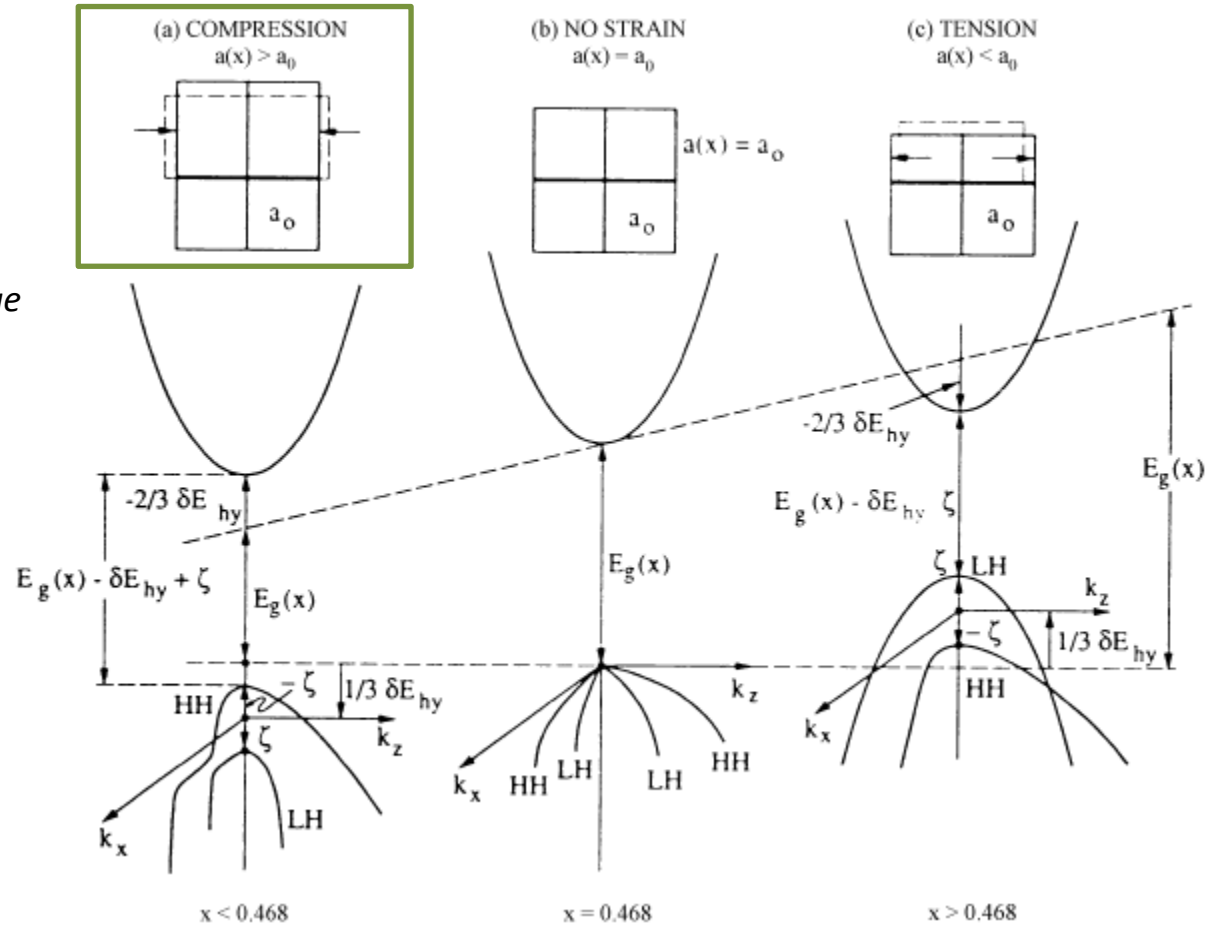
Prog. Quant. Electr. Vol. 21, No. 5, pp. 361±419, 1998

Bandgap engineering

The presence of the well changes the symmetry of the crystal (eg. quantum wells in the direction of [001] corresponds to an uniaxial pressure applied perpendicular to the layer). You have to solve the $\boldsymbol{kp}$ perturbation theory (Chemla 1983):

Effects of biaxial strain: decrease of the degeneracy of the valence band and change of the effective masses in the $Ga_xIn_{1-x}As$ / $Ga_xIn_{1-x}As_yP_{1-y}$ *material system.*

S.L. Chuang, *Phys. Rev. B* 43, p. 9649 (1991). 9, 10



Potencjał harmoniczny

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+\frac{1}{2}m\omega_0^2 z^2\right]\psi(z)=E\psi(z) \qquad \varepsilon=\frac{E}{\hbar\omega_0} \qquad \xi=\sqrt{\frac{m\omega_0}{\hbar}}z$$

$$\left(\frac{d}{d\xi}-\xi\right)\left(\frac{d}{d\xi}+\xi\right)\mathrm{A}\,\mathrm{e}^{\frac{\xi^2}{2}}=(-2\varepsilon_0+1)\mathrm{A}\,\mathrm{e}^{\frac{\xi^2}{2}}=0 \qquad \Rightarrow -2\varepsilon_0+1=0 \Rightarrow \varepsilon_0=\frac{1}{2}$$

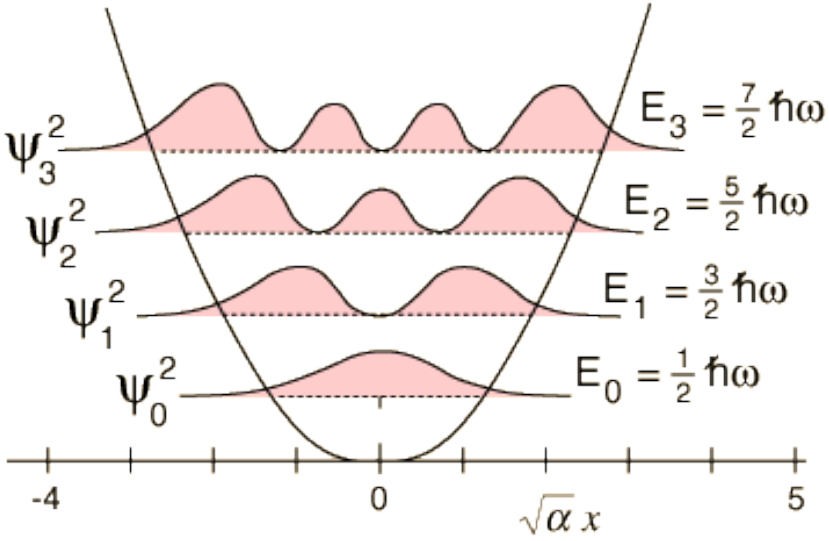
$$\varepsilon_n=n+\frac{1}{2}$$

$$E_n=\hbar\omega_0\left(n+\frac{1}{2}\right)$$

$$\psi_n(z)=A_n H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}z\right)\exp\left(-\frac{m\omega_0}{2\hbar}z^2\right)$$

H_n - wielomiany Hermite'a

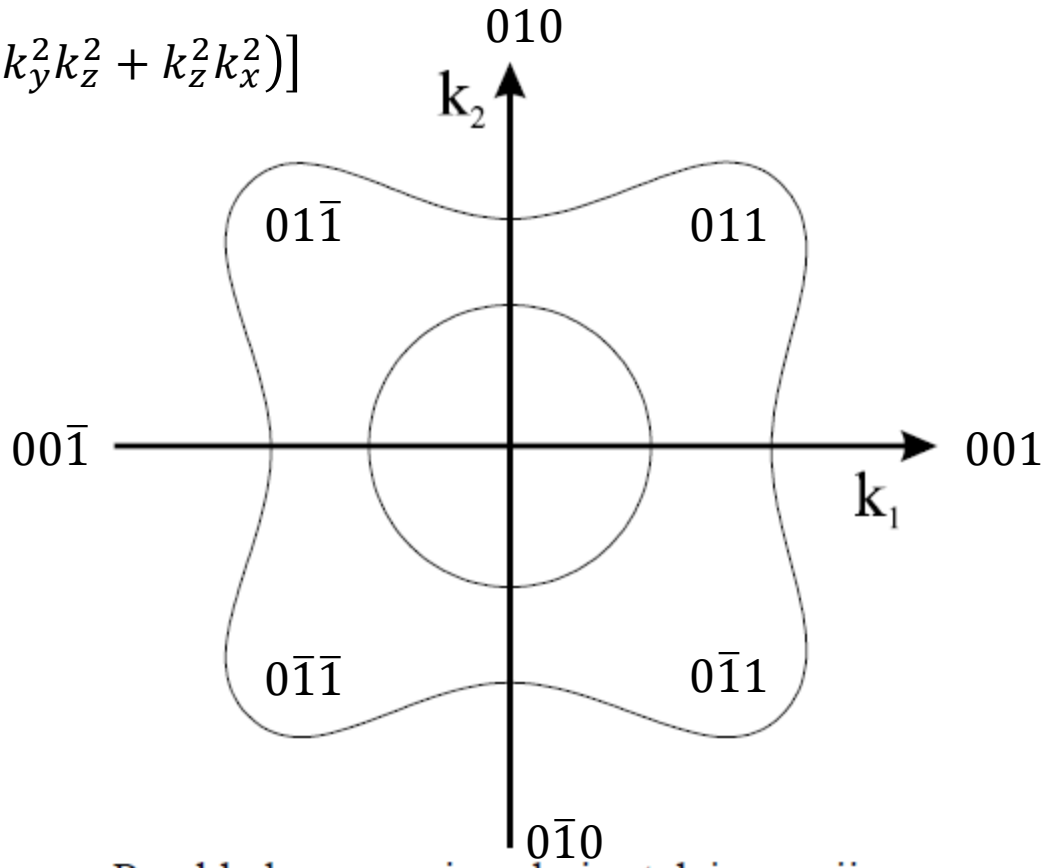
$$A_n=\left(2^n n!\sqrt{\frac{\pi\hbar}{m\omega}}\right)^{-1/2}$$



Comments on the valence band

From $\boldsymbol{kp}$ perturbation theory :

$$E_{3/2}(k) = Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]$$



Przykładowe powierzchnie stałej energii w dwuwymiarowej przestrzeni k.

Comments on the valence band

From $\boldsymbol{kp}$ perturbation theory :

$$E_{3/2}(k) = Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}$$

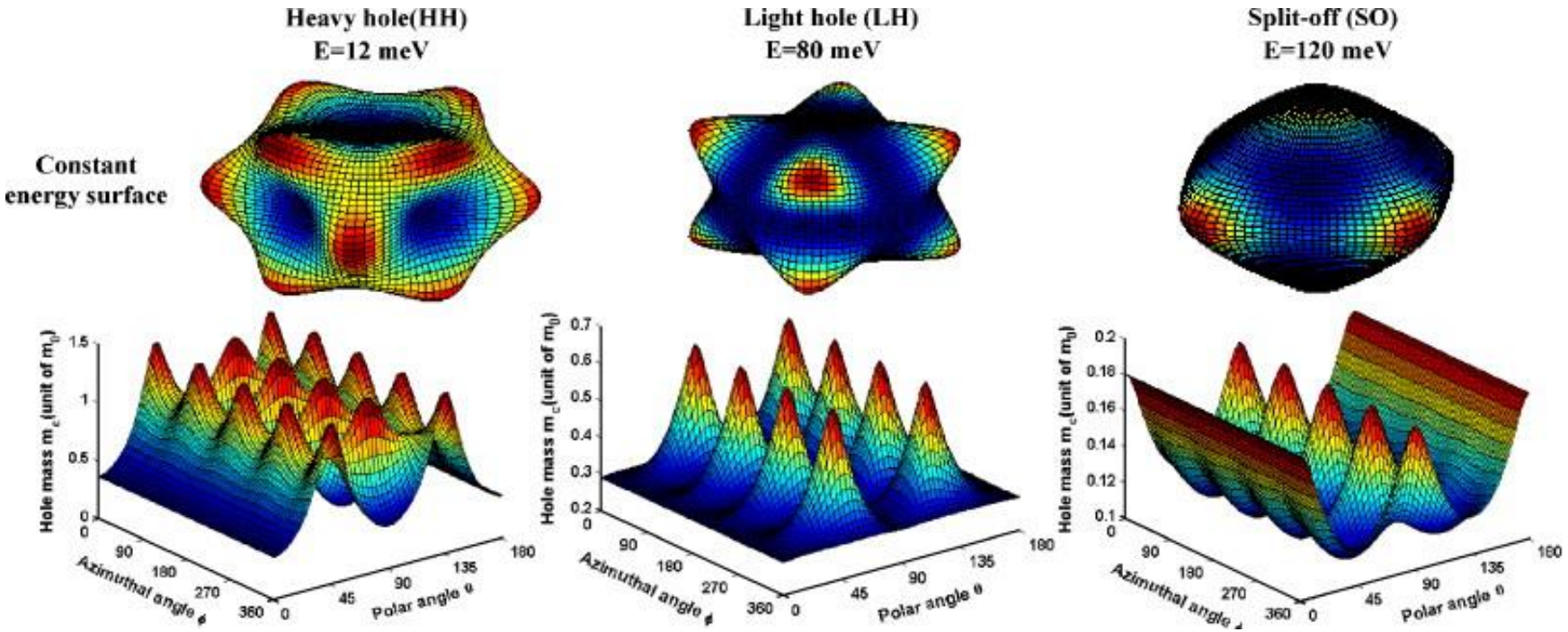


Fig. 7. The 3D constant-energy surfaces of the heavy hole (HH) band, the light hole (LH) band and the split-off (SO) band and their corresponding conductivity masses for unstrained silicon.

