ECE 162A
Mat 162A

Lecture #17

Heterostructures, Band diagrams, Quantum Structures

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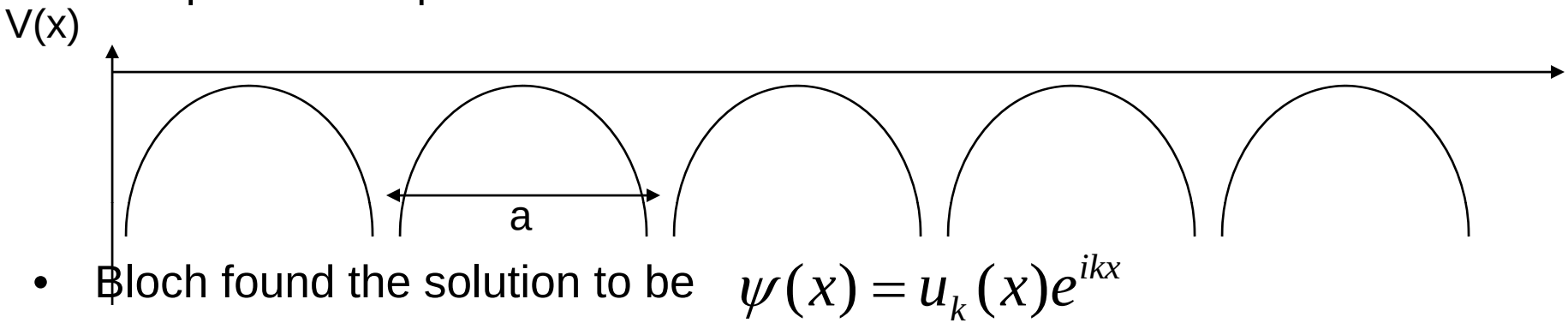
Final

- December 9, 12-3 p.m.
- 3 hours
- 2 sides of 8.5x11” crib sheet.
- 5 problems:
  - Band theory
  - Confined electron (in a compound semiconductor heterostructure)
  - Scattered electron (in a compound semiconductor heterostructure)
  - Angular momentum
  - Hydrogen atom
- Conceptual questions (short answers)
- Material covered: Eisberg/Resnick Chapters 1-9,11,13 plus lecture notes.

How do electrons move through a lattice?

- The potential is periodic:



- Bloch found the solution to be $\psi(x) = u_k(x)e^{ikx}$

$$\Psi(x,t) = u_k(x)e^{ikx-\omega t}$$

- The uk(x) are the Bloch functions.

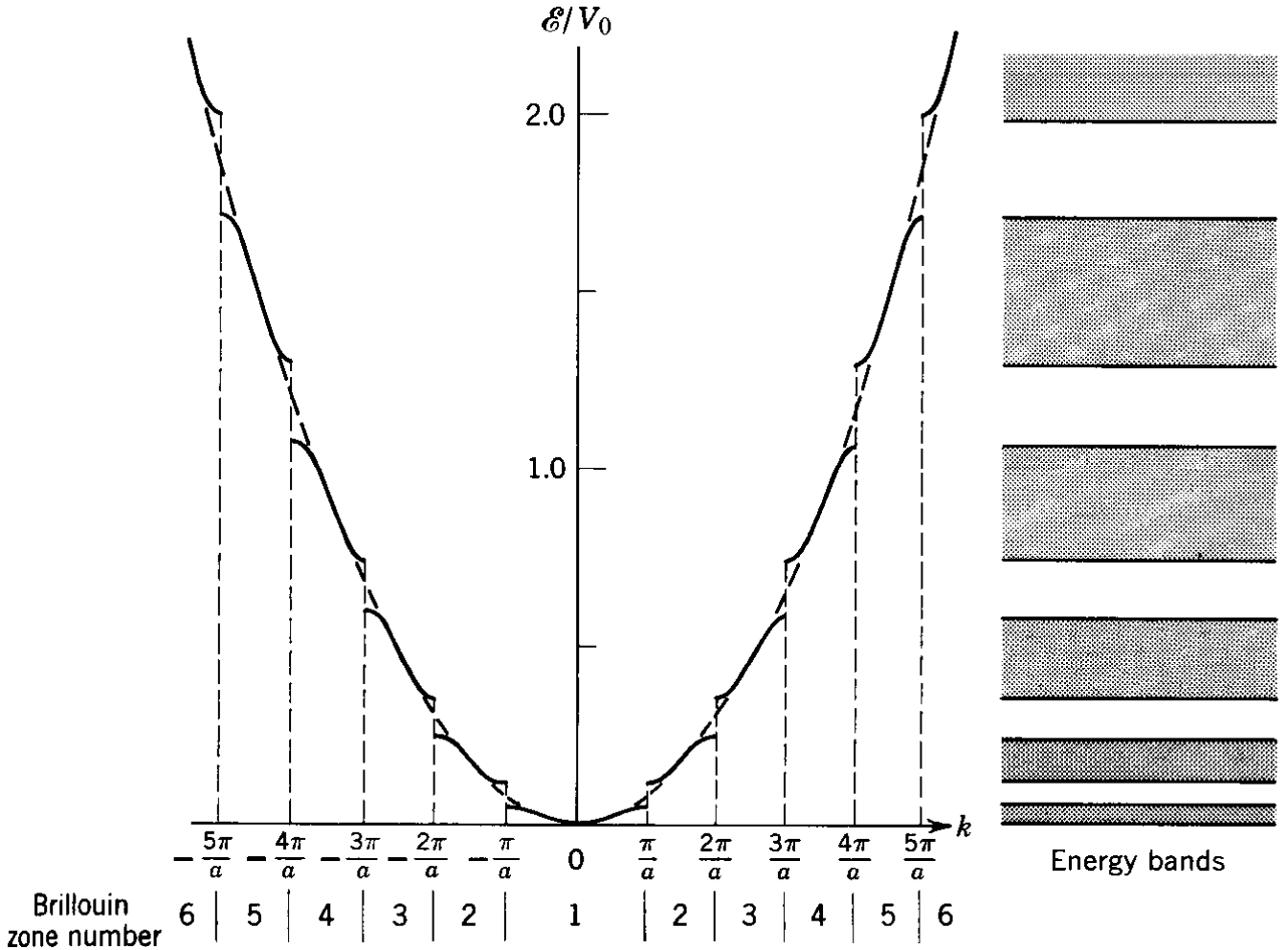
$$u_k(x) = u_k(x+a) = u_k(x+na)$$

- The free motion of the electron through the lattice is given by

$$e^{ikx-\omega t}$$

Energy Bands

- Extended zone



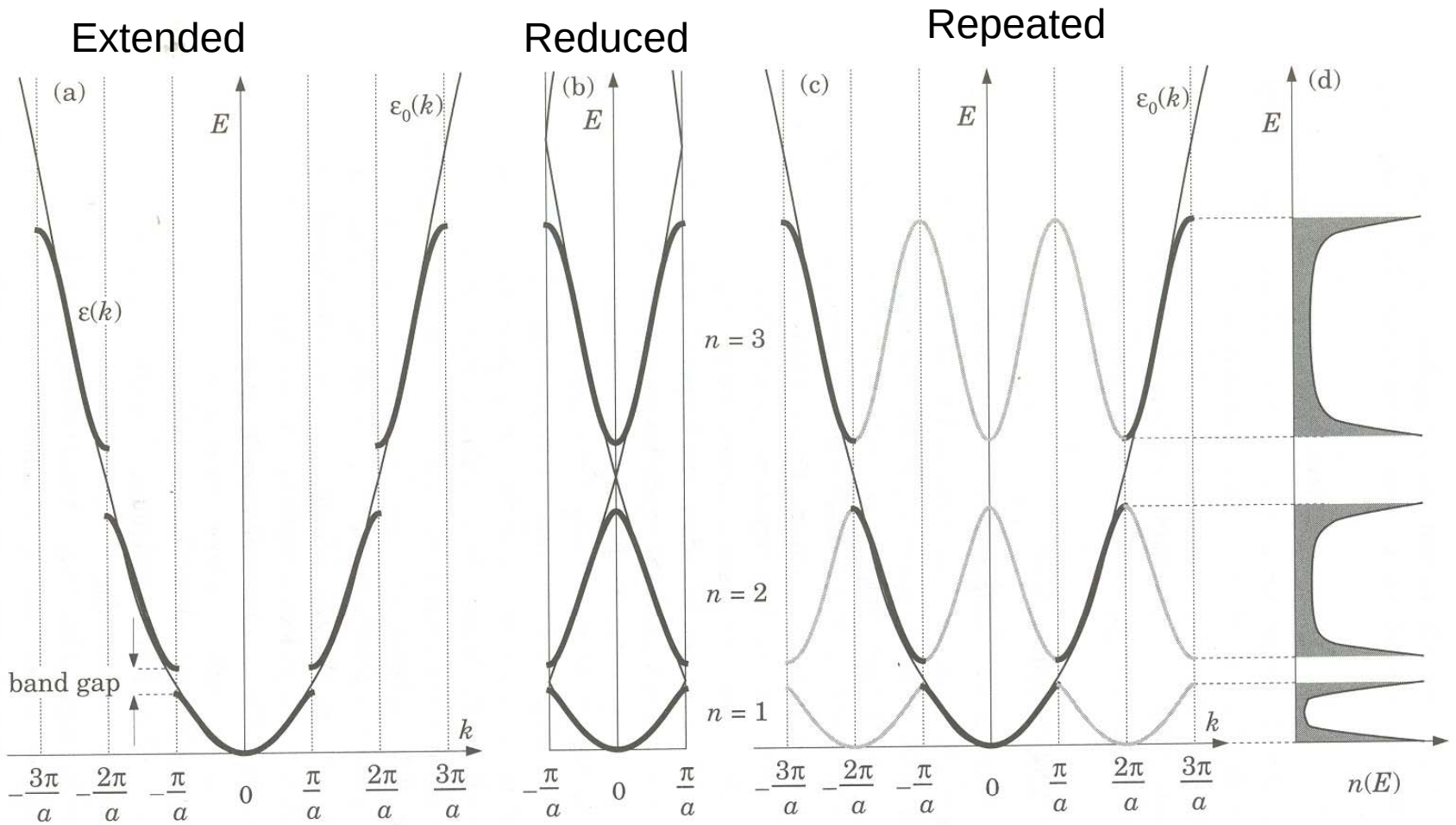


Figure 2.2. Band structure of a one-dimensional crystal in the (a) extended, (b) reduced, and (c) repeated zone schemes, and (d) the density of states as a function of energy. The thick lines show $\varepsilon(k)$ in a weak periodic potential, with bands labelled by n, while the thin parabola is $\varepsilon_0(k)$ for free electrons. The grey lines are periodic repeats.

