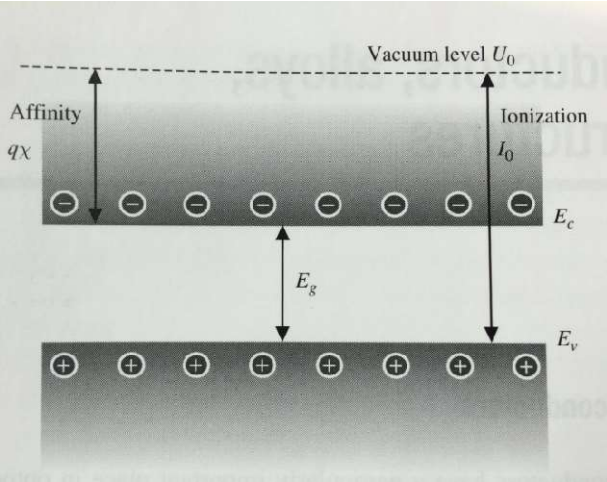
Lecture 2

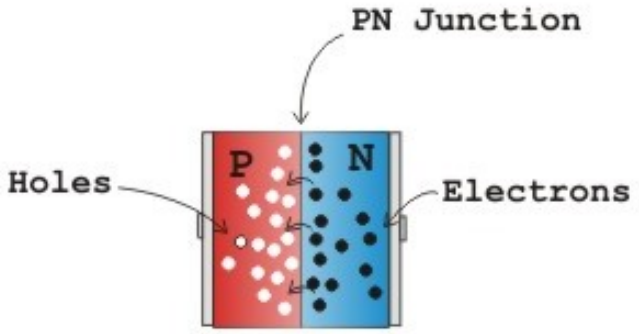
- Semiconductor basics

Valence and conduction bands



- In semiconductors, the energy gap is on the order of 1-2 eV, so some electrons have enough energy to reach the conduction band, leaving holes in the valence band.

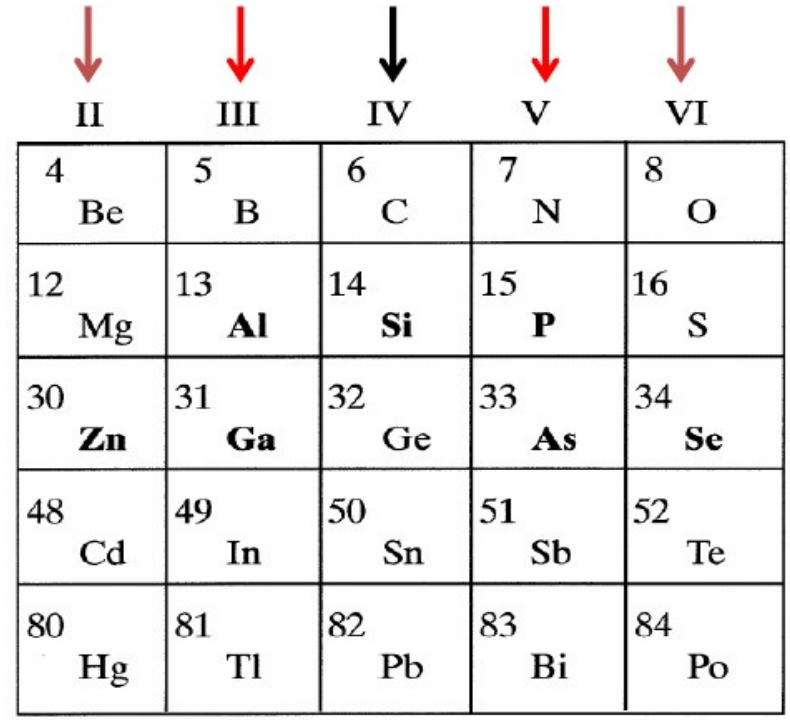
- In pure (intrinsic) semiconductors, charge transport is bipolar (electrons and holes), the conductivity is low, and dependent on the gap.



- Dopants can be added to provide large numbers of electrons to the conduction band (donors, n-type) or holes to the valence band (acceptors, p-type).