X.X. Wei,Y. Yu, Y. Bi; Int. J. of Mechanical Sciences Vol. 50, 1499–1509 (2008),

Comments on the valence band

From $\boldsymbol{kp}$ perturbation theory :

$$E_{3/2}(k) = Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}$$

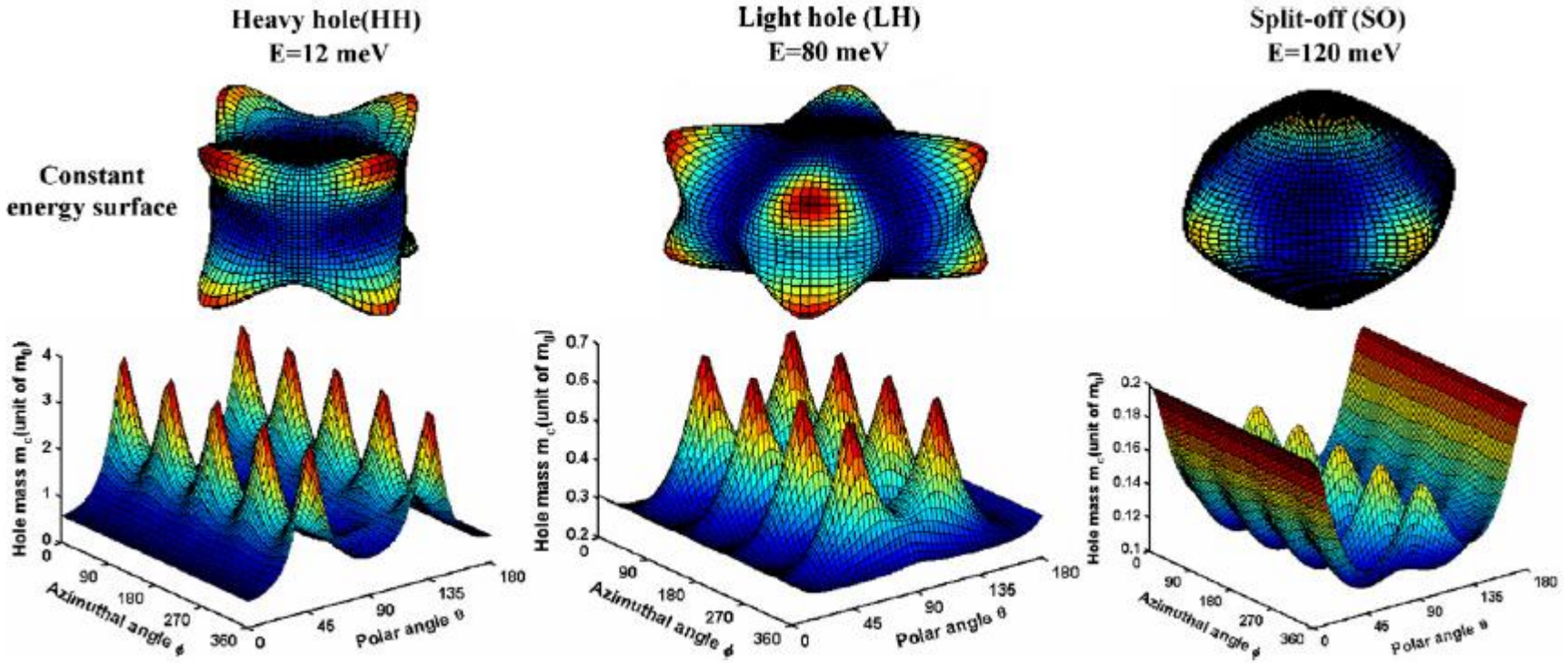


Fig. 8. The 3D constant-energy surfaces of the heavy hole (HH) band, the light hole (LH) band and the split-off (SO) band and the corresponding conductivity masses for silicon under the uniaxial compression P ¼ 500kN. .

X.X. Wei,Y. Yu, Y. Bi; Int. J. of Mechanical Sciences Vol. 50, 1499–1509 (2008),

Comments on the valence band

From $\boldsymbol{kp}$ perturbation theory :

$$E_{3/2}(k) = Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}$$

Luttinger dimensionless *parameters*:

$$\gamma_1 = -\frac{2m}{\hbar^2}A \qquad \gamma_2 = -\frac{m}{\hbar^2}B \qquad \gamma_3 = \frac{m}{\hbar^2}\sqrt{\frac{1}{3}C^2 + B^2}$$

$$E_{l,h}(\boldsymbol{k}) = -\frac{\hbar^2}{2m}\left[\gamma_1 k^2 \pm \sqrt{4\gamma_2^2k^4 + 12(\gamma_3^2 - \gamma_2^2)\left[k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right]}\right]$$

\+ heavy holes
– light holes

Expanding around $k = 0$

$$E_{hh}(\boldsymbol{k}) = -\frac{\hbar^2}{2m}\left[(\gamma_1 + 2\gamma_2)\boldsymbol{k}_\perp^2 + (\gamma_1 + 2\gamma_2)k_z^2\right]$$

$$E_{lh}(\boldsymbol{k}) = -\frac{\hbar^2}{2m}\left[(\gamma_1 - 2\gamma_2)\boldsymbol{k}_\perp^2 + (\gamma_1 - 2\gamma_2)k_z^2\right]$$

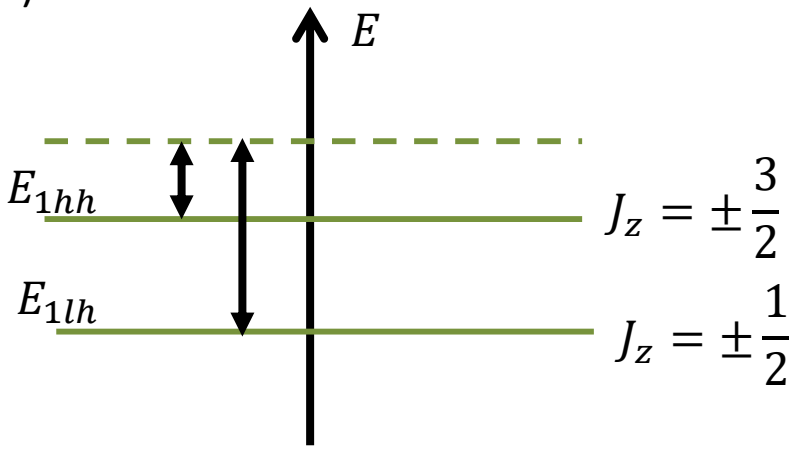
Symmetry!

Comments on the valence band

The presence of the well changes the symmetry of the crystal (eg. quantum wells in the direction of [001] corresponds to an uniaxial pressure applied perpendicular to the layer). You have to solve the $\boldsymbol{kp}$ perturbation theory (Chemla 1983):

$$E_{hh}(\boldsymbol{k}) = -\frac{\hbar^2}{2m}[(\gamma_1 + \gamma_2)\boldsymbol{k}_\perp^2 + (\gamma_1 - 2\gamma_2)k_z^2]$$

$$E_{lh}(\boldsymbol{k}) = -\frac{\hbar^2}{2m}[(\gamma_1 - \gamma_2)\boldsymbol{k}_\perp^2 + (\gamma_1 + 2\gamma_2)k_z^2]$$



It follows that the heavy holes have a "light" mass $\frac{m}{(\gamma_1+\gamma_2)}$ in the plane $(x-y)$, while light holes have heavy mass $\frac{m}{(\gamma_1-\gamma_2)}$

Comments on the valence band

The presence of the well changes the symmetry of the crystal (eg. quantum wells in the direction of [001] corresponds to an uniaxial pressure applied perpendicular to the layer). You have to solve the $\boldsymbol{kp}$ perturbation theory (Chemla 1983):

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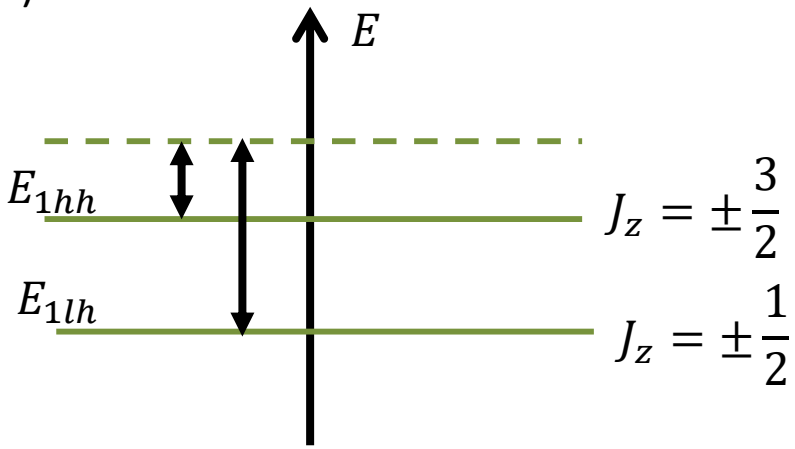
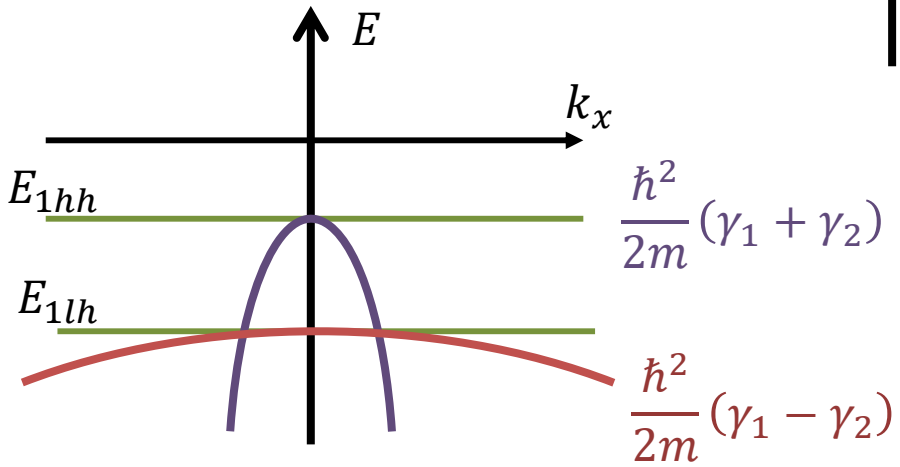
$$E_{lh}(\boldsymbol{k}) = -\frac{\hbar^2}{2m}[(\gamma_1 - \gamma_2)\boldsymbol{k}_\perp^2 + (\gamma_1 + 2\gamma_2)k_z^2]$$





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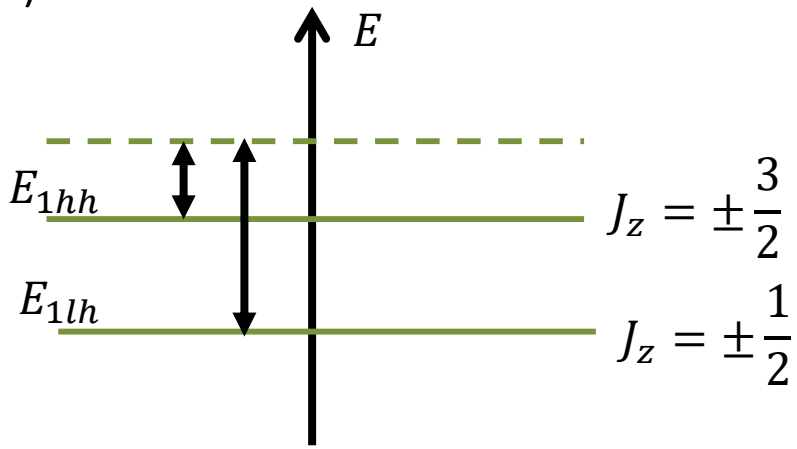
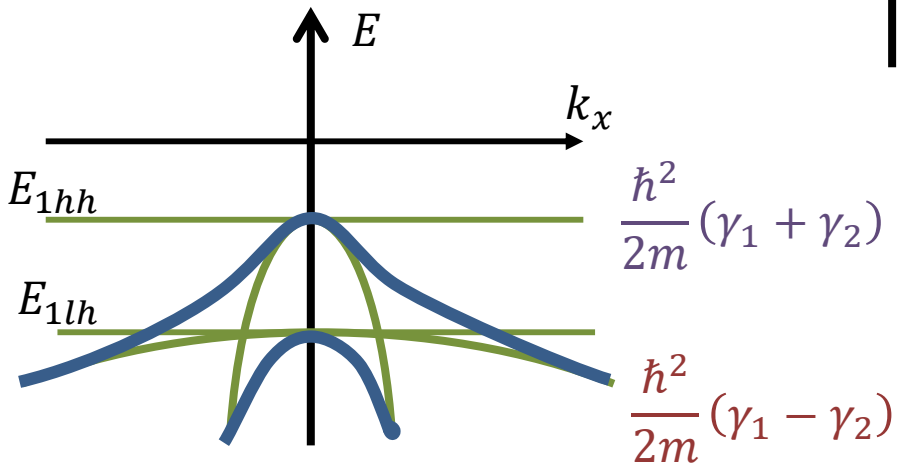