Actual Crystal Lattices

Γ: k=0
L: [111] direction
X: [100] direction

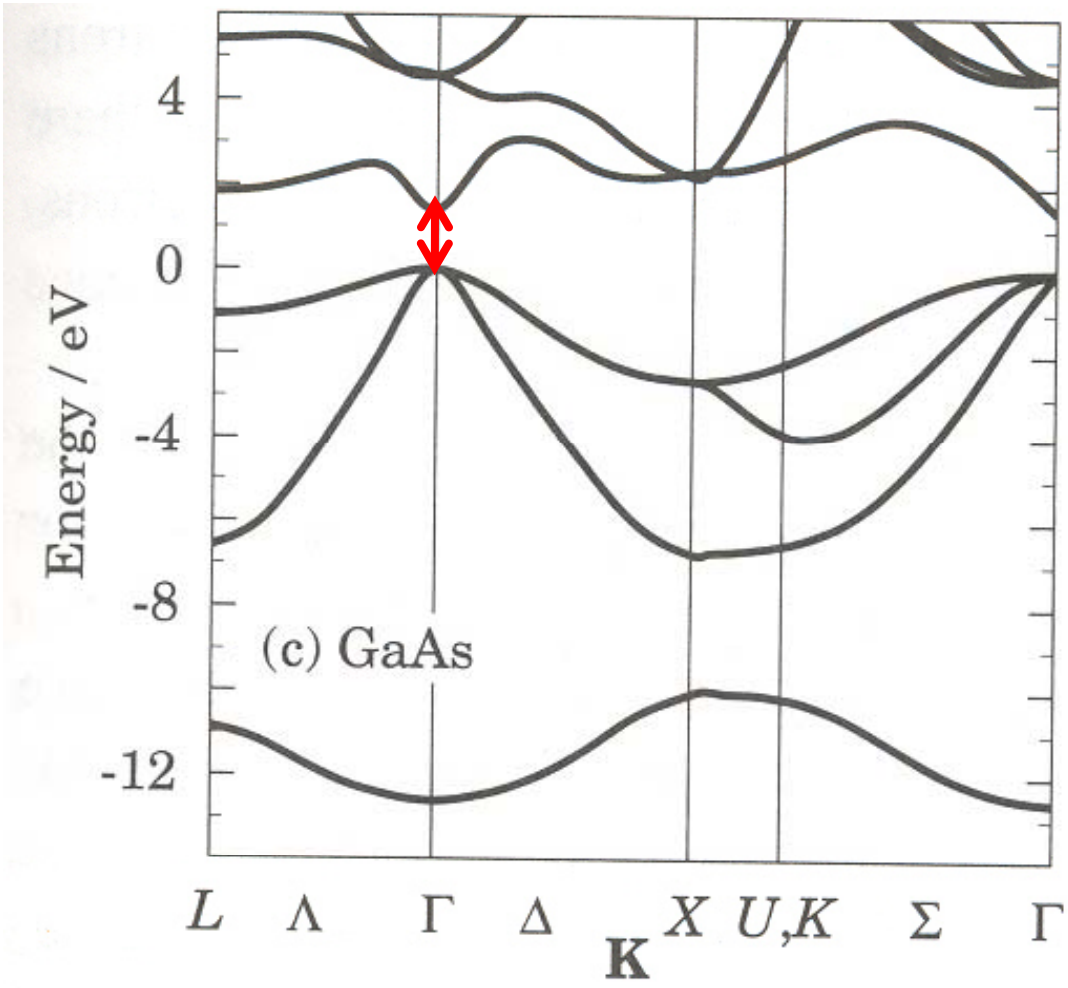


FIGURE 2.16. Band structure of four common arsenide, and aluminium arsenide. The calculations kindly supplied by Prof. G. P. Srivastava, Universit

Actual Crystal Lattices

G: k=0
L: [111] direction
X: [100] direction

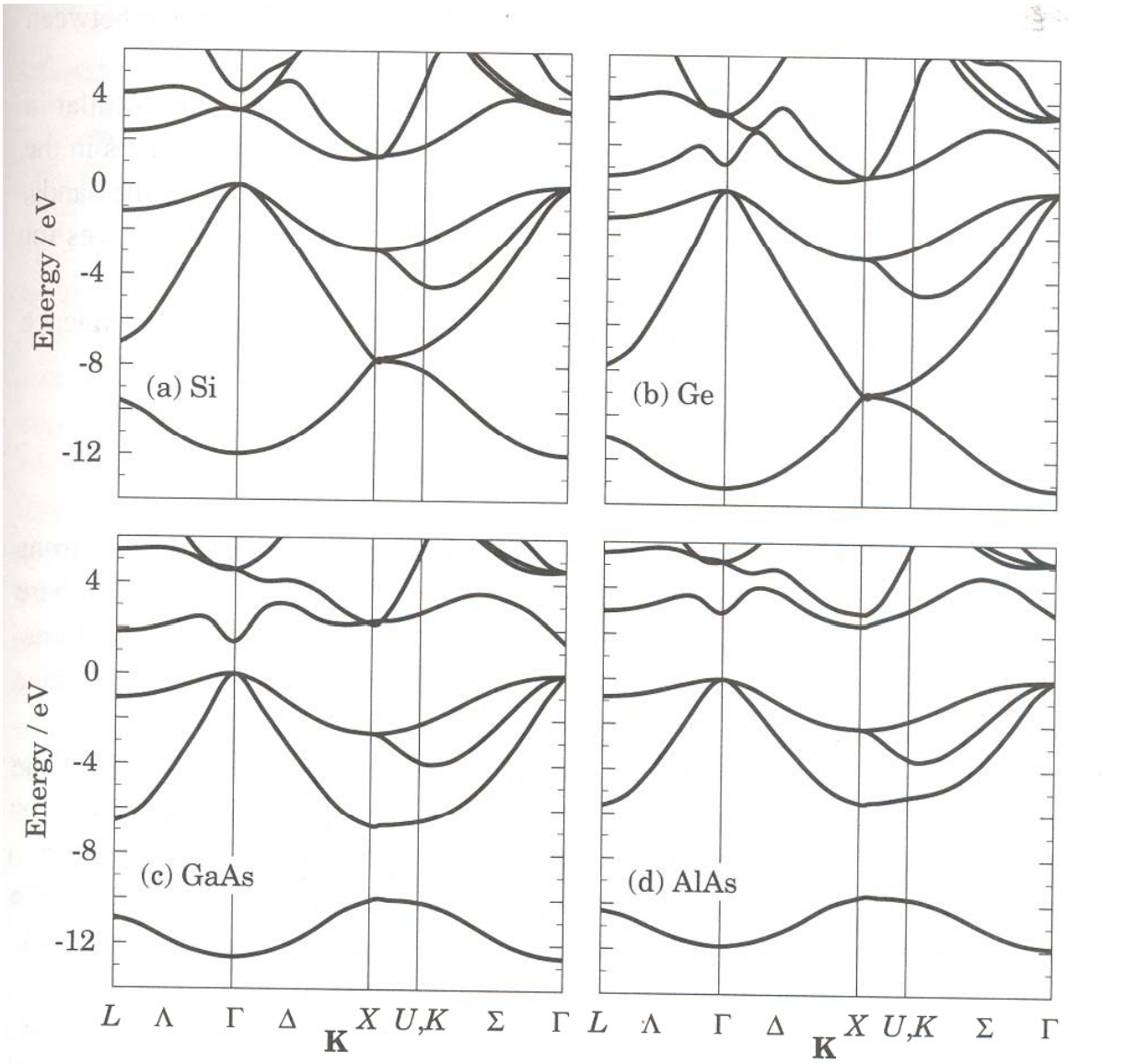


FIGURE 2.16. Band structure of four common semiconductors: silicon, germanium, gallium arsenide, and aluminium arsenide. The calculations do not include the spin–orbit coupling. [Results kindly supplied by Prof. G. P. Srivastava, University of Exeter.]

GaAs Valence Band Structure

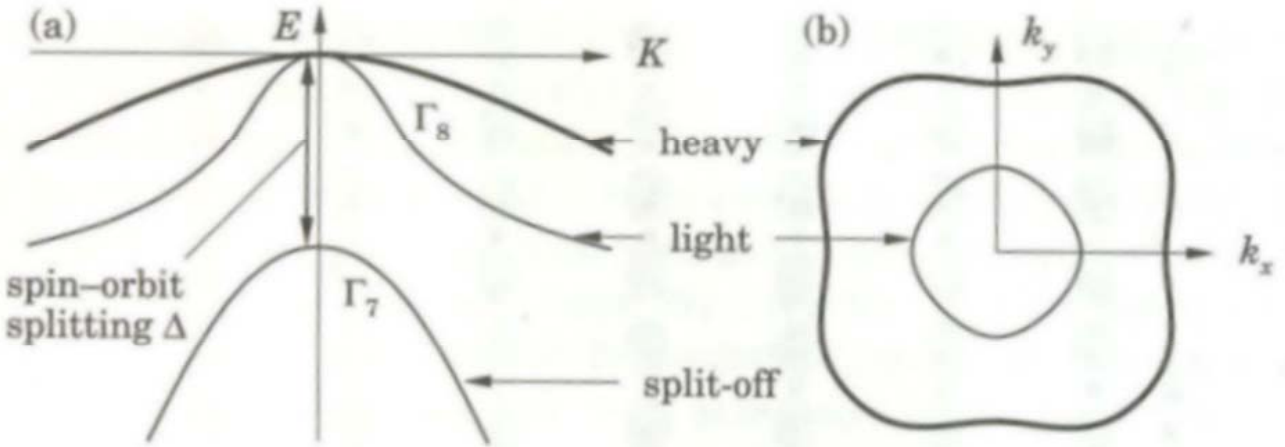


FIGURE 2.18. (a) Top of the valence band showing light and heavy holes, and the split-off band. (b) Constant-energy surfaces or 'warped spheres' for light and heavy holes in GaAs.