Energy bands

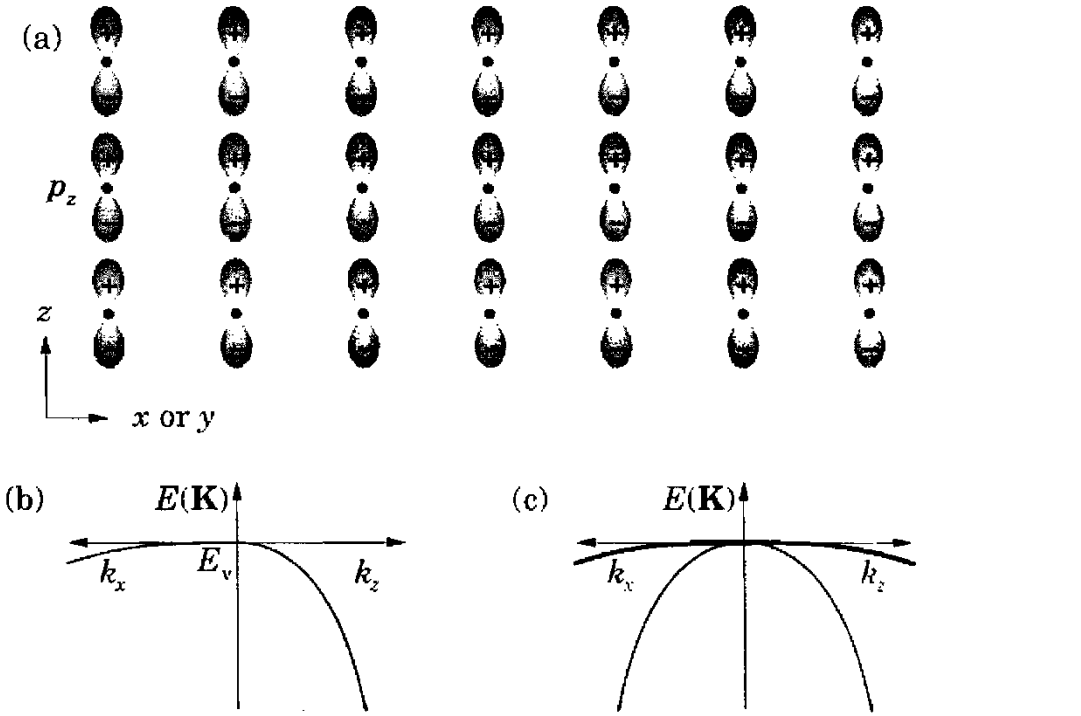
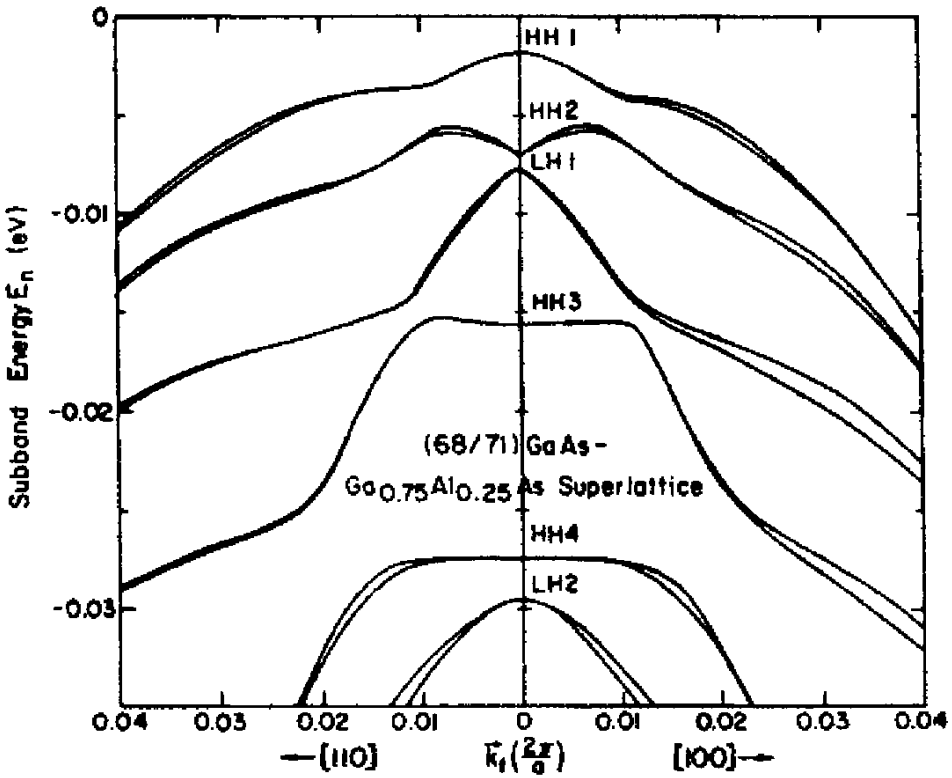


FIGURE 2.17. Valence bands constructed from p orbitals. (a) Lattice of p_z orbitals. (b) Band structure of the p_z orbitals only; the band is 'light' along k_z to the right and 'heavy' along k_x (or k_y) to the left. (c) Total bands from all three p orbitals, showing a doubly degenerate 'heavy' band and a single 'light' band.

Energy bands

Example:



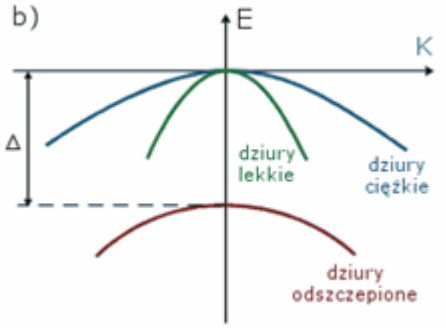
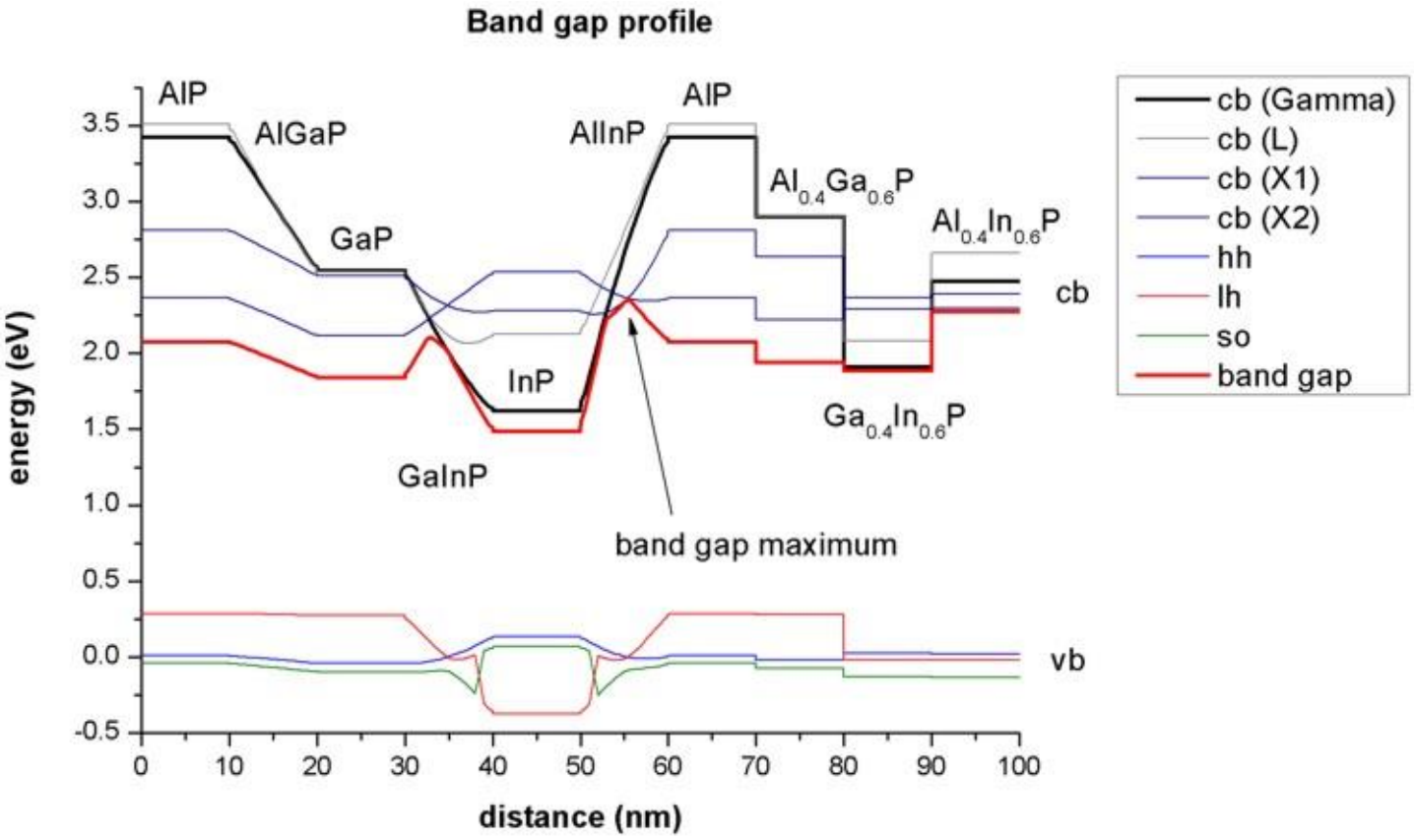


FIGURE 10.4. Valence-band structure in a multiquantum well as a function of **k** along two directions. The wells comprise 68 atomic layers of GaAs with barriers of 71 atomic layers of $Al_{0.25}Ga_{0.75}As$. [From Chang and Schulman (1985).]

D. Wasik.

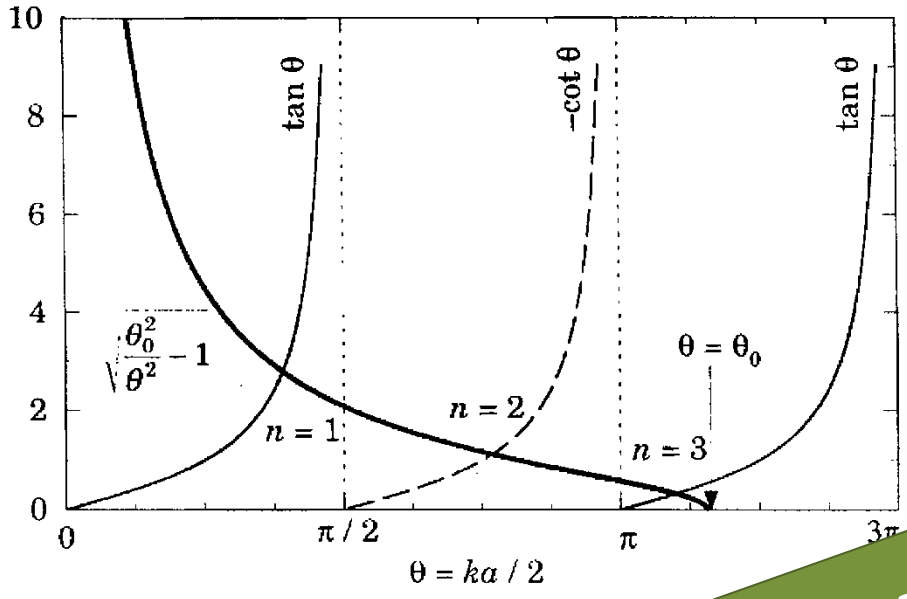
Quantum well



http://www.nextnano.de/nextnano3/tutorial/1Dtutorial_AlGaInP_onGaAs.htm

Finite potential well – square well

Simply example has been already calculated



On exercises

Finite potential well – square well

Heterostructures can have different effective masses in different regions:

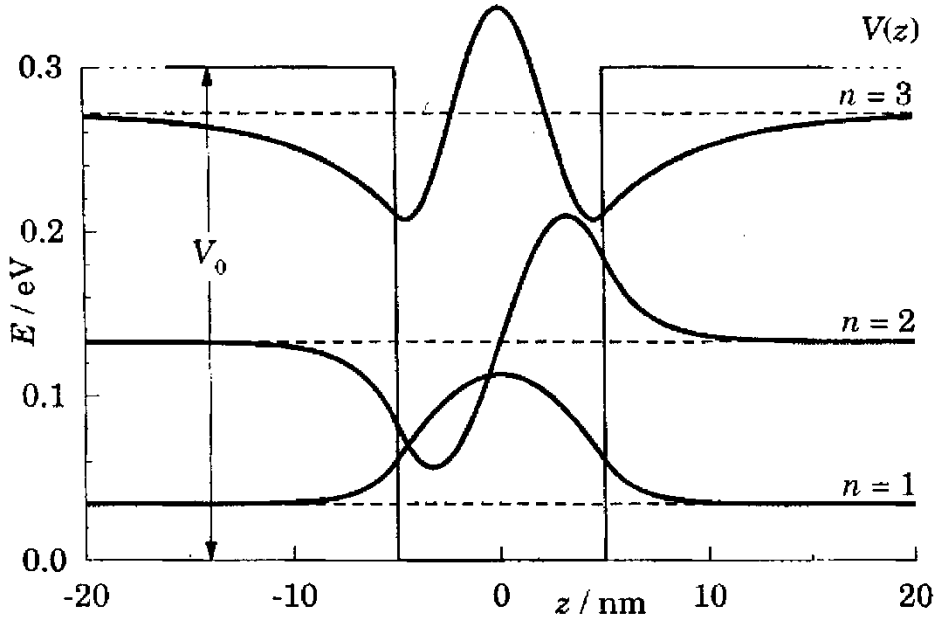
$$-\frac{\hbar^2}{2m_0 m^*}\frac{d^2}{dz^2}\psi(z) + \mathrm{V_0(z)}\psi(z) = \varepsilon\psi(z)$$

It turns that the conversion $m^* \rightarrow m(z)$ is not a good solution of the problem (equation ceases to be Hermitean). It has to be done diferently, eg.:

$$-\frac{\hbar^2}{2m_0}\frac{d}{dz}\left[\frac{1}{m(z)}\frac{d}{dz}\right]\psi(z) + \mathrm{V_0(z)}\psi(z) = \varepsilon\psi(z)$$

Matching conditions at the interface must be modified (equation has to conserve current $I_W = I_B$ thus $v_W = v_B$):

$$\left.\frac{1}{m_B}\frac{d\psi}{dz}\right|_{\mathrm{z}=\frac{\mathrm{a}}{2}} = \left.\frac{1}{m_W}\frac{d\psi}{dz}\right|_{\mathrm{z}=\frac{\mathrm{a}}{2}}$$



Finite potential well – square well

Inside the well: $-\frac{a}{2} < z < \frac{a}{2}$

$$-\frac{\hbar^2}{2m_0 m_W}\frac{d^2}{dz^2}\psi(z) = (E_n - E_W)\psi(z)$$

$$\psi(z,t) = C\begin{cases}\cos(k_n z)\\ \sin(k_n z)\end{cases} e^{-i\omega_n t}$$

$$k_n = \frac{1}{\hbar}\sqrt{2mm_W(E_n - E_W)}$$

$$\kappa_n = \frac{1}{\hbar}\sqrt{2mm_B(E_B - E_n)}$$

The barrier:

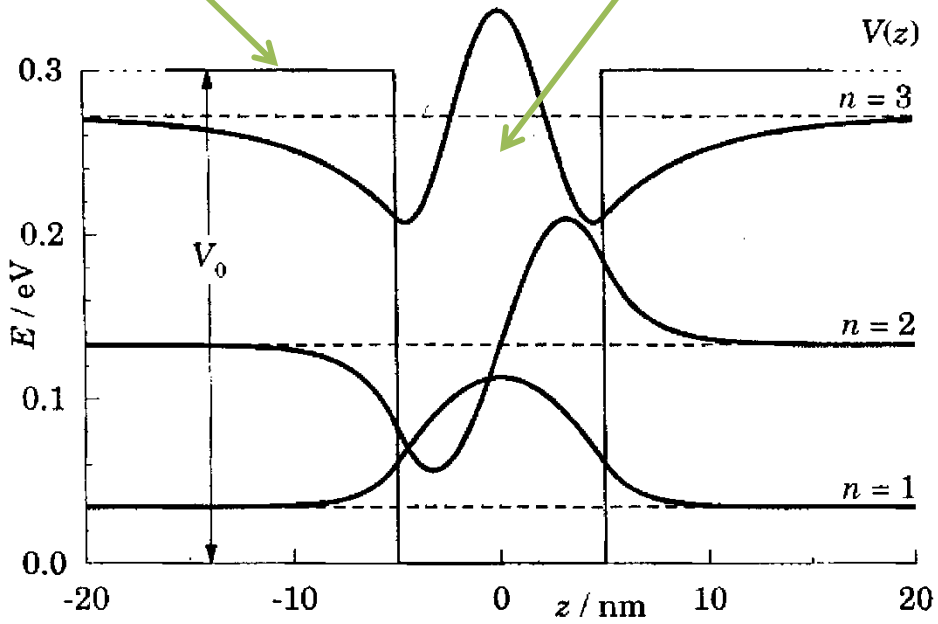
$$\frac{\hbar^2\kappa^2}{2m\, m_B} = E_B - E_n = B$$

$$\psi(z) = D\exp(\pm\kappa_n z)$$

Matching conditions:

$$\frac{1}{m_B}\frac{d\psi}{dz}\bigg|_{z=\frac{a}{2}} = \frac{1}{m_W}\frac{d\psi}{dz}\bigg|_{z=\frac{a}{2}}$$

$$\frac{Ck}{m_W}\begin{cases}-\sin\left(k_n\frac{a}{2}\right)\\ \cos\left(k_n\frac{a}{2}\right)\end{cases} = -\frac{D\kappa}{m_B}\exp\left(k_n\frac{a}{2}\right)$$



Finite potential well – square well

We calculate:

$$\begin{cases} \psi_B(z)\Big|_{z=\frac{a}{2}} = \psi_W(z)\Big|_{z=\frac{a}{2}} \\ \dfrac{1}{m_B}\dfrac{d\psi}{dz}\Big|_{z=\frac{a}{2}} = \dfrac{1}{m_W}\dfrac{d\psi}{dz}\Big|_{z=\frac{a}{2}} \end{cases}$$

$$\frac{Ck}{m_W}\begin{cases} -\sin\left(k_n\dfrac{a}{2}\right) \\ \cos\left(k_n\dfrac{a}{2}\right) \end{cases} = -\frac{D\kappa_n}{m_B}\exp\left(\kappa_n\frac{a}{2}\right)$$

$$\begin{cases} \tan\left(k_n\dfrac{a}{2}\right) \\ \cot\left(k_n\dfrac{a}{2}\right) \end{cases} = \frac{m_W\kappa_n}{m_B k_n} = \sqrt{\frac{m_W}{m_B}\left(\frac{2m_0 m_W V_0}{\hbar^2 k_n^2} - 1\right)}$$

Substituting $\theta = \dfrac{k_n a}{2}$, and $\theta_0^2 = \dfrac{m_0 m_W V_0 a^2}{2\hbar^2}$ (depends only on m_W)

$$\begin{cases} \tan\theta \\ -\cot\theta \end{cases} = \sqrt{\frac{m_W}{m_B}\left(\frac{\theta_0^2}{\theta^2} - 1\right)}$$

Finite potential well – square well

THE SAME mass in the well and in the barrier:

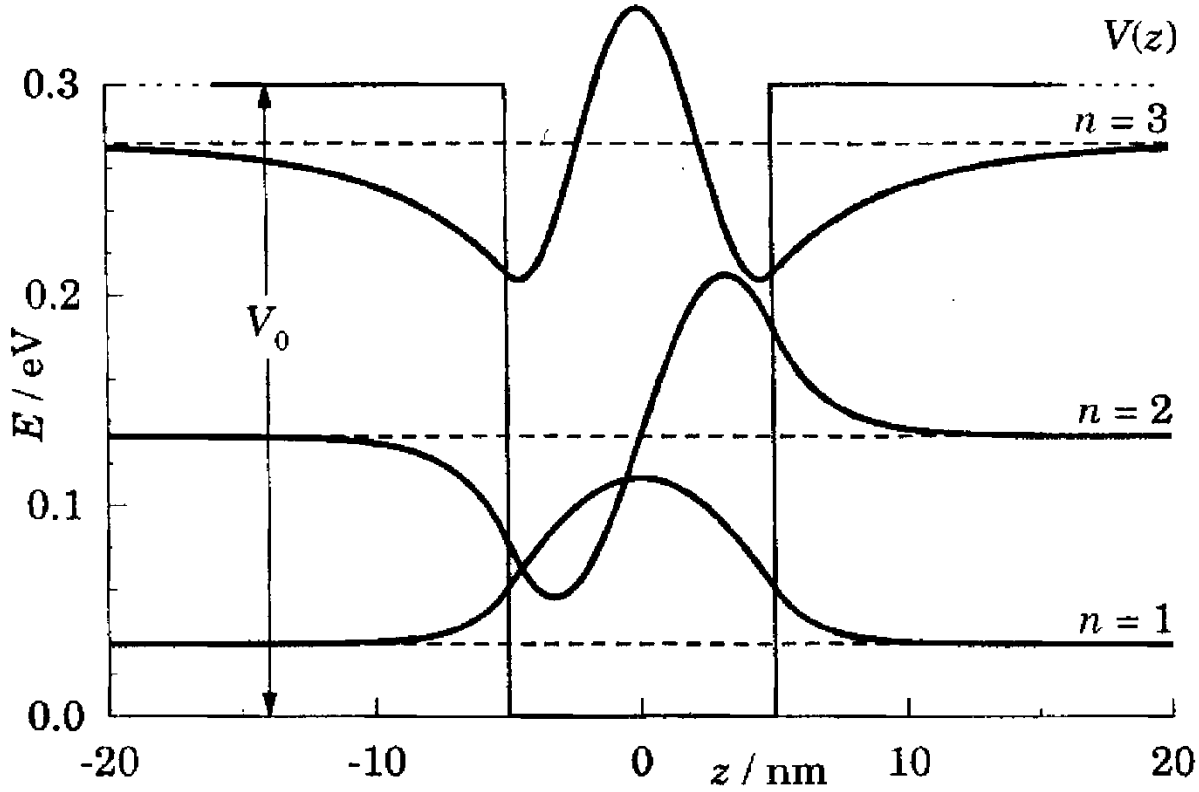


FIGURE 4.1. Finite square well in GaAs of depth $V_0 = 0.3\,\text{eV}$ and width $a = 10\,\text{nm}$, showing three bound states.

Finite potential well – square well

THE DIFFERENT mass in the well and in the barrier:

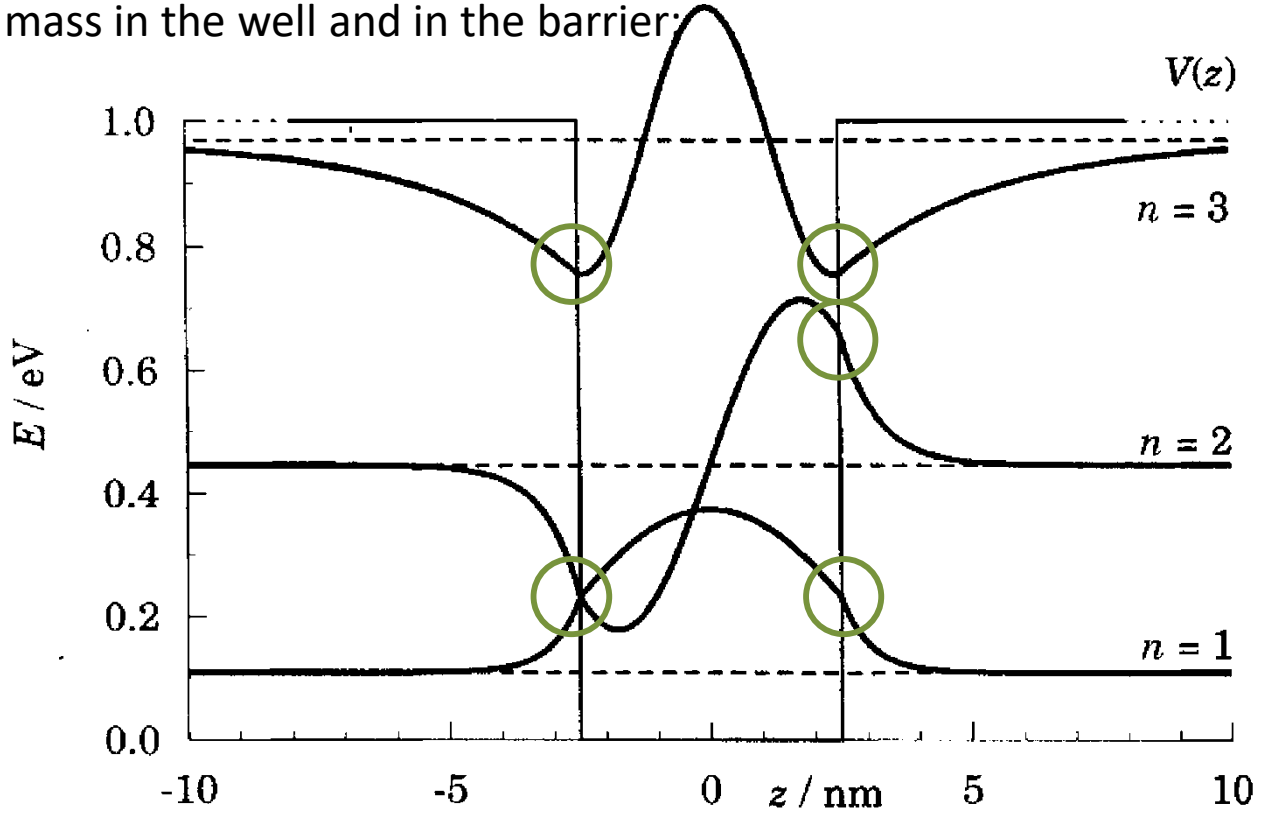
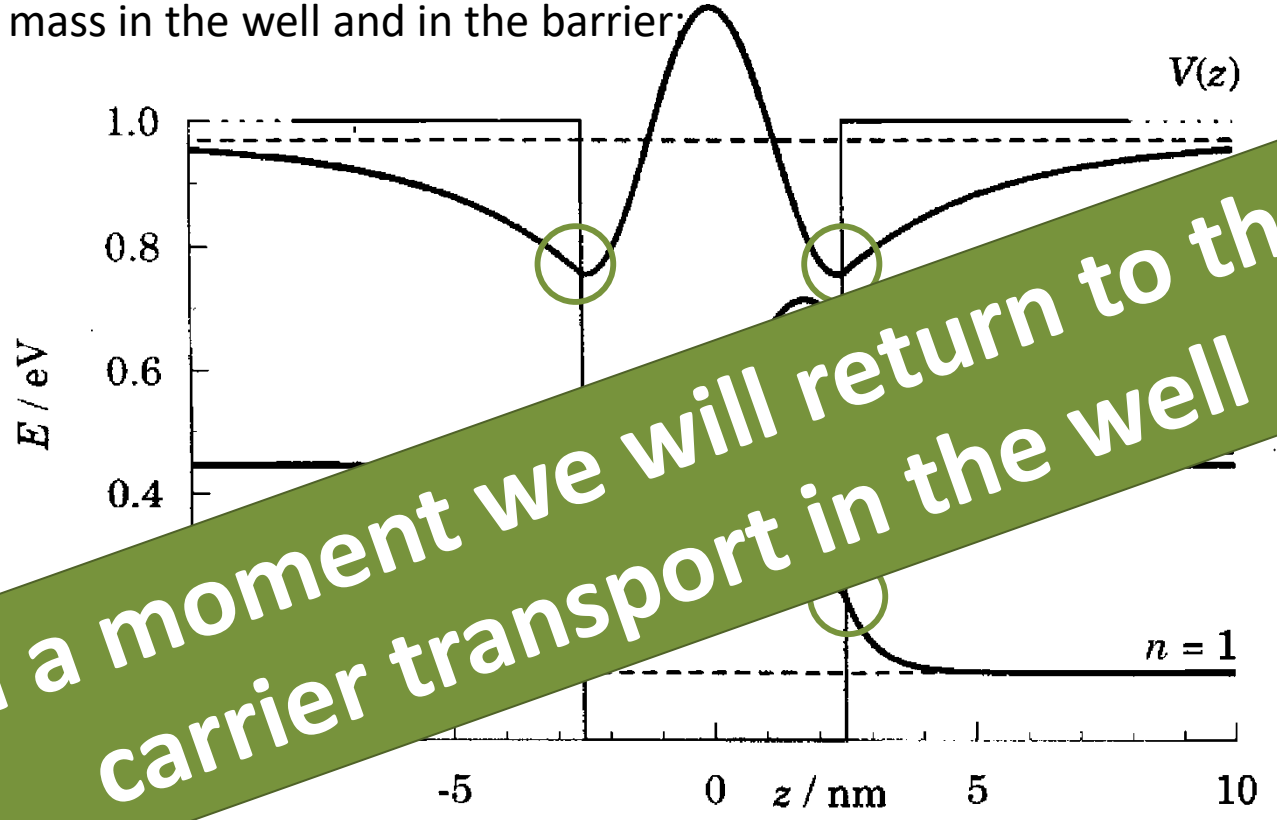


FIGURE 4.12. Finite square well of depth $V_0 = 1$ eV, width $a = 5$ nm along z, and effective masses $m_W = 0.067$ in the well and $m_B = 0.15$ in the barrier.

Finite potential well – square well

THE DIFFERENT mass in the well and in the barrier:



In a moment we will return to the carrier transport in the well

4.12. Finite square well of depth $V_0 = 1$ eV, width $a = 5$ nm along z, and effective masses $m_W = 0.067$ in the well and $m_B = 0.15$ in the barrier.