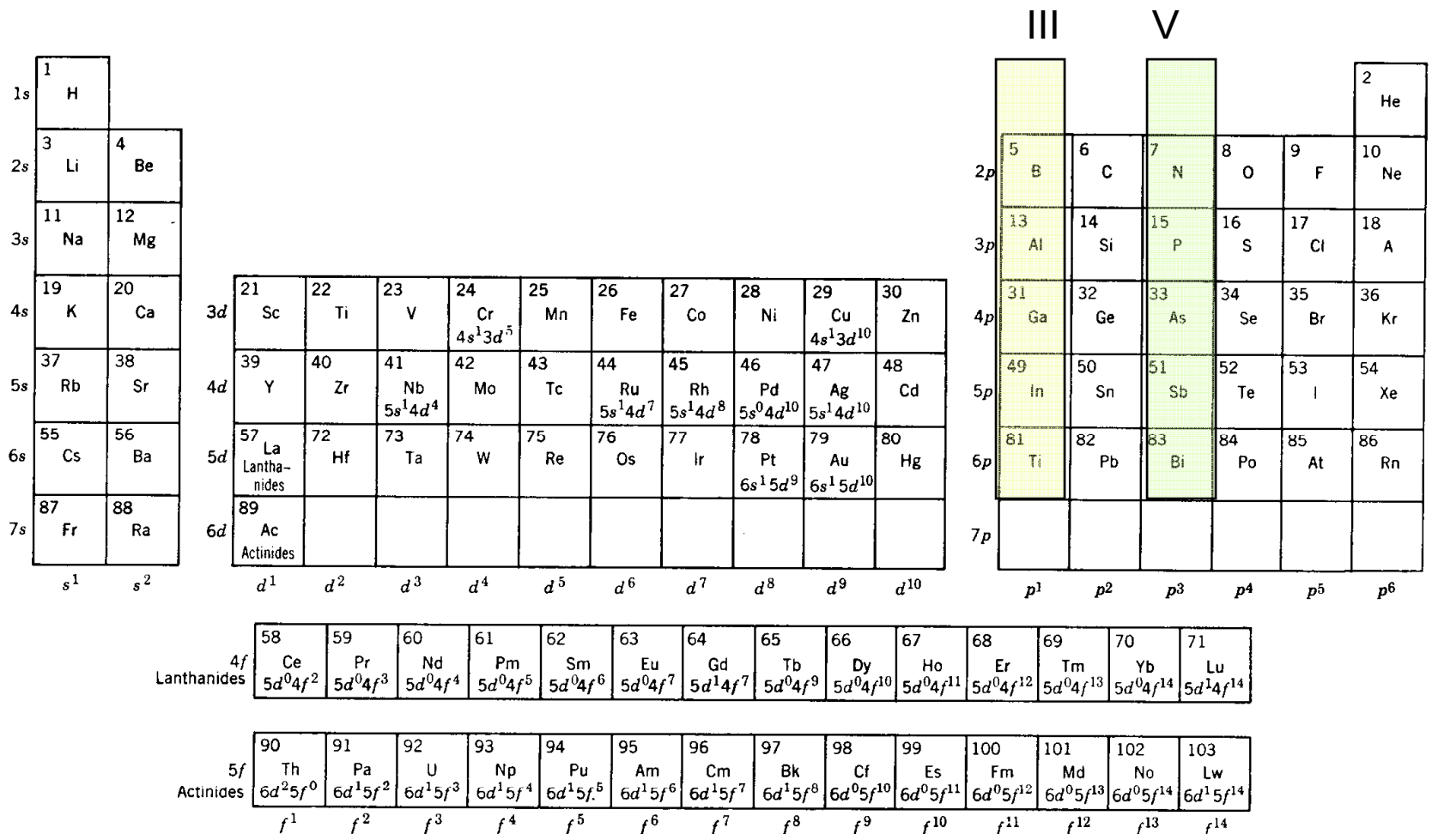
derived already. Near Γ their dispersion is *very roughly* described by

$$\varepsilon(\mathbf{K}) = E_v - \frac{\hbar^2 K^2}{2m_0 m_h}, \tag{2.20}$$

Compound Semiconductors

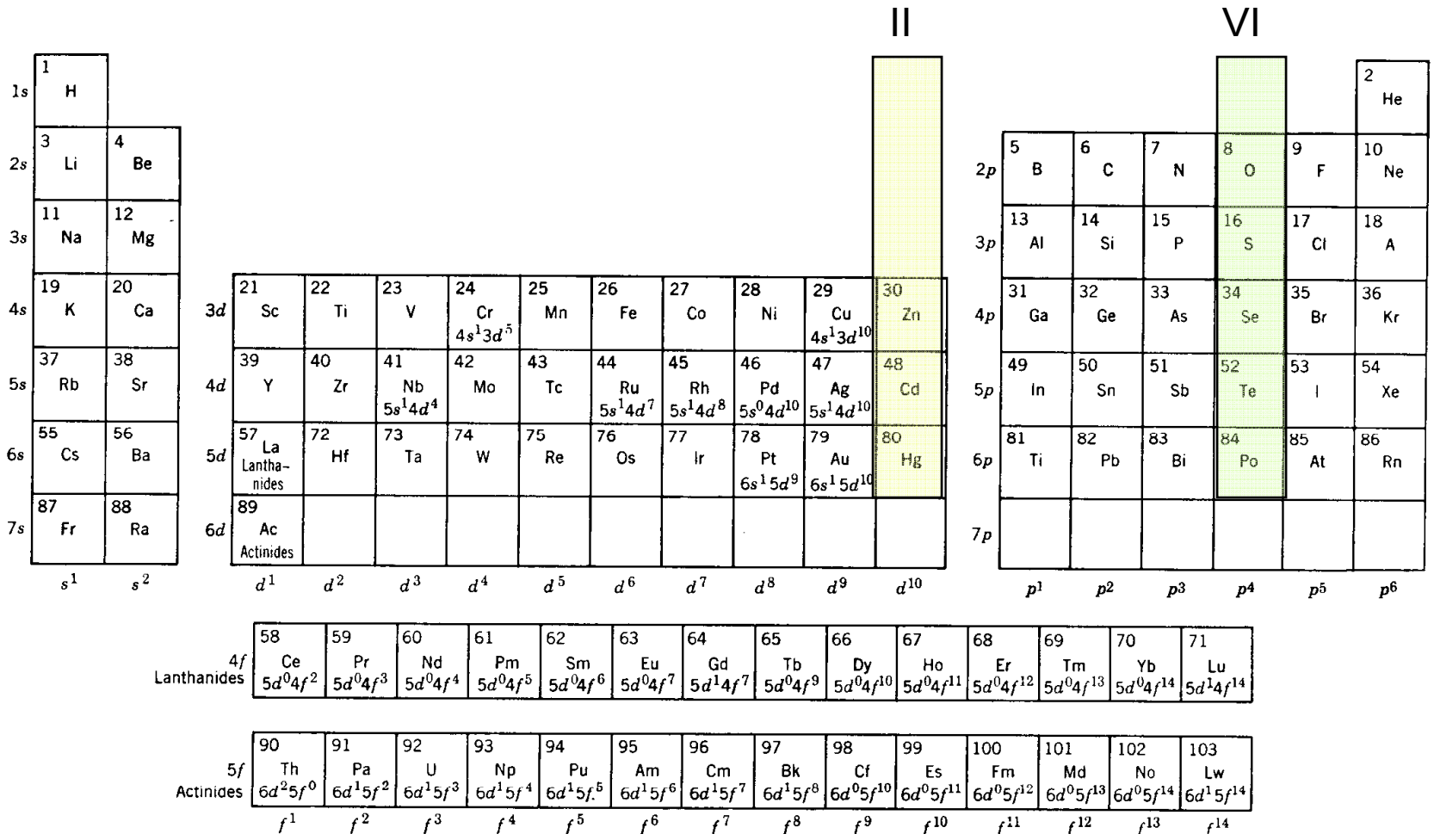
- Tetrahedrally bonded in a zinc blende structure.
- Several varieties: III-V compounds
- II-VI compounds.