Finite potential well – square well

THE DIFFERENT mass in the well and in the barrier:

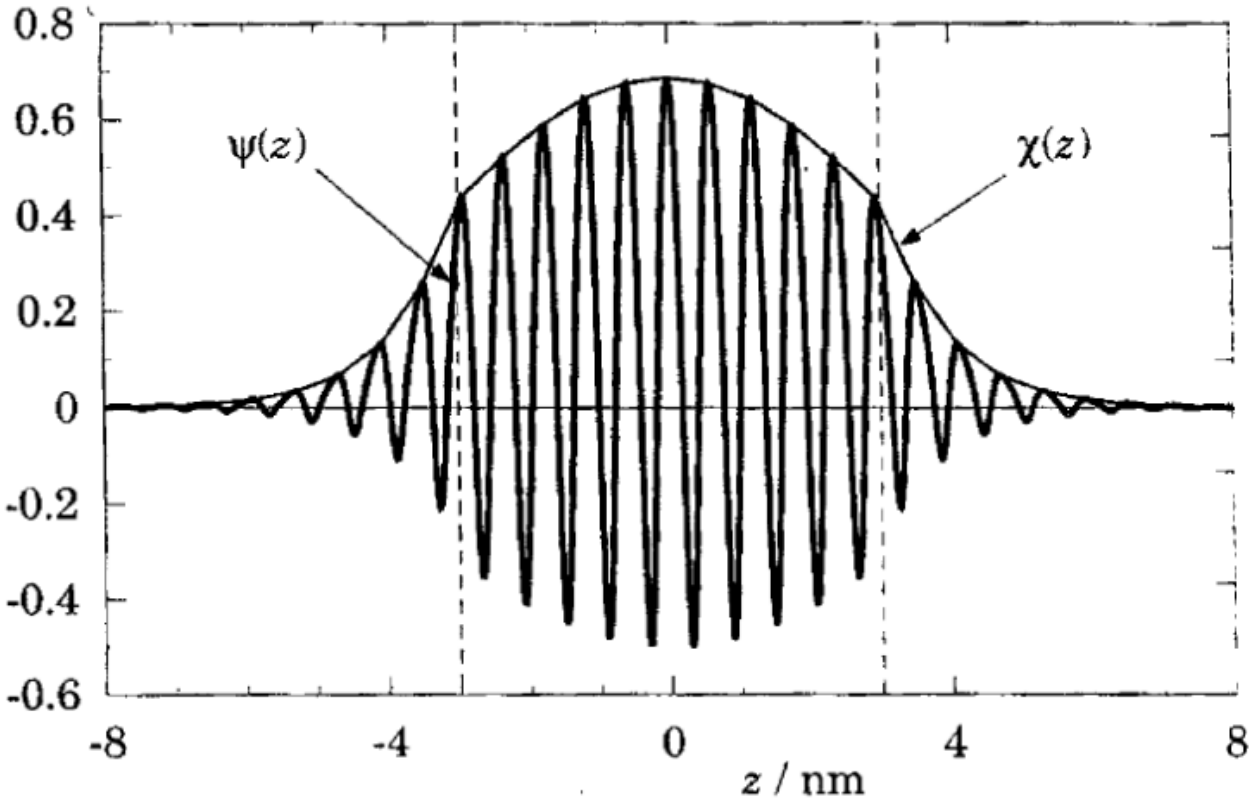
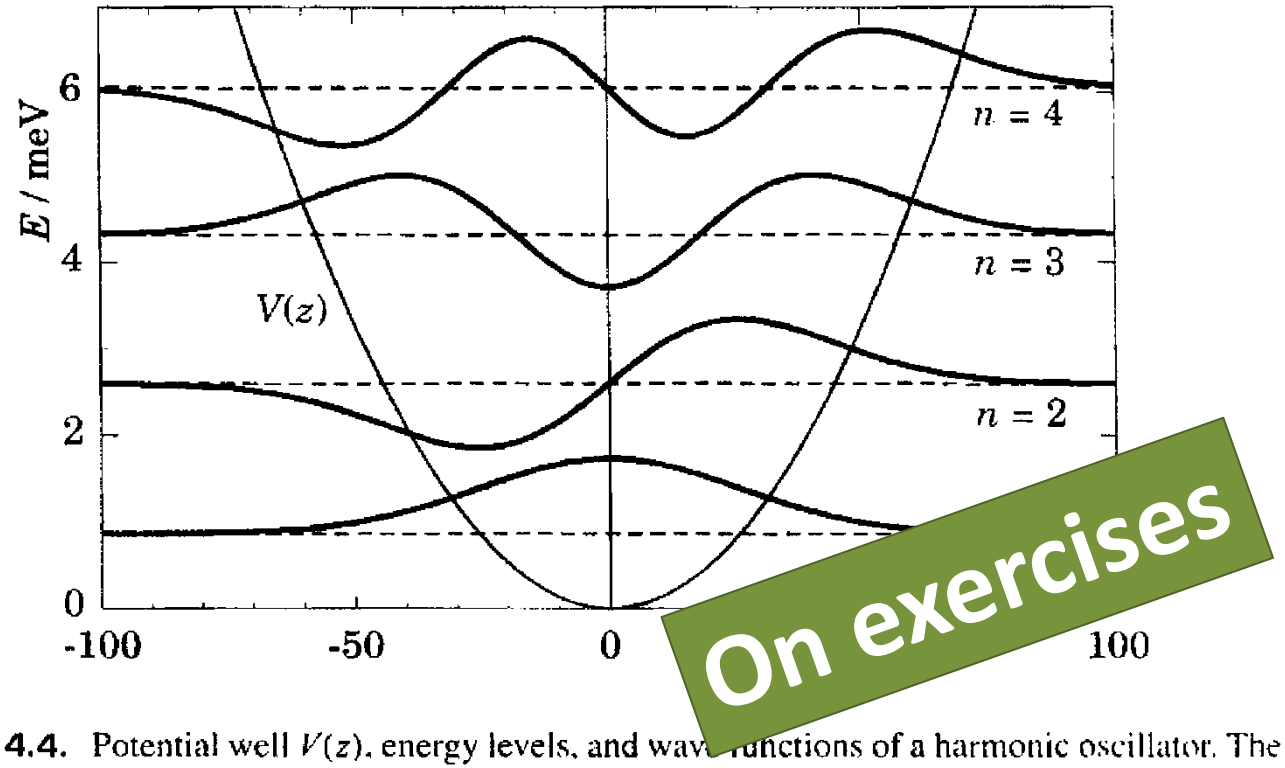


FIGURE 3.22. Wave function for the lowest state in a 6 nm quantum well in a heterostructure, including the Bloch functions. The thin curve is an approximate envelope function joining the peaks of the full wave function. [Redrawn from Burt (1994).]

Harmonic potential

Harmonic potential

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V(z)\right]\psi(z)=\varepsilon\psi(z) \qquad V(z)=\frac{1}{2}Kz^2=\frac{1}{2}m\omega_0^2z^2 \qquad \varepsilon_n=\left(n-\frac{1}{2}\right)\hbar\omega_0$$



On exercises

FIGURE 4.4. Potential well $V(z)$, energy levels, and wave functions of a harmonic oscillator. The potential is generated by a magnetic field of 1 T acting on electrons in GaAs.

Harmonic potential

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+\frac{1}{2}m\omega_0^2 z^2\right]\psi(z)=\varepsilon\psi(z)$$

$$\varepsilon_n=\left(n-\frac{1}{2}\right)\hbar\omega_0$$

Wavefunction

$$\phi_{n+1}(z)=\frac{1}{\sqrt{2^n n!}}\left[\frac{m\omega_0}{\hbar\pi}\right]^{1/4}\exp\left(-\frac{m\omega_0 z^2}{2\hbar}\right)H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}z\right)$$

Hermite polynomials

$$H_0(t)=1$$
$$H_1(t)=t$$
$$H_2(t)=4t^2-2$$
$$H_3(t)=8t^3-12t$$

The ground state is a Gauss package – does the packet diffuse?

$$|\phi_1(z)|^2=\sqrt{\frac{m\omega_0}{\pi\hbar}}\exp\left(-\frac{m\omega_0 z^2}{\hbar}\right)$$

Harmonic potential

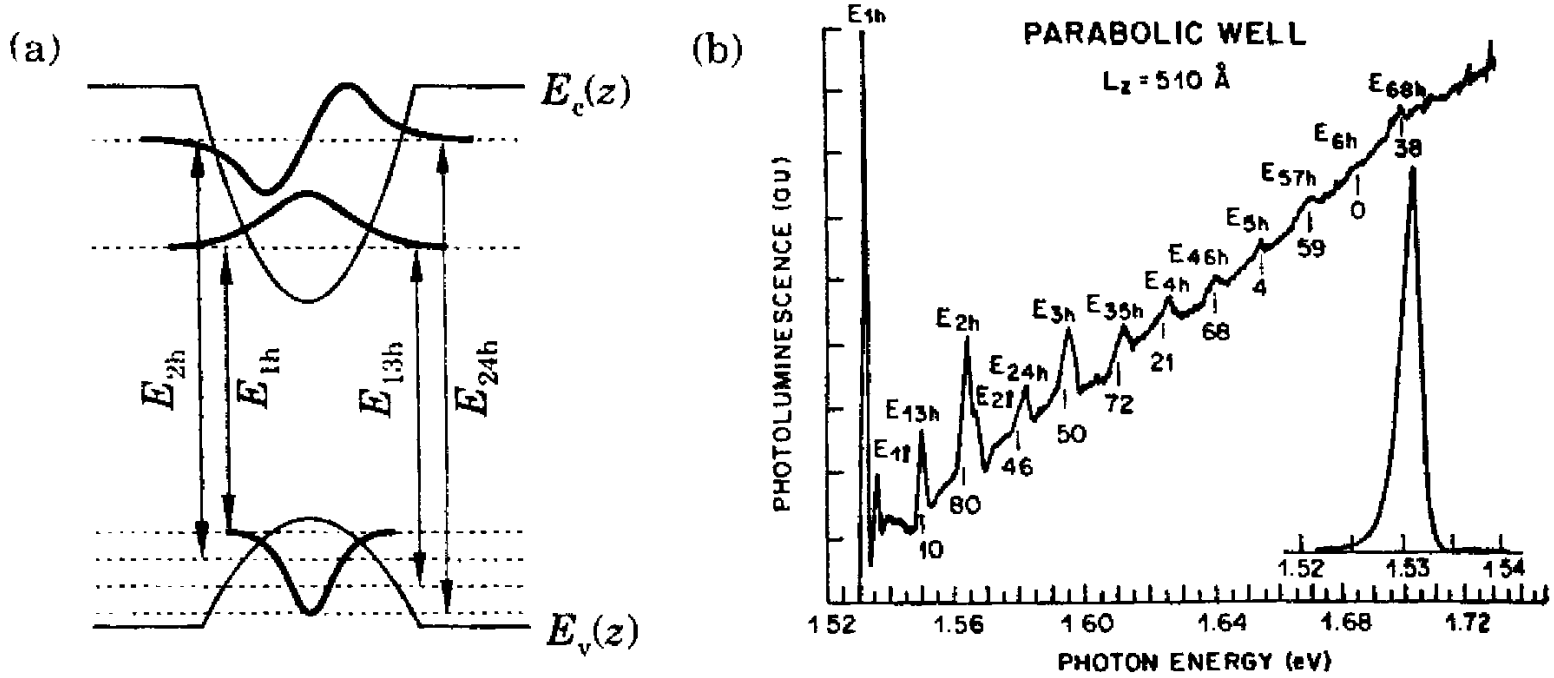


FIGURE 4.5. (a) Parabolic potential in both conduction and valence bands grown into GaAs by a graded composition of $Al_xGa_{1-x}As$. The band gap has been reduced in this sketch, and only heavy holes are shown. (b) Photoluminescence in parabolic wells. [From Miller et al. (1984).]

Triangular well

Triangular well

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + eFz\right]\psi(z) = \varepsilon\psi(z)$$

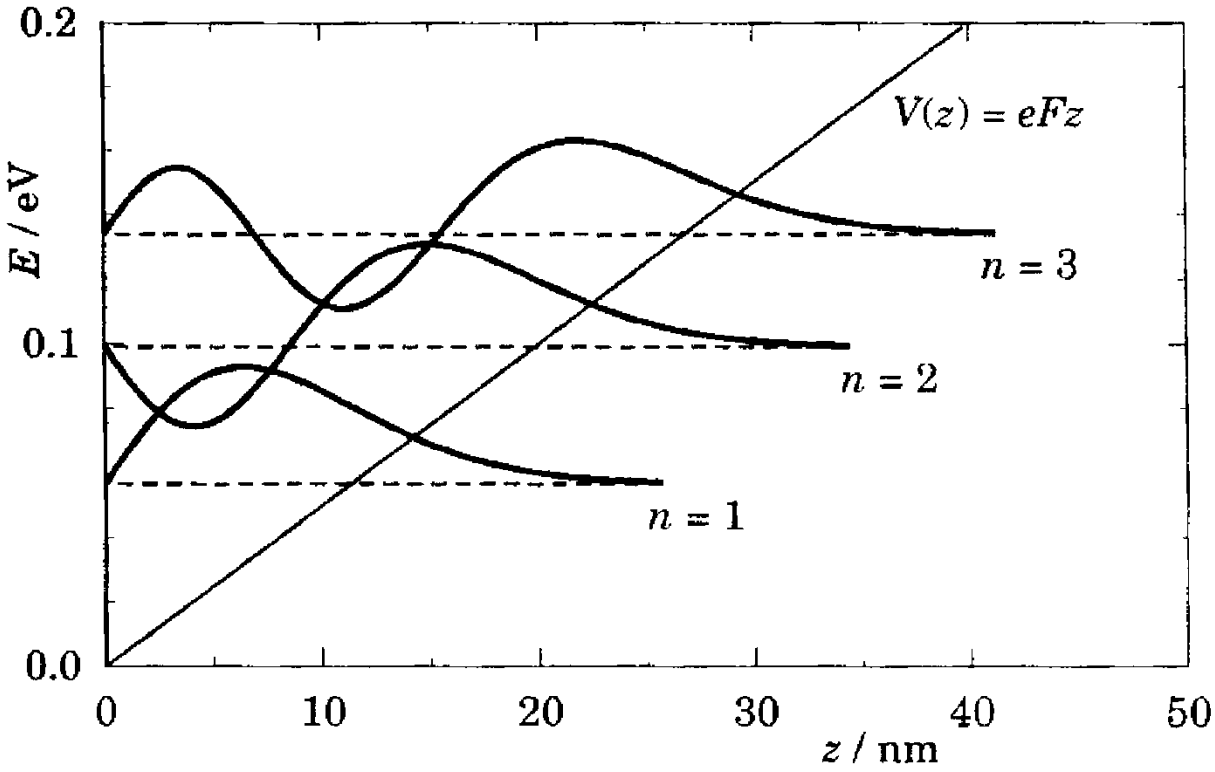


FIGURE 4.6. Triangular potential well $V(z) = eFz$, showing the energy levels and wave functions. The scales are for electrons in GaAs and a field of 5 MV m^{-1}.

Triangular well

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+eFz\right]\psi(z)=\varepsilon\psi(z)$$

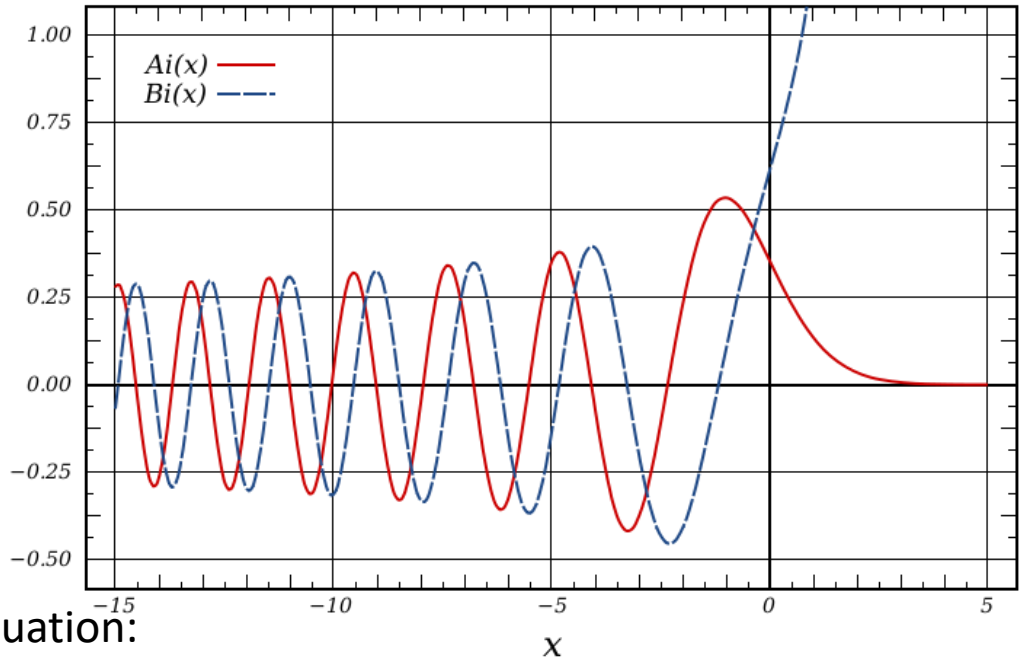
Transformation:

$$\frac{d^2}{dz^2}\psi(z)=\frac{2m}{\hbar^2}(eFz-\varepsilon)\psi(z)$$

Substituting: $z_0=\left(\frac{\hbar^2}{2meF}\right)^{1/3}$

$$\varepsilon_0=eFz_0=\left[\frac{(eF\hbar)^2}{2m}\right]^{1/3},\ \bar{z}=\frac{z}{z_0},\ \bar{\varepsilon}=\frac{\varepsilon}{\varepsilon_0}$$

$$\frac{d^2}{dz^2}\psi(z)=\frac{2m}{\hbar^2}(eFz-\varepsilon)\psi(z)$$



The equation reduces to Stokes or Airy equation:

$$\frac{d^2}{dz^2}f(z)=zf(z)$$

Its two independent solutions the Airy functions $Ai(z)$ and $Bi(z)$. The solutions of the equation are the zeros of a function $Ai(z)$ (after some rearrangements).

Triangular well

$$V(z) = eFz$$

$$\varepsilon_n = c_n \left[\frac{(eFz)^2}{2m}\right]^{1/3}$$

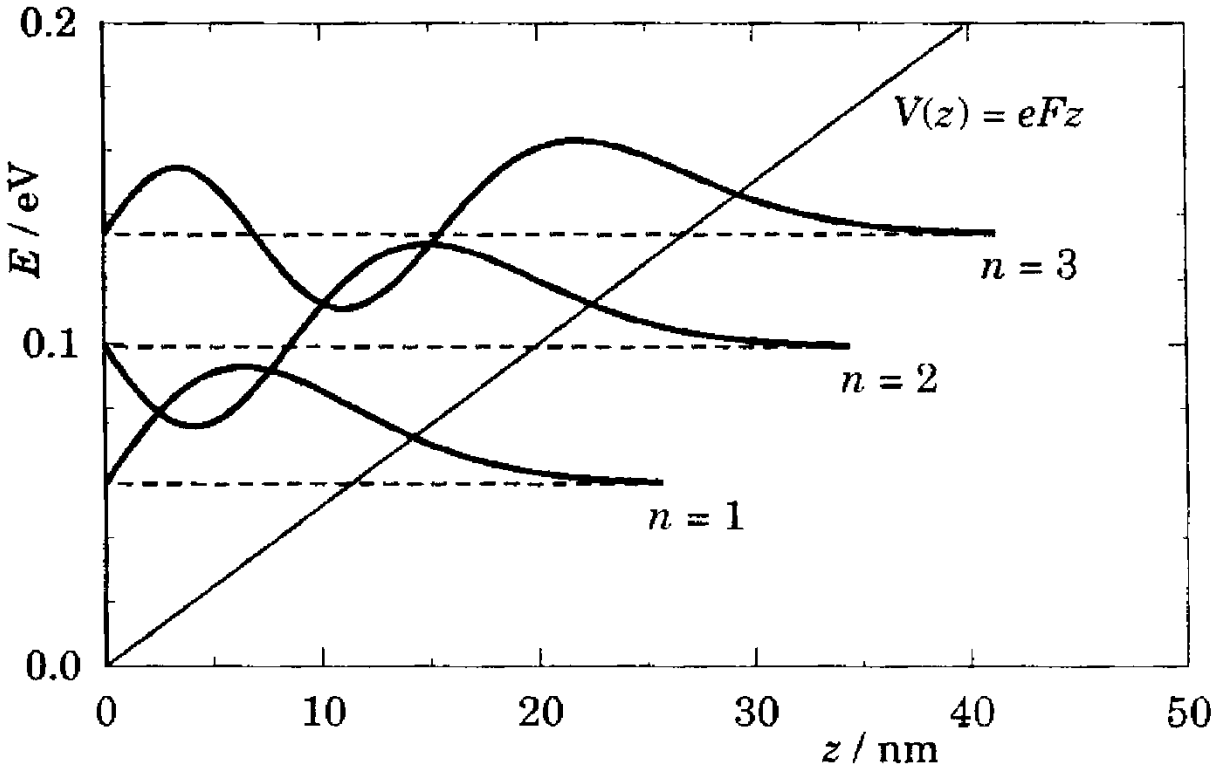


FIGURE 4.6. Triangular potential well $V(z) = eFz$, showing the energy levels and wave functions. The scales are for electrons in GaAs and a field of 5 MV m^{-1}.

WKB approximation

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly changing potential

It is also known as the **LG** or **Liouville–Green** method or **JWKB** and **WKBJ**, where the "J" stands for Jeffreys or *phase integral method* **or** *semi-classical approximation*.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x)$$

What is slowly varing potential? It is for sure $V(x)=V_0=const$. The solution for this potential is a plane wave $\psi(x)=e^{ikx}$ - phase of the wavefunction $k(x)=k=const$ is constant in the whole space $k^2=\frac{2m}{\hbar}[E-V_0]$

Let's define $k^2(x)=\frac{2m}{\hbar}[E-V(x)]$ - we want the phase $k(x)$ to be slowly varying in space, i.e.

$$\left|\frac{dk}{dx}\right| \ll k^2$$

(such condition).

We are looking for the solution $\psi(x)=e^{i\chi(x)}$ where $\chi(x)$ is the phase of the wavefunction.

WKB approximation

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly changing potential

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x)$$

Let's define $k^2(x)=\frac{2m}{\hbar}[E-V(x)]$ - slowly varing in real space $k(x)$.

We are looking for the solutuion $\psi(x)=e^{i\chi(x)}$ where $\chi(x)$ its the phase of the wavefunction.

Inserting into Schrodinger equation:

$[\chi'(x)]^2-i\chi''(x)=\frac{2m}{\hbar}[E-V(x)]\equiv k^2(x)$ - this is rigorous.

Zero-order WKB approximation assumes $[\chi'(x)]^2 \gg |\chi''(x)|$ czyli $\chi''(x)\approx 0$

$[\chi'(x)]^2=k^2(x)$ czyli

$$\chi(x)=\pm\int^x k(x')dx'$$

Usually we expand more

$$[\chi'(x)]^2=k^2(x)+i\chi''(x)=k^2(x)+i[\chi'(x)]'\approx k^2(x)\pm i[k(x)]'$$

Thus:

$$\chi'(x)\approx\pm k(x)\sqrt{1+\frac{ik'(x)}{k^2(x)}}\approx\pm\, k(x)+\frac{ik'(x)}{2k(x)}$$

WKB approximation

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly changing potential

Typically, the WKB method continues into

$$[\chi'(x)]^2 = k^2(x) + i\chi''(x) = k^2(x) + i[\chi'(x)]' \approx k^2(x) \pm i[k(x)]'$$

Thus:

$$\chi'(x) \approx \pm k(x)\sqrt{1 + \frac{ik'(x)}{k^2(x)}} \approx \pm\, k(x) + \frac{ik'(x)}{2k(x)}$$

therefore:

$$\chi(x) = \pm \int^x k(x')dx' + \frac{i}{2}\ln k(x)$$

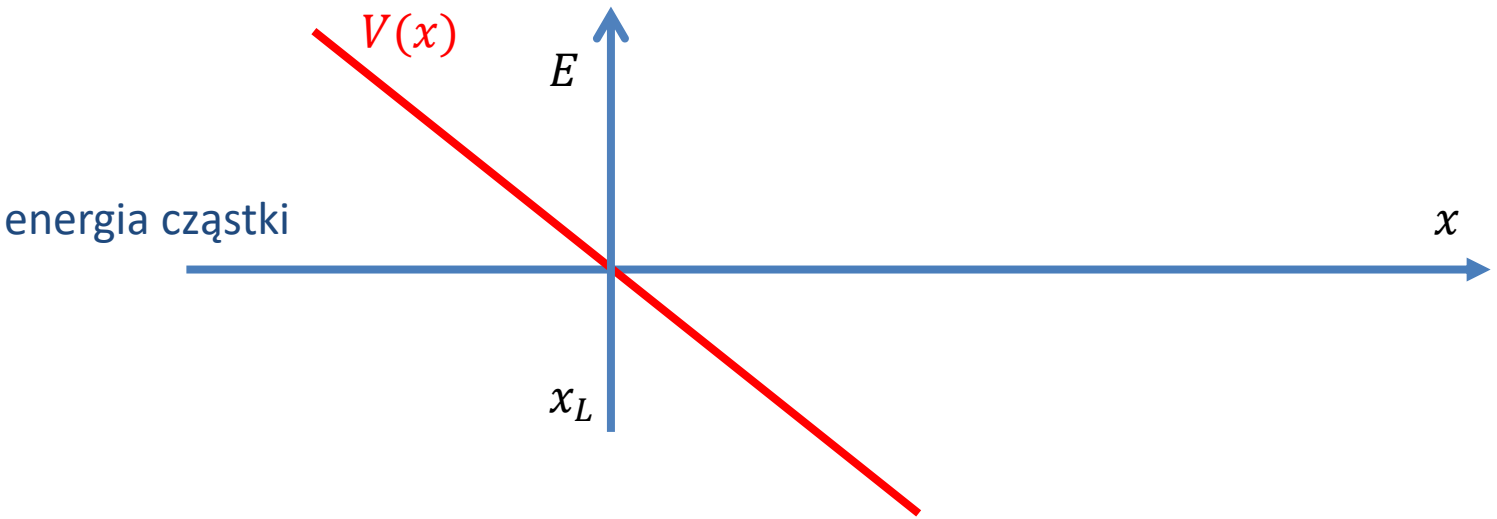
We get:

$$\psi(x) \approx \frac{1}{\sqrt{k(x)}} \exp\left[\pm i \int^x k(x')dx'\right]$$

The term $1/\sqrt{k(x)}$ - the density of probability of fast-moving particles is small for large k - OK!