III-V Compound Semiconductors



GaN, GaP, GaAs, GaSb, InN, InP, InAs, InSb, AlN, AlP, AlSb, …

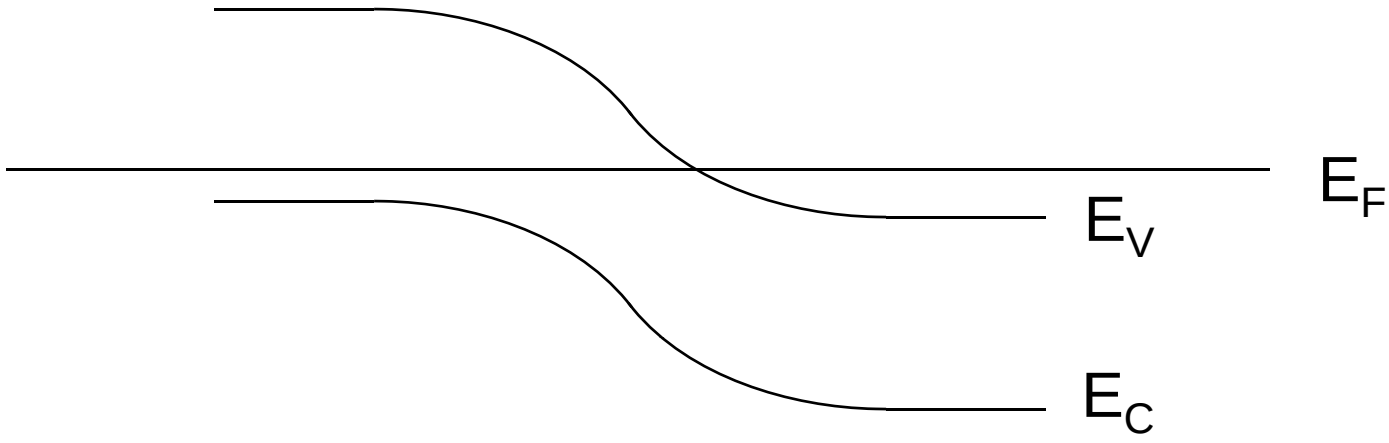
II-Vi Compound Semiconductors



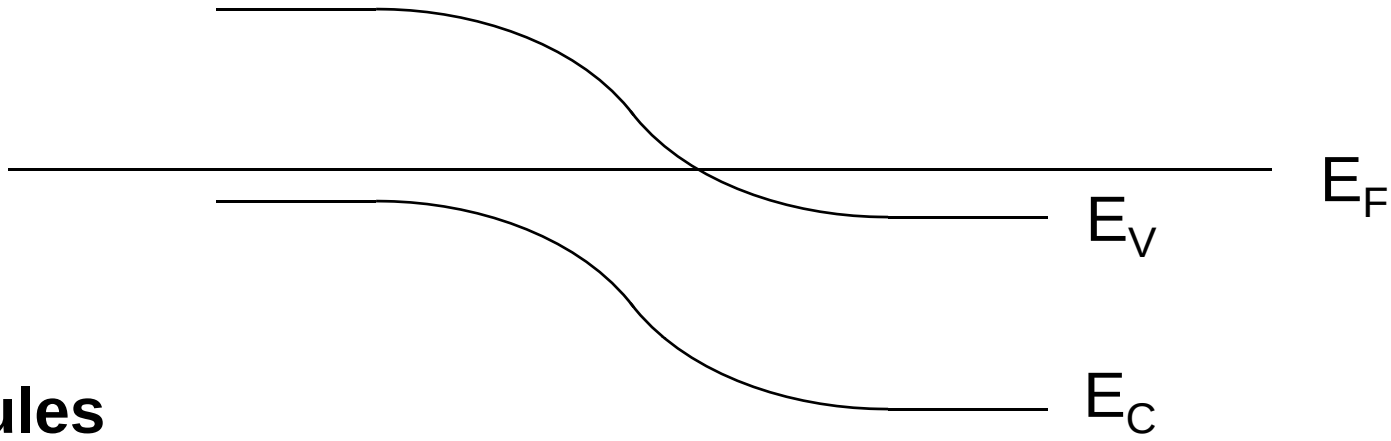
Semiconductor Problems

- p-n junction in GaAs
- E_G=1.42 eV
- N_C=4.7 x 10^{17} cm^{-3}
- N_V=7x10^{18} cm^{-3}
- n_i=2.1x10^{6} cm^{-3}
- In equilibrium, the Fermi level is constant across the structure.
- Draw a p-n junction in GaAs for N_D=10^{18} cm^{-3} and N_A=10^{17} cm^{-3}

p-n junction in GaAs



p-n junction in GaAs



Rules

1. Valence bands and conduction bands equadistant and parallel everywhere (constant bandgap).
2. Fermi energy E_F is constant in equilibrium.
3. Quadratic variation of band edge (constant doping, depletion edge approximation).
4. Fermi level to band edge separation appropriate for doping.

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho}{\varepsilon} = -\frac{p - n + N_D - N_A}{\varepsilon}$$

Binaries

- Bandgap always fixed.
- Lattice constant always fixed.
- Consequently, you can grow large boules of binaries, and cut identical substrates out of the boule.
- Fermi level depends on doping.

Ternary Materials

- Binary materials always have a particular bandgap and a particular lattice constant.
- However, many times we need intermediate bandgaps, not provided in nature. Or we wish to make a square well, or some other heterostructure.
- Ternaries:
  - $Ga_xAl_{1-x}As$
  - $Hg_xCd_{1-x}Te$
  - These are both mixtures on the group III site. Mixtures on the group V site are also possible.

Ternary Materials

- Mix two binaries together. The bandgap is approximately the arithmetic average of the two (Vegard's law) e.g. $Ga_xAl_{1-x}As$
- There are two types of sites: group III and group V. (II-VI compounds also possible).
- Ternaries cannot be grown on binary substrates in general because the lattice constants don't line up and dislocations occur. Special case: $Ga_xAl_{1-x}As$ because the lattice constants of GaAs and AlAs are almost equal.

Quaternary materials

- To match bandgap and lattice constant, two degrees of freedom are required.
- Example: $Ga_xIn_{1-x}As_yP_{1-y}$
  - X is the fraction of group III sites occupied by Ga.
  - Y is the fraction of group V sites occupied by As.
- In a bandgap chart, the dots are binaries, the lines are ternaries, and the regions bounded by 4 lines are quaternaries.

Need for lattice matching: Small amounts of strain can be accommodated. Large amounts of strain result in dislocations.

3.6.1 STRUCTURAL ASPECTS OF STRAINED LAYERS

Two extreme outcomes are possible if a material is grown on one with a different lattice constant, say, InGaAs on GaAs. In equilibrium InGaAs has a larger lattice constant (Figure 3.12(a)). Assume that the GaAs substrate is so thick that it cannot be distorted significantly. If the InGaAs is thin, it can strain to conform to the GaAs in the plane of the junction as in Figure 3.12(b). Thus its lattice constant in the plane is

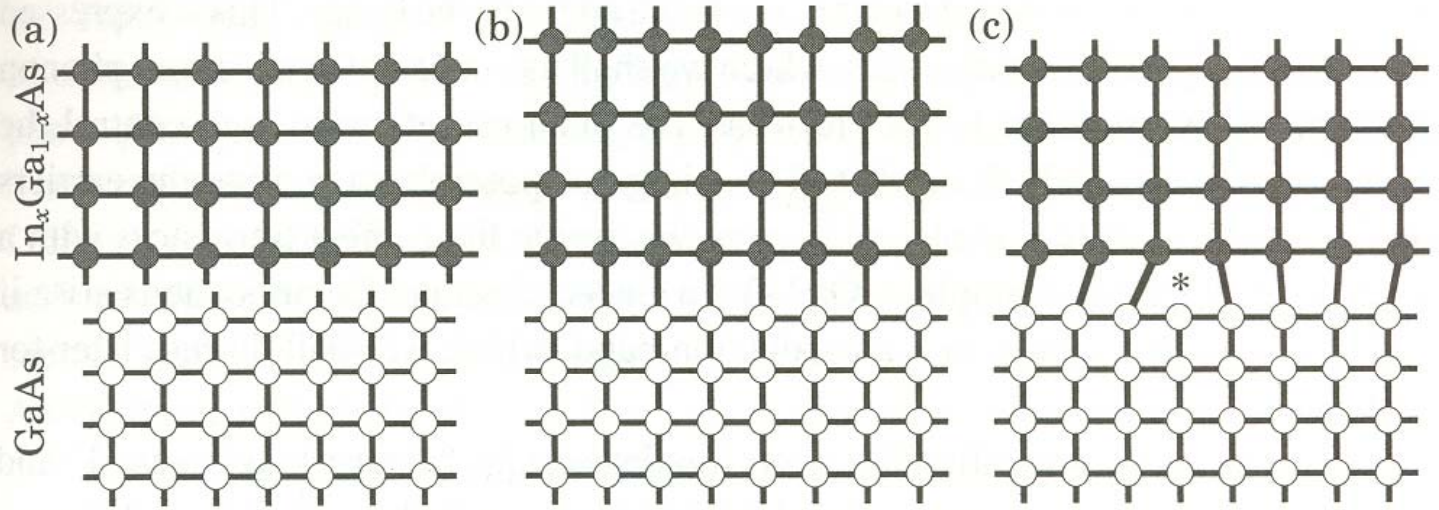
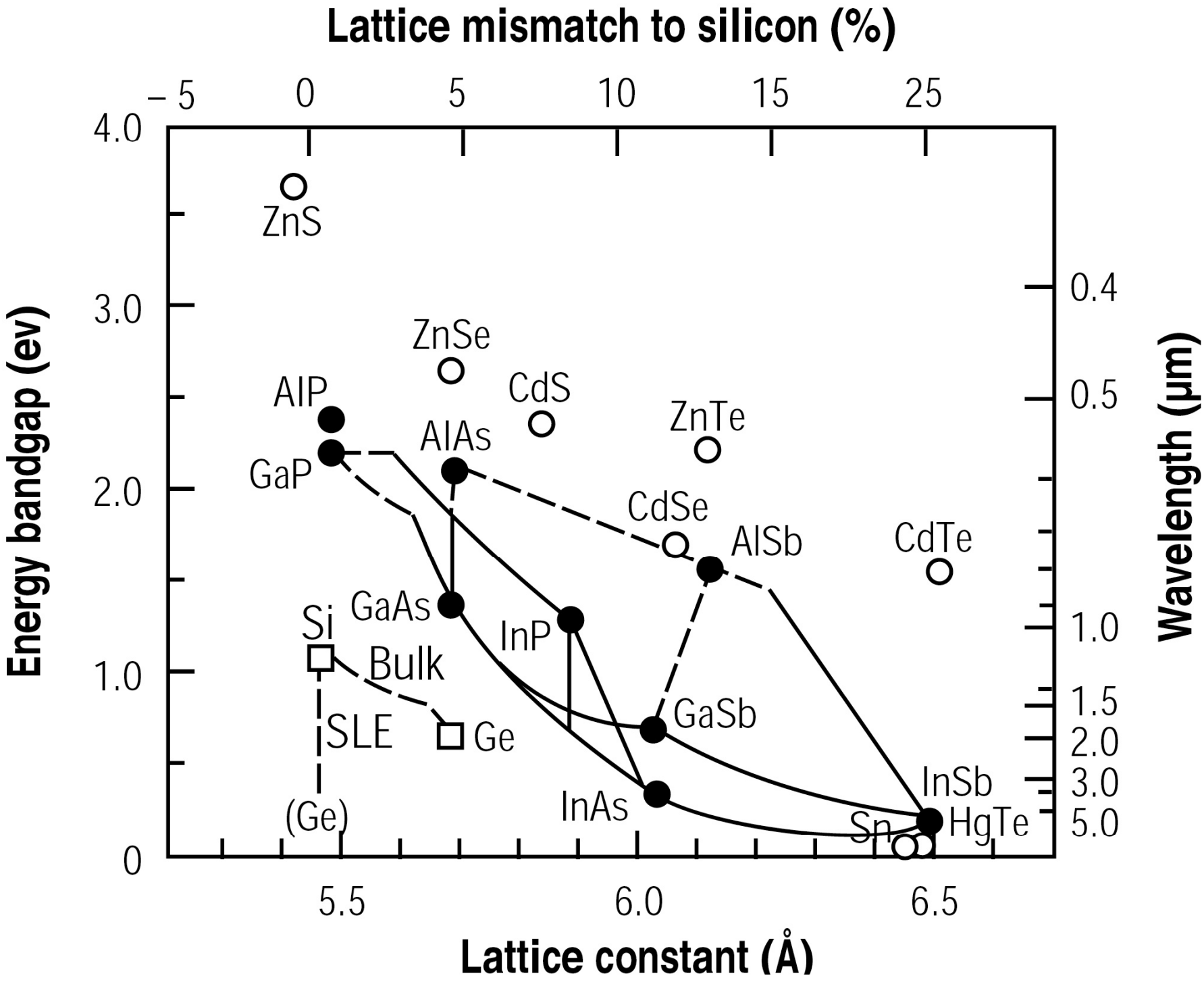