WKB approximation

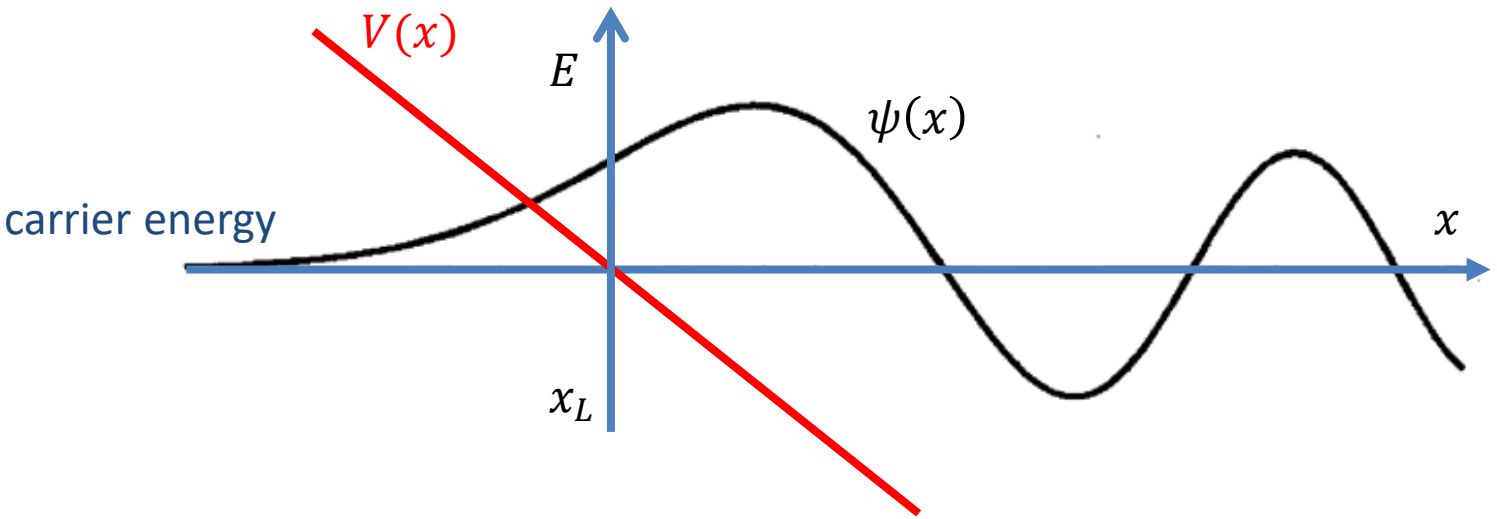
WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential



In the case of turning points (ie. the edges of the barriers well) potential changes rapidly compared with the wavelength $k(x)$ - WKB approximation is not valid (a rigorous approach avoids it by moving into the complex plane). Another way is to note that the potential is linear for a small region around the turning point Δx_L - and the Airy functions are the exact solutions. Then the solution must match on both regions near x_L.
The problem sounds complicated but fortunately the results are simple (we got additional phase).

WKB approximation

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential



$$\psi(x) \sim \frac{2}{\sqrt{k(x)}} \cos\left[\int_{x_L}^{x} k(x')dx' - \frac{\pi}{4}\right], \qquad x \gg x_L$$

$$\psi(x) \sim \frac{1}{\sqrt{\kappa(x)}} \exp\left[-\int_{x_L}^{x} \kappa(x')dx'\right], \qquad x \ll x_L$$

WKB approximation

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential

$$\psi(x) \sim \frac{2}{\sqrt{k(x)}} \cos\left[\int_{x_L}^{x} k(x')dx' - \frac{\pi}{4}\right], \qquad x \gg x_L$$

Examples:

1. „Hard" (infinitely steep) wall – the wave function goes to zero at the boundaries, so an exact number of half-wavelengths must fit between them

$$\int_{x_L}^{x_R} k(x')dx' = n\pi$$

For : $k(x) = const$ we have $k_n = \frac{n\pi}{L}$

2. „Soft wall" – an allowed state must obey the matching conditions ($x \gg x_L$, above) and at x_L it has additional phase $\left(-\frac{\pi}{4}\right)$ and similarly at x_R - next $\left(-\frac{\pi}{4}\right)$. Altogether:

$$\int_{x_L}^{x_R} k(x')dx' = \left(n - \frac{1}{2}\right)\pi$$

WKB approximation

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential

$$\psi(x) \sim \frac{2}{\sqrt{k(x)}} \cos\left[\int_{x_L}^{x} k(x')dx' - \frac{\pi}{4}\right], \qquad x \gg x_L$$

3. Triangular well of „hard" and „soft" well:

$$\int_{x_L}^{x_R} k(x')dx' = \left(n - \frac{1}{4}\right)\pi$$

Eg. Triangular well: $V(x) = eFx$ wtedy $k_n(x) = \frac{1}{\hbar}\sqrt{2m\big(E_n - V(x)\big)} = \frac{1}{\hbar}\sqrt{2m(E_n - eFx)}$

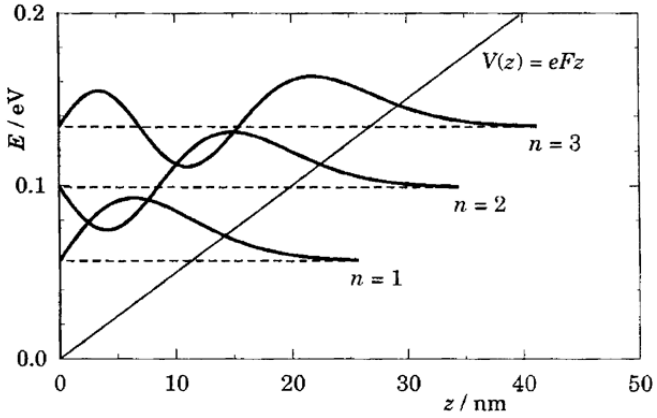
$$\int_{x_L}^{x_R} k_n(x')dx' = \int_0^{E_n/eF} \frac{1}{\hbar}\sqrt{2m(E_n - eFx')}dx' = \left[\frac{2mE_n}{\hbar^2}\right]^{1/2} \frac{E_n}{eF} \int_0^1 \sqrt{1-s}\, ds =$$

$s = \frac{x}{x_R}$

$$\left[\frac{2mE_n}{\hbar^2}\right]^{1/2} \frac{E_n}{eF} \int_0^1 \sqrt{1-s}\, ds = \frac{2}{3}\left[\frac{2mE_n}{\hbar^2}\right]^{1/2} \frac{E_n}{eF}$$

$$\int \sqrt{1-x}\, dx = -\frac{2}{3}(1-x)^{3/2} + \text{constant}$$

$$E_n = \left[\frac{3}{2}\pi\left(n - \frac{1}{4}\right)\right]^{2/3} \left[\frac{(eF\hbar)^2}{2m}\right]^{1/3}$$



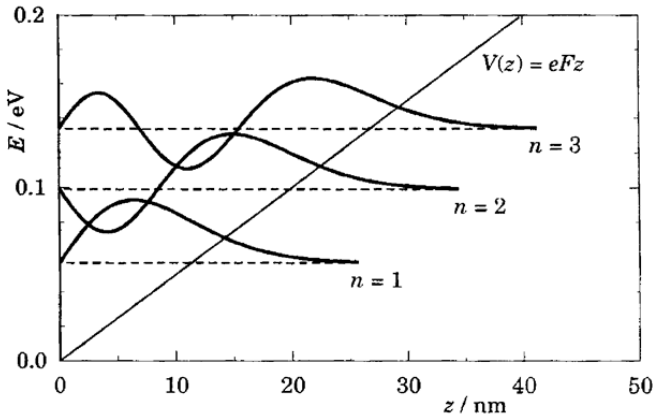
Triangular well

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential

TABLE 7.1 A comparison of various approximate methods for energy levels in a triangular potential, in units of $\varepsilon_0 = [(eF\hbar)^2/(2m)]^{1/3}$, and the exact results from the Airy function.

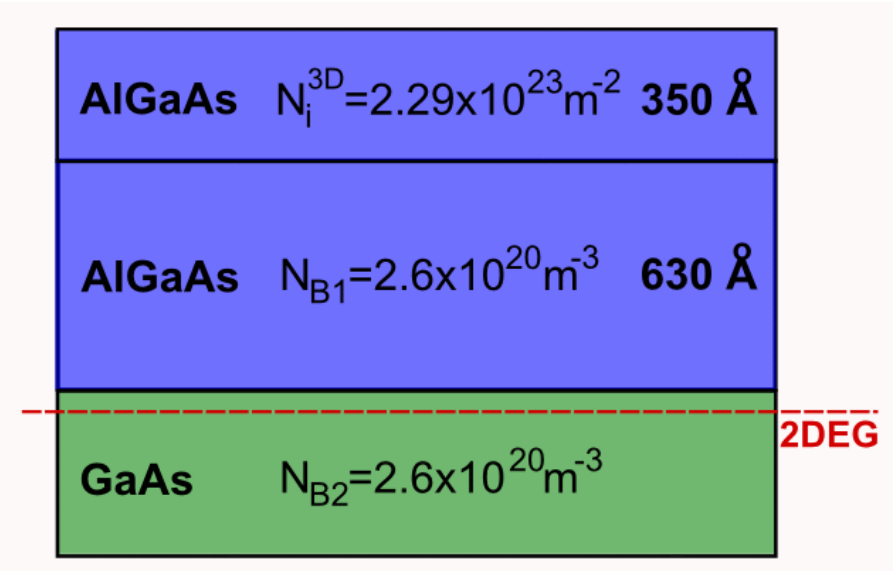
n	Airy function (exact)	WKB	Variational (Fang–Howard)	Variational (Gaussian)
1	2.3381	2.3203	2.4764	2.3448
2	4.0879	4.0818		
3	5.5206	5.5172		
⋮	⋮	⋮		
10	12.8288	12.8281		

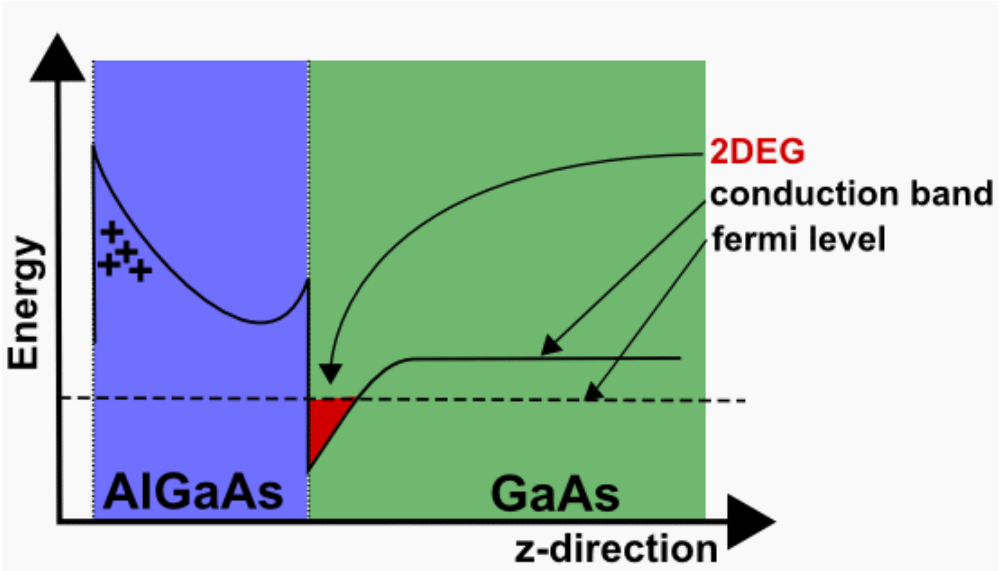
$$E_n = \left[\frac{3}{2}\pi\left(n-\frac{1}{4}\right)\right]^{2/3}\left[\frac{(eF\hbar)^2}{2m}\right]^{1/3}$$



Triangular well

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential





http://www.phys.unsw.edu.au/QED/research/2D_scattering.htm

$$E_n = \left[\frac{3}{2}\pi\left(n-\frac{1}{4}\right)\right]^{2/3}\left[\frac{(eF\hbar)^2}{2m}\right]^{1/3}$$

WKB approximation

$$V(x) = V_b\left[1 - \left(\frac{x}{d}\right)^2\right]$$

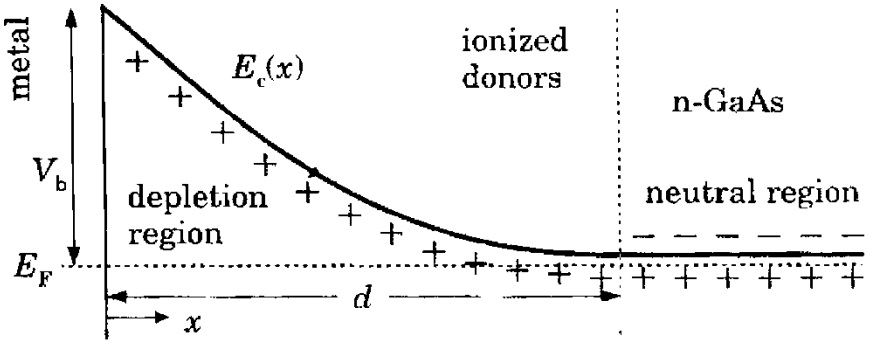


FIGURE 7.7. Schottky barrier in the conduction band $E_c(x)$ between a metal and n-GaAs. The potential is parabolic with height V_b and thickness d.

$$k_n(x) = \frac{1}{\hbar}\sqrt{2mV(x)} = \frac{1}{\hbar}\sqrt{2mV_b\left[1 - \left(\frac{x}{d}\right)^2\right]}$$

We will return discussing the transport

Low dimensional structures

Full Hamiltonian in our universe has three spatial dimensions $(x, y, z, t) = (\vec{R}, t)$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{R})\right]\psi(\vec{R}) = E\psi(\vec{R})$$

For $V(\vec{R}) = V(z)$ we obtain:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(z)\right]\psi(x, y, z) = E\psi(x, y, z)$$

Along directions x and y mamy ruch swobodny:

$$\psi(x, y, z) = \exp(ik_x x)\exp(ik_y y)\,u(z)$$

We can show (on the blackboard!), that final eigenenergies of the potential $V(z)$ are:

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

$$\varepsilon = E - \frac{\hbar^2 k_x^2}{2m} - \frac{\hbar^2 k_y^2}{2m}$$

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Low dimensional structures

$$\psi_{k_x,k_y,n}(x,y,z) = \exp(ik_x x)\exp(ik_y y)\,u_n(z) = \psi_{\boldsymbol{k},n}(\boldsymbol{r},z) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})\,u_n(z)$$

$$E_n(k_x,k_y) = \varepsilon_n + \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} \qquad E_n(\boldsymbol{k}) = \varepsilon_n + \frac{\hbar^2 \boldsymbol{k}^2}{2m}$$