FIGURE 3.12. Growth of $In_xGa_{1-x}As$ on a GaAs substrate. (a) Separate layers at equilibrium. (b) Thin layer of InGaAs on GaAs. The InGaAs is strained to conform to the lattice constant of GaAs in the plane of the heterojunction. (c) Thicker layer, where the strain has relaxed due to a misfit dislocation at the heterointerface, shown by an asterisk.

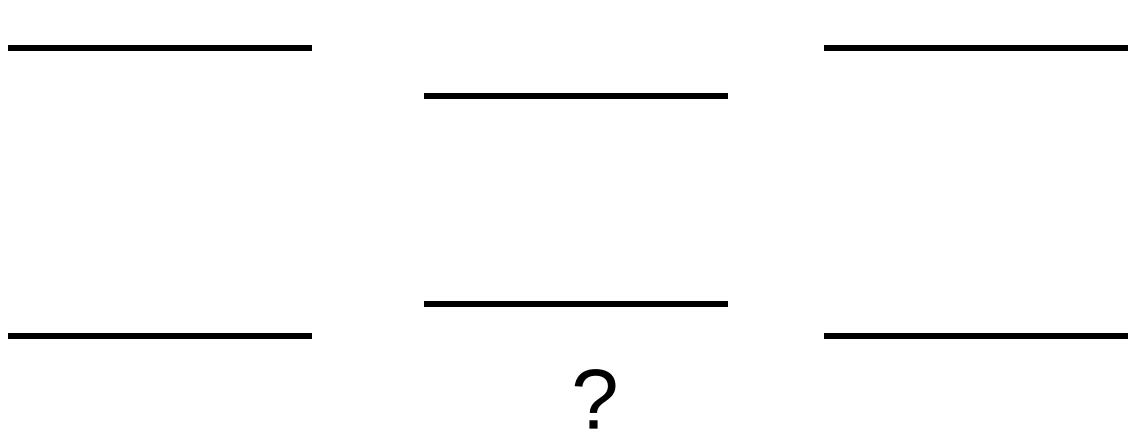

Lattice mismatch to silicon (%)
– 5
0
5
10
15
25
4.0
3.0
2.0
1.0
0
Energy bandgap (ev)
ZnS
ZnSe
CdS
ZnTe
AlP
AlAs
GaP
CdSe
AlSb
CdTe
GaAs
Si
InP
Bulk
GaSb
SLE
Ge
(Ge)
InAs
InSb
Sn
HgTe
0.4
0.5
1.0
1.5
2.0
3.0
5.0
Wavelength (μm)
5.5
6.0
6.5
Lattice constant (Å)

Epitaxial Layers

- Epitaxial layers of different compound semiconductors can be grown on top of each other.
- Small differences in lattice constants can be accommodated for thin layers (strained layers: Compressive or tensile).
- Too much accumulated strain results in dislocations.

InP/InGaAs/InP Square Well

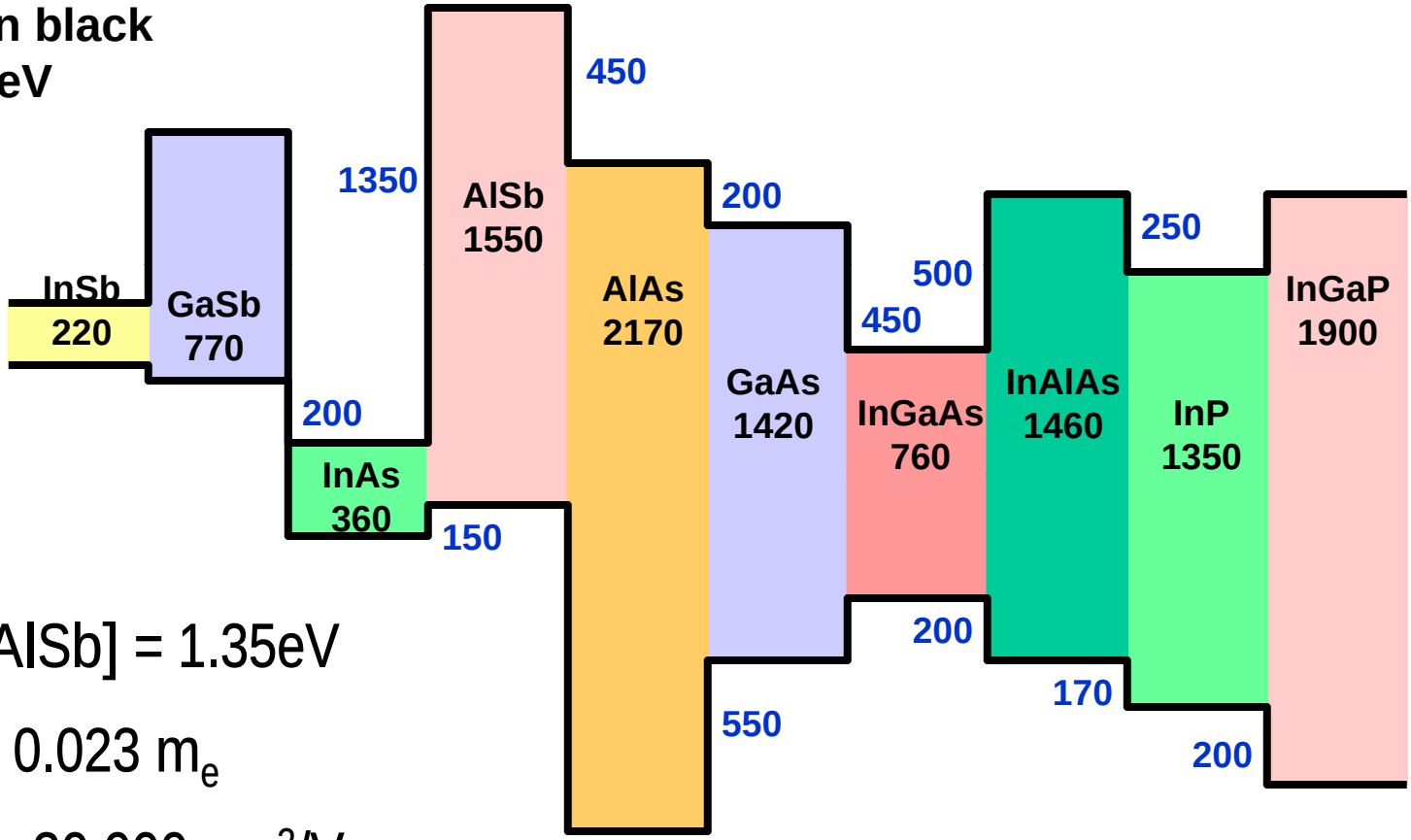
- InGaAs: E_g=.76 eV
- InP: E_g=1.35 eV



How do bands line up?
It depends on the electron affinity: Energy to bring an electron from the conduction band edge to vacuum.

Bandgap Heaven

- Offsets in blue #s
- Bandgaps in black
- Units are meV



ΔE_C [InAs-AlSb] = 1.35eV

m* [InAs] = 0.023 m_e

InAs RT μ > 30,000 cm^2/Vs

Guidelines

- Figure out bandgaps. (draw horizontal where there is no depletion).
- Figure out conduction band and valence band discontinuity.
- Figure out Fermi level for each material.
- Draw flat band first, then flaten out the Fermi level.
- Keep the band separation constant for any region where the bandgap is not changing.

AlAs/GaAs Heterostructure

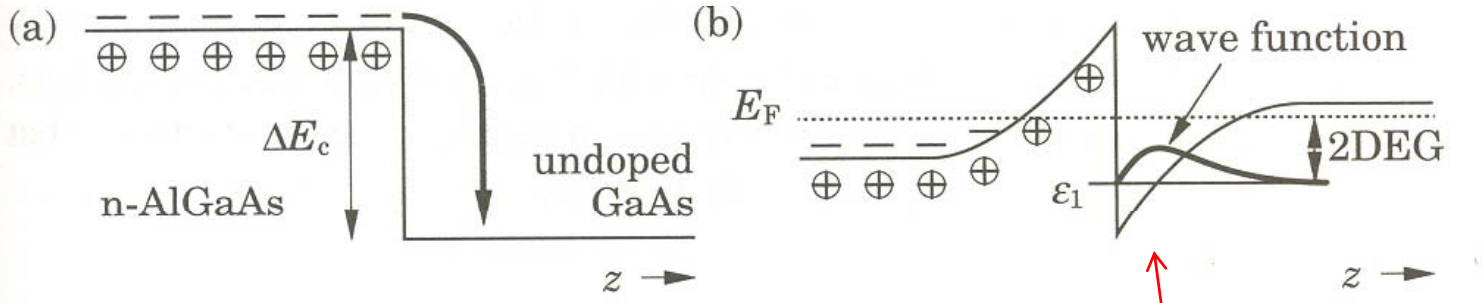


FIGURE 3.9. Conduction band around a heterojunction between n-AlGaAs and undoped GaAs, showing how electrons are separated from their donors to form a two-dimensional electron gas.

High mobility channel because there are carriers but no dopants (which cause scattering, which reduces the mobility). Important for HEMTs (High electron mobility transistor).

Heterostructure Band Diagram Construction

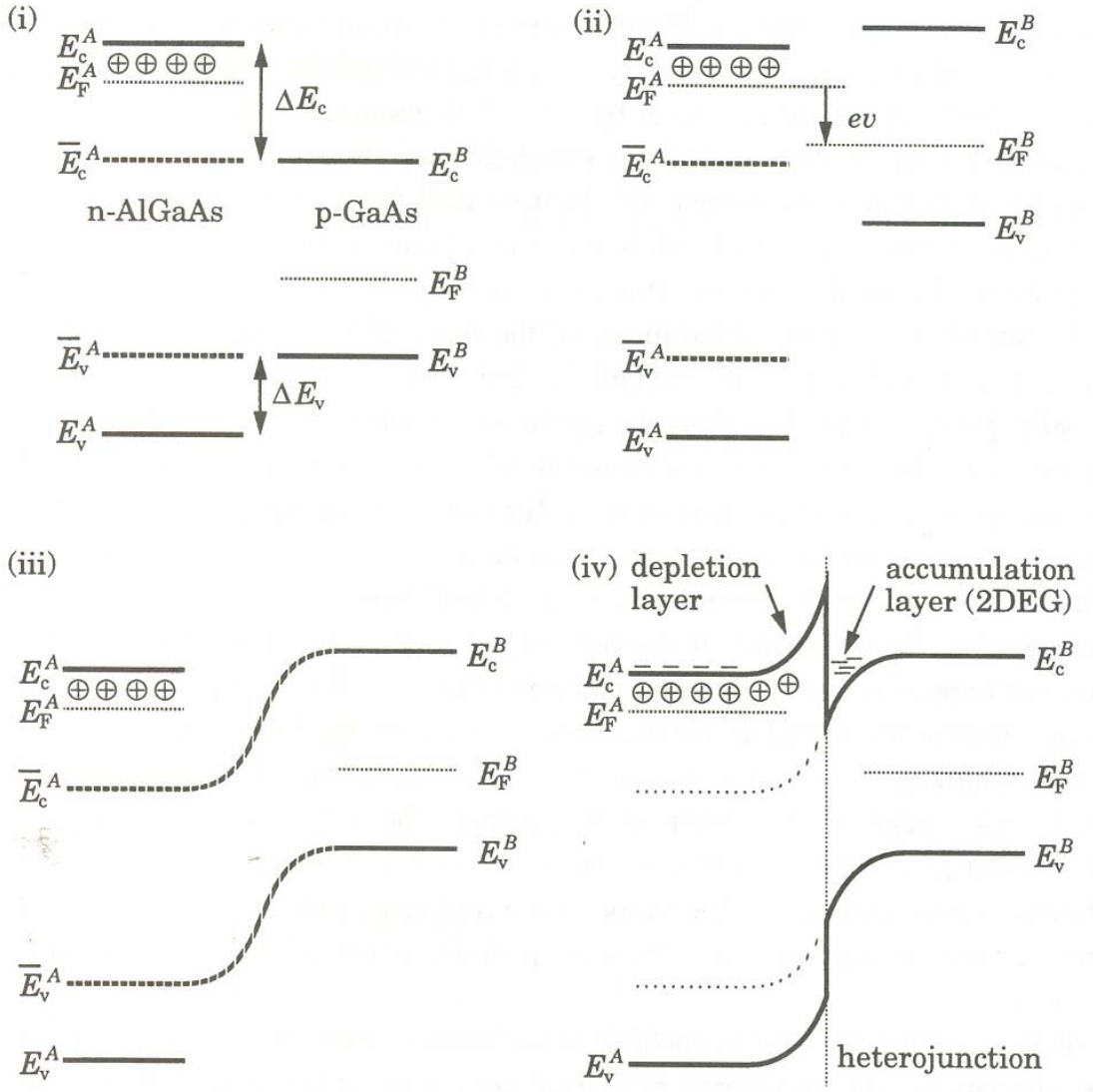
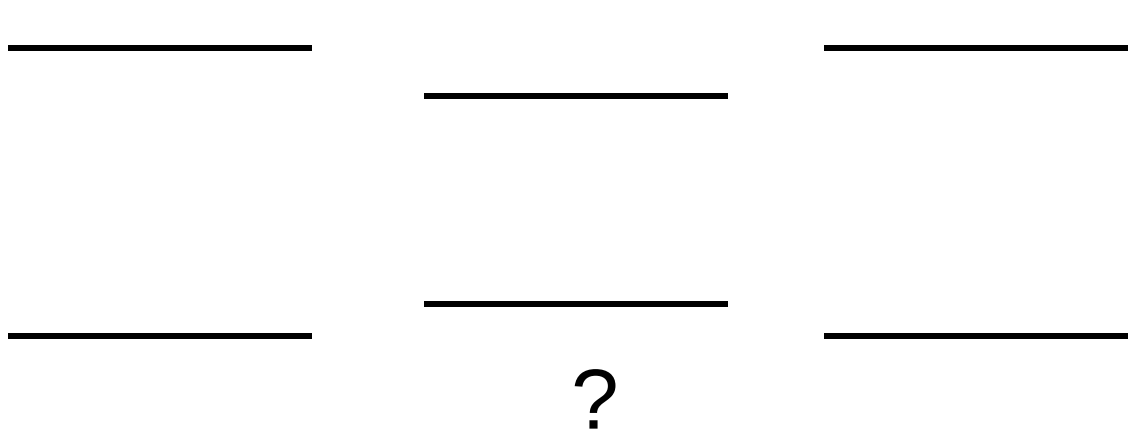


FIGURE 3.10. Steps in the construction of the band diagram for a doped heterojunction between material A, n-type AlGaAs, and material B, p-GaAs.

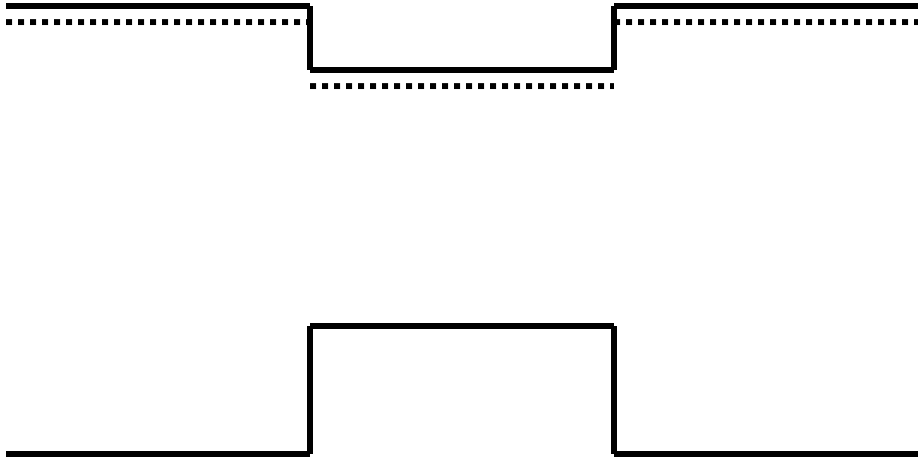
InP/InGaAs/InP Square Well

- N+ InGaAs: E_g=.76 eV
- N+ InP: E_g=1.35 eV



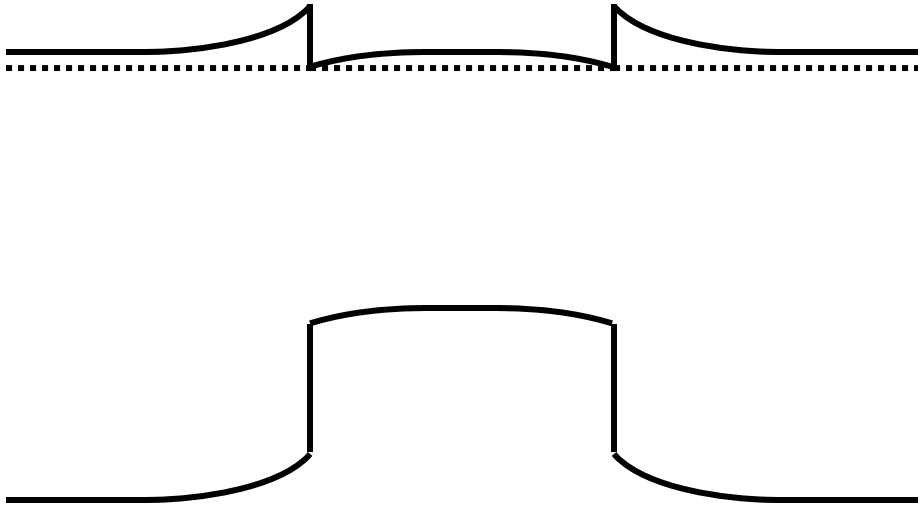
InP/InGaAs/InP Square Well

- N+ InGaAs: E_g=.76 eV
- N+ InP: E_g=1.35 eV
- ΔE_g=.59 eV
- ΔE_c=.25 eV
- ΔE_v=.34 eV
- Draw the flatband diagram first, ignoring doping.