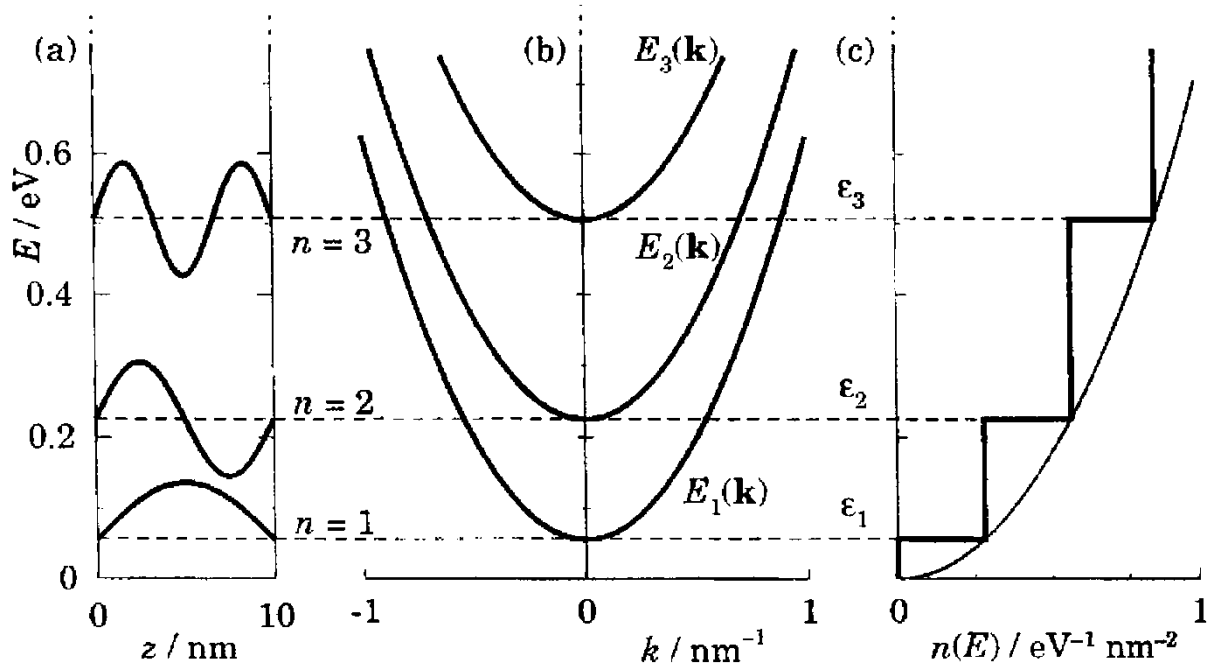


FIGURE 4.7. (a) Potential well with energy levels, (b) total energy including the transverse kinetic energy for each subband, and (c) steplike density of states of a quasi-two-dimensional system. The example is an infinitely deep square well in GaAs of width 10 nm. The thin curve in (c) is the parabolic density of states for unconfined three-dimensional electrons.

Low dimensional structures

$$\psi_{k_x,k_y,n}(x,y,z) = \exp(ik_x x)\exp(ik_y y)\,u_n(z) = \psi_{\boldsymbol{k},n}(\boldsymbol{r},z) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})\,u_n(z)$$

$$E_n(k_x,k_y) = \varepsilon_n + \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} \qquad E_n(\boldsymbol{k}) = \varepsilon_n + \frac{\hbar^2 \boldsymbol{k}^2}{2m}$$

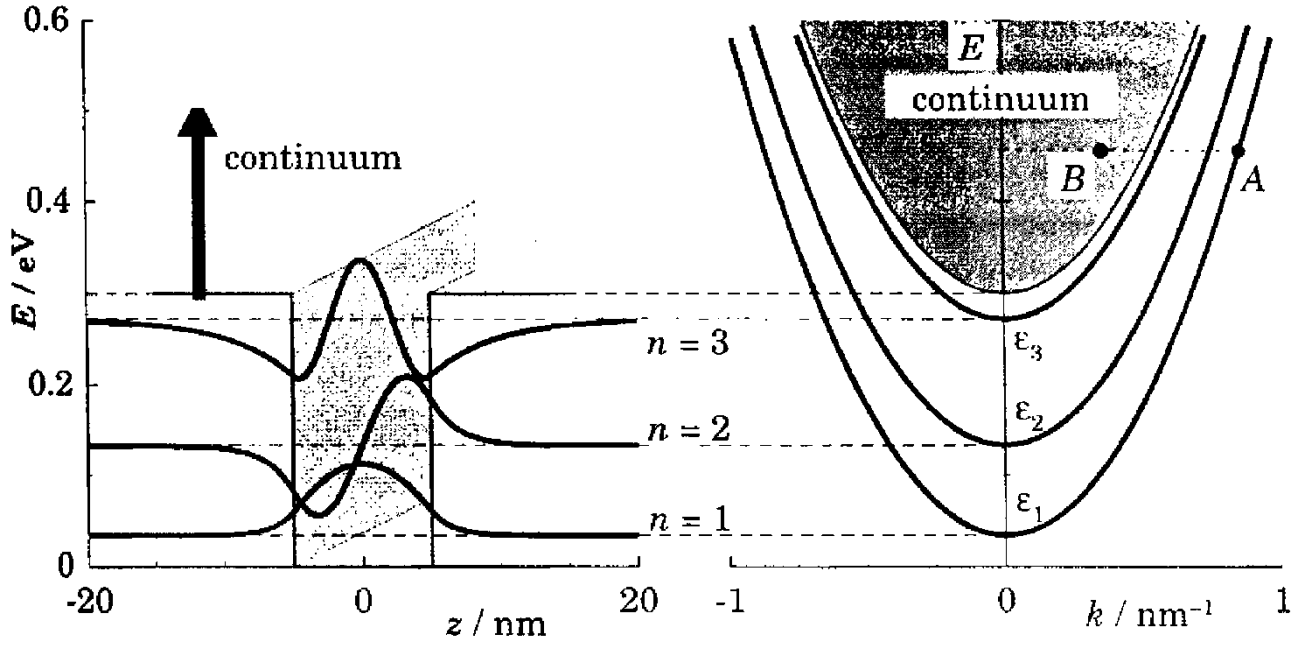
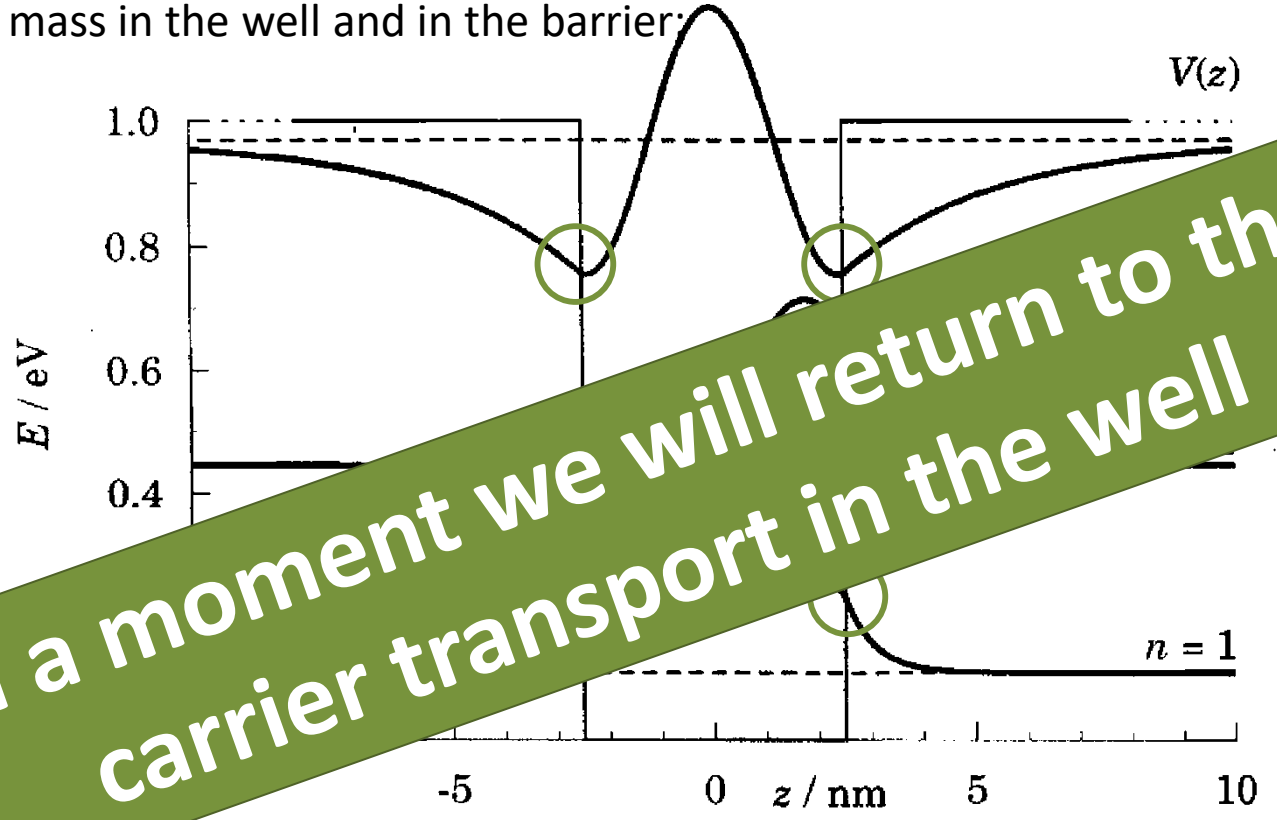


FIGURE 4.9. Quasi-two-dimensional system in a potential well of finite depth. Electrons with the same total energy can be bound in the well (*A*) or free (*B*).

Finite potential well – square well

THE DIFFERENT mass in the well and in the barrier:



In a moment we will return to the carrier transport in the well

4.12. Finite square well of depth $V_0 = 1$ eV, width $a = 5$ nm along z, and effective masses $m_W = 0.067$ in the well and $m_B = 0.15$ in the barrier.

Low dimensional structures

Effective mass in the barrier m_B and in the well m_W

$$\left[-\frac{\hbar^2}{2m_0\, m_{W,B}}\nabla^2 + V(\vec{R})\right]\psi(\vec{R}) = E\psi(\vec{R})$$

For separated wave functions: $\psi(\vec{R}) = \psi_{\boldsymbol{k},n}(\boldsymbol{r}, z) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})\, u_n(z)$

$$\left[-\frac{\hbar^2}{2m_0\, m_W}\nabla^2 + E_W\right]\psi(\vec{R}) = E\psi(\vec{R})$$

$$\left[-\frac{\hbar^2}{2m_0\, m_B}\nabla^2 + E_B\right]\psi(\vec{R}) = E\psi(\vec{R})$$

We got (on the blackboard!):

$$\left[-\frac{\hbar^2}{2m_0\, m_W}\frac{d^2}{dz^2} + \frac{\hbar^2\boldsymbol{k}^2}{2m_0\, m_W} + E_W\right]u_n(z) = \varepsilon u_n(z)$$

$$\left[-\frac{\hbar^2}{2m_0\, m_B}\frac{d^2}{dz^2} + \frac{\hbar^2\boldsymbol{k}^2}{2m_0\, m_B} + E_B\right]u_n(z) = \varepsilon u_n(z)$$

Low dimensional structures

The particle moves in the well which potentiald depends on $\boldsymbol{k}$, in fact $k = |\boldsymbol{k}|$

$$\left[-\frac{\hbar^2}{2m_0\, m_W}\frac{d^2}{dz^2} + \frac{\hbar^2\boldsymbol{k}^2}{2m_0\, m_W} + E_W\right] u_n(z) = \varepsilon u_n(z)$$

$$\left[-\frac{\hbar^2}{2m_0\, m_B}\frac{d^2}{dz^2} + \frac{\hbar^2\boldsymbol{k}^2}{2m_0\, m_B} + E_B\right] u_n(z) = \varepsilon u_n(z)$$

$$V_0(k) = (E_B - E_W) + \frac{\hbar^2 k^2}{2m_0}\left(\frac{1}{m_B} - \frac{1}{m_W}\right)$$

Np. w strukturze GaAs-AlGaAs $m_B > m_W$ więc studnia robi się „płytsza”

The particle gains partially the effective mass of the barrier:

$$E_n(k) = \varepsilon_n(k) + \frac{\hbar^2 k^2}{2m_0 m_W} \approx \varepsilon_n(k=0) + \frac{\hbar^2 k^2}{2m_0 m_{eff}}$$

energy of the bond state depends on k

$$m_{eff} \approx m_W P_W + m_B P_B$$

prawdopodobieństwo znalezienia cząstki

Low dimensional structures

The particle moves in the well which potentiald depends on $\boldsymbol{k}$, in fact $k = |\boldsymbol{k}|$

$$\left[-\frac{\hbar^2}{2m_0\, m_W}\frac{d^2}{dz^2} + \frac{\hbar^2\boldsymbol{k}^2}{2m_0\, m_W} + E_W\right] u_n(z) = \varepsilon u_n(z)$$

$$\left[-\frac{\hbar^2}{2m_0\, m_B}\frac{d^2}{dz^2} + \frac{\hbar^2\boldsymbol{k}^2}{2m_0\, m_B} + E_B\right] u_n(z) = \varepsilon u_n(z)$$

$$V_0(k) = (E_B - E_W) + \frac{\hbar^2 k^2}{2m_0}\left(\frac{1}{m_B} - \frac{1}{m_W}\right)$$

Np. w strukturze GaAs-AlGaAs $m_B > m_W$ więc studnia robi się „płytsza”

TABLE 4.2 Dependence on transverse wave vector $\mathbf{k}_\perp$ of the energies of the states bound in a well 5 nm wide and 1 eV deep, with effective mass $m_W = 0.067$ inside the well and $m_B = 0.15$ outside.

k	$\frac{\hbar^2k^2}{2m_0m_W}$	$\frac{\hbar^2k^2}{2m_0m_B}$	$V_0(k)$	ε_1	ε_2	ε_3	m_{eff}
(nm^{-1})	(eV)	(eV)	(eV)	(eV)	(eV)	(eV)	
0.0	0.000	0.000	1.000	0.108	0.446	0.969	0.067
0.5	0.142	0.064	0.921	0.106	0.435	0.919	0.069
1.0	0.570	0.254	0.685	0.096	0.397	—	0.076