InP/InGaAs/InP Square Well

- N+ InGaAs: E_g=.76 eV
- N+ InP: E_g=1.35 eV
- ΔE_g=.59 eV
- ΔE_c=.20 eV
- ΔE_v=.39 eV



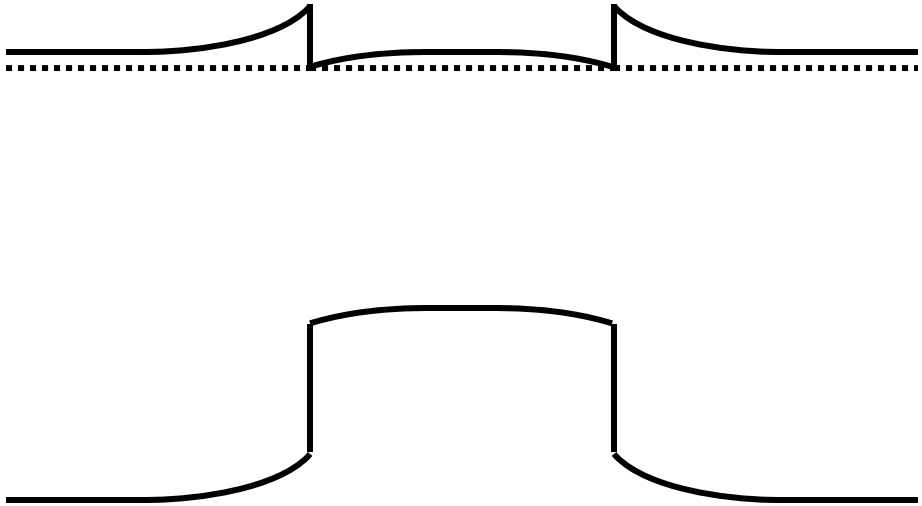
General comments

- If the composition is constant, the bandgap is constant. Hence, the separation of conduction band and valence band are constant.
- If there is no field, the bands are horizontal.
- Use the depletion edge approximation; either the material is depleted of free carriers (and the bands are bent) or there is no field and the bands are flat.
- Depleted doped material has a quadratic bend and linearly increasing field.
- Depleted undoped material has constant electric field and linear band bending.

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho}{\varepsilon} = -\frac{p - n + N_D - N_A}{\varepsilon}$$

InP/InGaAs/InP Square Well

- N+ InGaAs: E_g=.76 eV
- N+ InP: E_g=1.35 eV
  - ΔE_g=.59 eV
  - ΔE_c=.20 eV
  - ΔE_v=.39 eV
- Adjust Fermi level to account for bias.
- Keep bandgaps constant.



Calculate the absorption bandedge assuming a 100 Angstrom quantum well and m_e*=0.1 m_e and m_h*=1 m_e
Calculate the absorption bandedge assuming a 100 Angstrom quantum dot and m_e*=0.1 m_e and m_h*=1 m_e
Check the validity of your assumptions.

Quantum well confinement (1 D)

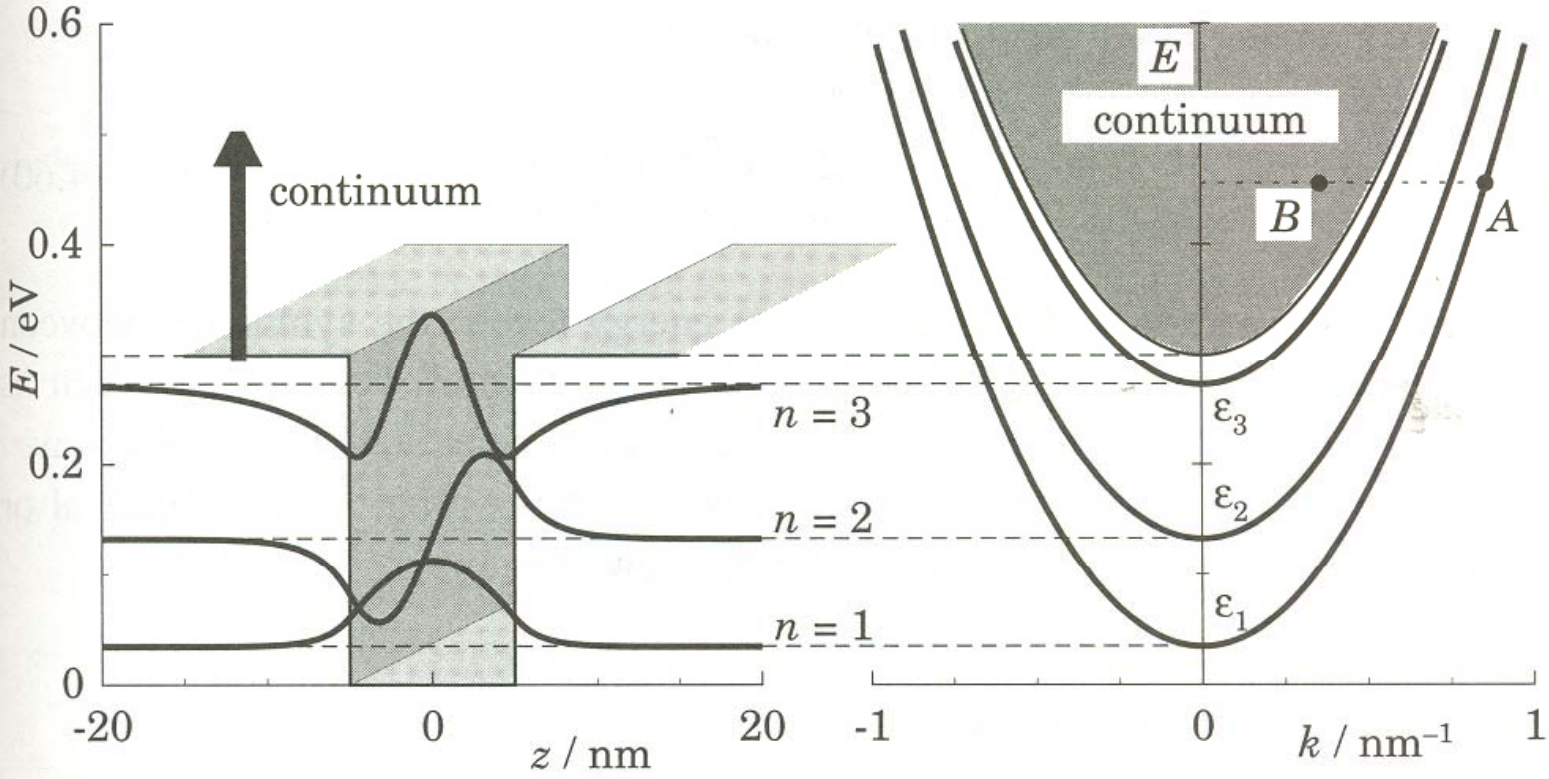
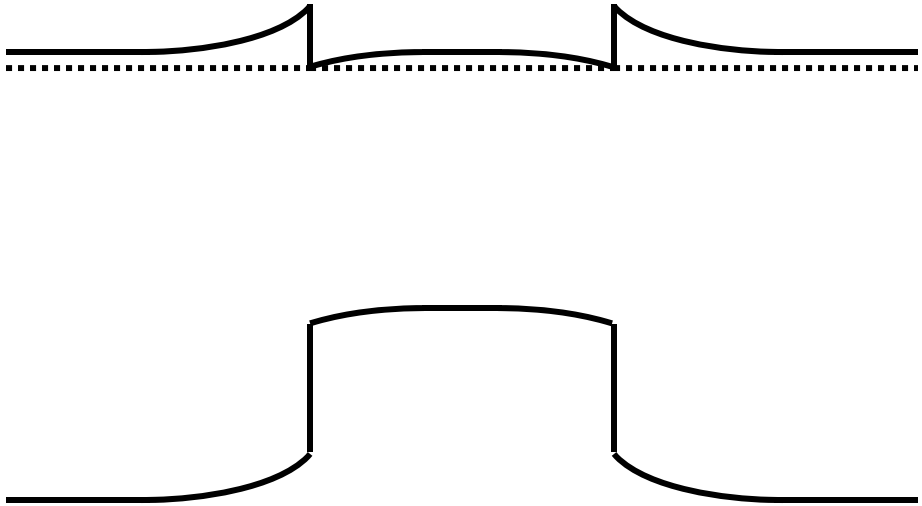


FIGURE 4.9. Quasi-two-dimensional system in a potential well of finite depth. Electrons with the same total energy can be bound in the well (A) or free (B).

InP/InGaAs/InP Square Well

- N+ InGaAs: E_g=.76 eV
- N+ InP: E_g=1.35 eV
  - ΔE_g=.59 eV
  - ΔE_c=.20 eV
  - ΔE_v=.39 eV
- Adjust Fermi level to account for bias.
- Keep bandgaps constant.



Calculate the absorption bandedge assuming a 100 Angstrom quantum well and m_e*=0.1 m_e and m_h*=1 m_e
Calculate the absorption bandedge assuming a 100 Angstrom quantum dot and m_e*=0.1 m_e and m_h*=1 m_e
Check the validity of your assumptions.

1D case

For simplicity, assume an infinite square well, then see if that is valid.

Electron and hole levels:

$$E = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{a}\right)^2 + \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2\right)$$

$$1D\ electron:$$

$$E_1 = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{a}\right)^2 = 0.03eV$$

$$\Delta E_c = 0.2eV$$

$$1D\ hole:$$

$$E_1 = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{a}\right)^2 = 0.003eV$$

$$\Delta E = h\upsilon = \frac{hc}{\lambda} = .76 + .03 + .003 = .79eV$$

$$\lambda = \frac{1.24eV\mu m}{.79eV} = 1.57\mu m$$

3D case

For simplicity, assume an infinite square well, then see if that is valid.
Electron and hole levels:

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

$3D\ electron:$

$$E_1 = \frac{3\hbar^2}{2m^*}\left(\frac{\pi}{a}\right)^2 = 0.09eV$$

Infinite square well approximation poor, Even for the lowest electron energy level.

$3D\ hole:$

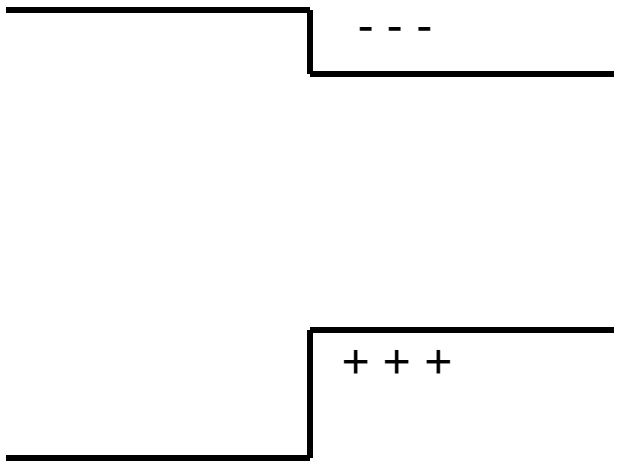
$$E_1 = \frac{3\hbar^2}{2m^*}\left(\frac{\pi}{a}\right)^2 = 0.009eV$$

$$\Delta E = h\upsilon = \frac{hc}{\lambda} = .76 + .09 + .009 = .86eV$$

$$\lambda = \frac{1.24eV\mu m}{.86eV} = 1.44\mu m$$

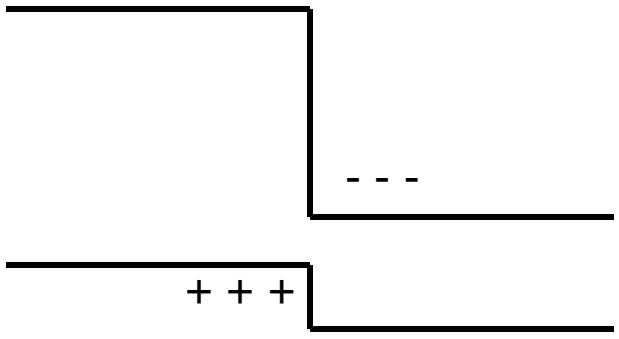
Three types of heterojunctions

- Type I (Straddling)
  - Free electrons and holes reside in the same region of space.
  - Examples: AlGaAs/GaAs, InP/GaInAs



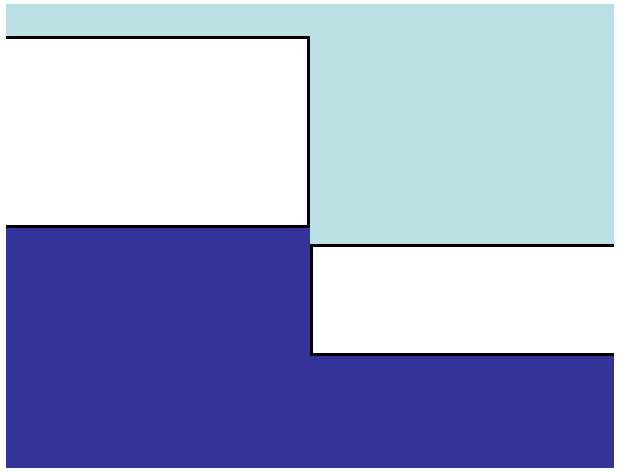
Three types of heterojunctions

- Type I (Straddling lineup)
- Type II (Staggered lineup)
  - ΔE_c and ΔE_c have the same sign.
  - Free electrons and holes reside in different regions of space.
  - Example: AlSb/InAs



Three types of heterojunctions

- Type I (Straddling lineup)
- Type II (Staggered lineup)
- Type III (Broken Gap Lineup)
  - ΔE_c and ΔE_c have the same sign.
  - Free electrons and holes reside in different regions of space.
  - Example: GaSb/InAs



Semiconductor Lasers

Need to confine electrons and holes

Need to guide light (confine photons in a waveguide)

Double Heterostructure

Separate confinement Heterostructure

GRINSCH

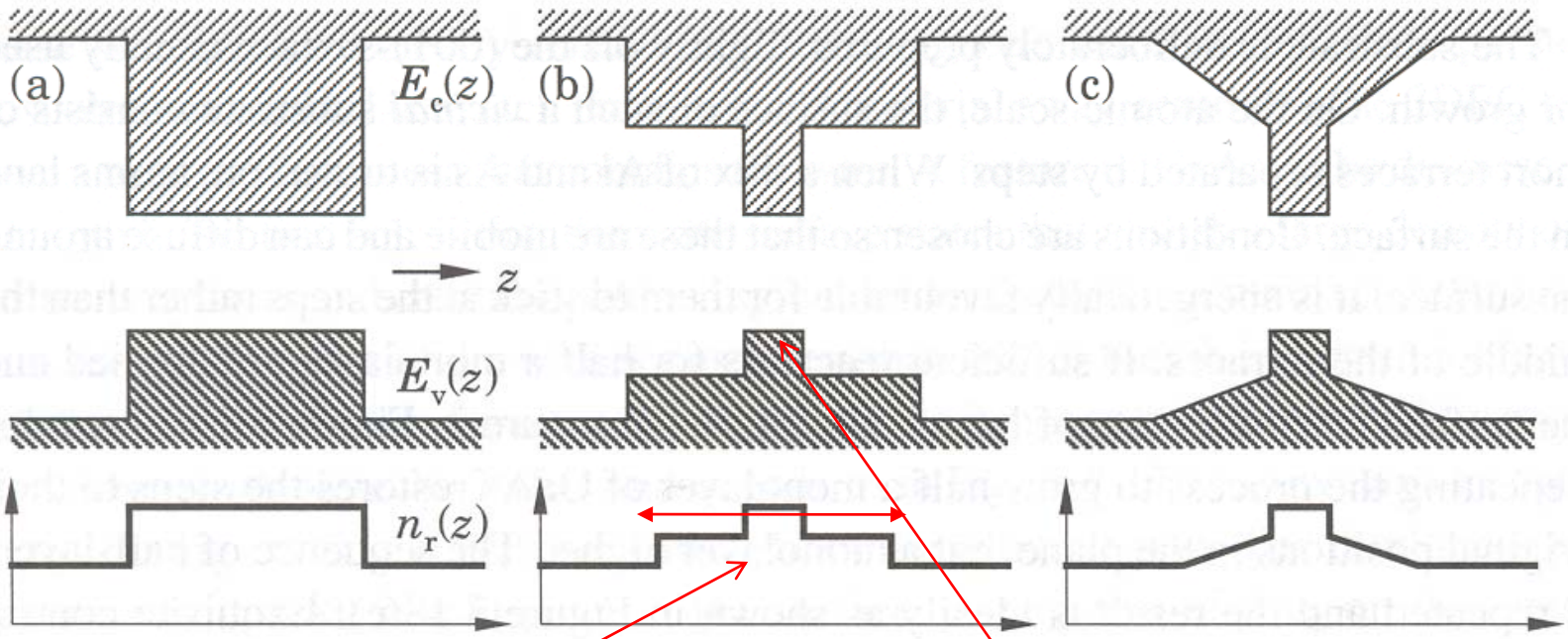


FIGURE 3.19. Profiles of conduction and valence bands and refractive index through layers designed both to guide light and trap carriers: (a) double heterostructure (DH), (b) separately confined heterostructure (SCH), (c) graded-index separately confined heterostructure (GRINSCH).

Optical confinement

Electron/hole confinement

Other examples

1. InAlAs/InGaAs/InAlAs
2. AlAs/GaAs/AlAs
3. GaSb/InAs/GaSb
4. GaSb/InSb/GaSb
5. AlSb/GaSb/AlSb
6. GaSb/InAs/GaSb
7. InGaP/GaAs/InGaP

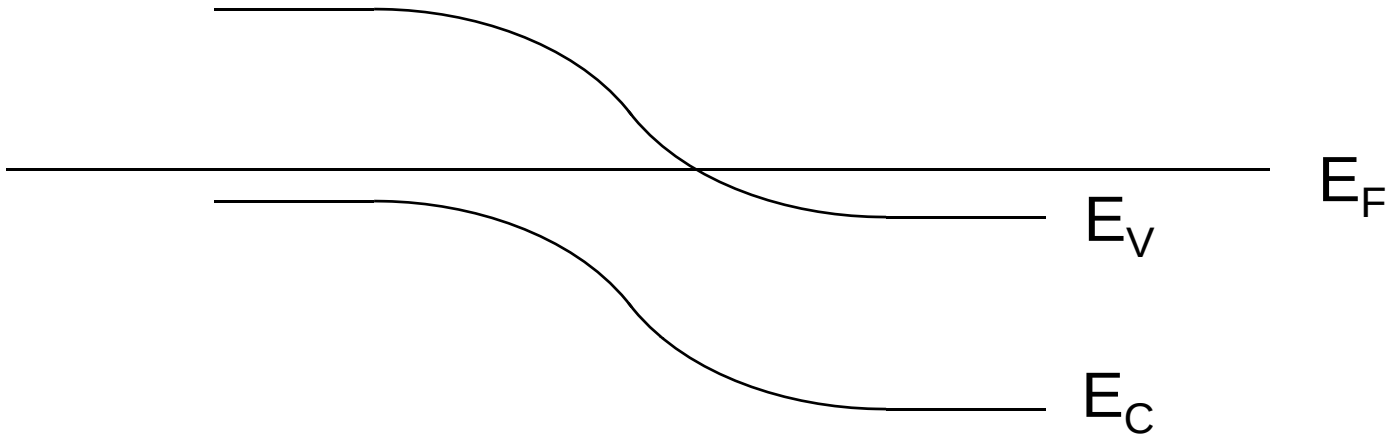
- Draw each for n- n+ n-.

Other examples

1. InAlAs/InGaAs/InAlAs
2. AlAs/GaAs/AlAs
3. GaSb/InAs/GaSb
4. GaSb/InSb/GaSb
5. AlSb/GaSb/AlSb

- Draw each for n- n+ n-, then draw each for p i n.

p-n junction in GaAs



$$\frac{d^2\Phi}{dx^2} = -\frac{\rho}{\varepsilon} = -\frac{p - n + N_D - N_A}{\varepsilon}$$