- PN junction is formed by n- and p-type doped semiconductors

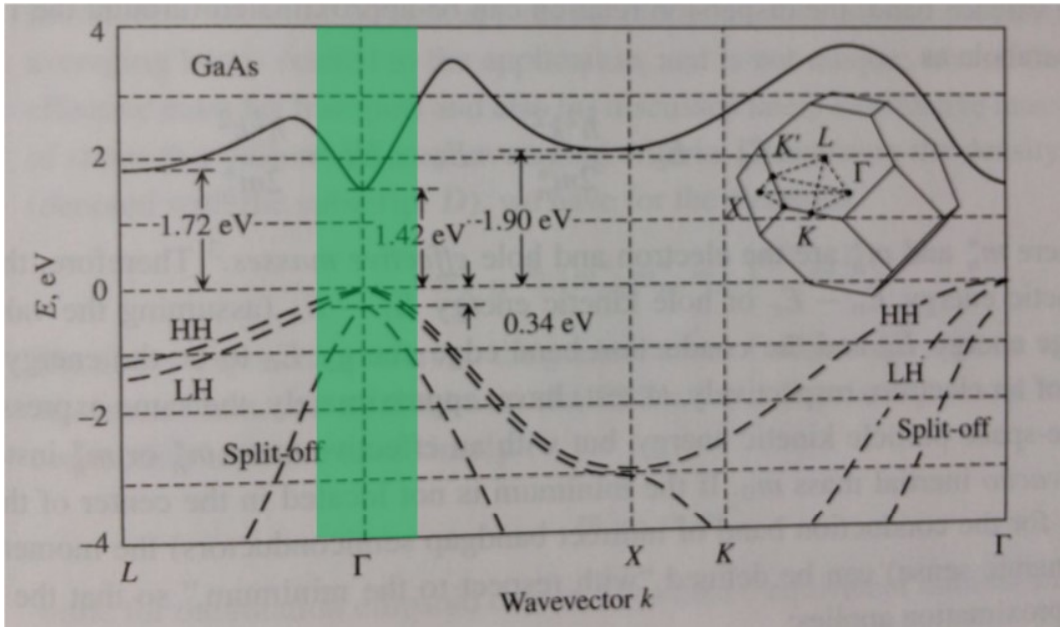
Semiconductor materials



II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 **Al**	14 **Si**	15 **P**	16 S
30 **Zn**	31 **Ga**	32 Ge	33 **As**	34 **Se**
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

- Types of Semiconductors:
  - ✓ Elemental: Silicon or Germanium (Si or Ge)
  - ✓ Compound: Gallium Arsenide (GaAs), Indium Phosphide (InP), Silicon Carbide (SiC), CdS and many others
- Note that the sum of the valence adds to 8, a complete outer shell. I.E. 4+4, 3+5, 2+6

The energy-momentum (E-k) relation (k-space)

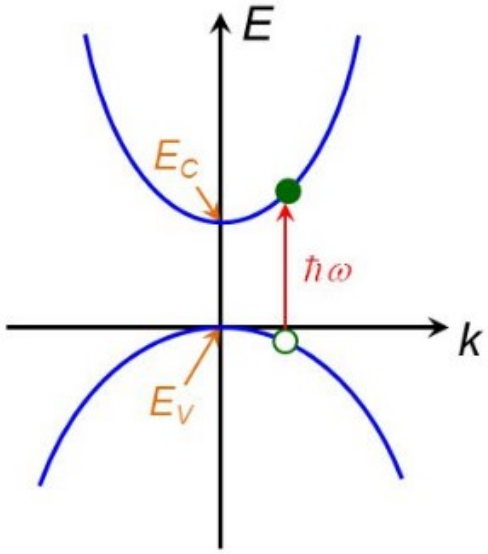


- Attention can be restricted to the branches of low-energy electrons in the conduction band, and low-energy holes in the valence band. Because most carriers are close the band edges.

- Only E-K relation near the Gamma point is of great interest, where locates the conduction band edge (Ec) and the valence band edge (Ev).
- Heavy hole (HH) and light hole (LH) bands dominate the optical processes, while the split-off band is negligible.

Parabolic band approximation

- Around the Gamma point, the E-k relation can be approximated by a parabolic function, using the effective mass.
- The electron's effective mass is smaller than the hole's effective mass. For GaAs, $m_{n*}=0.067m_0$, $m_h^*=0.47m_0$.

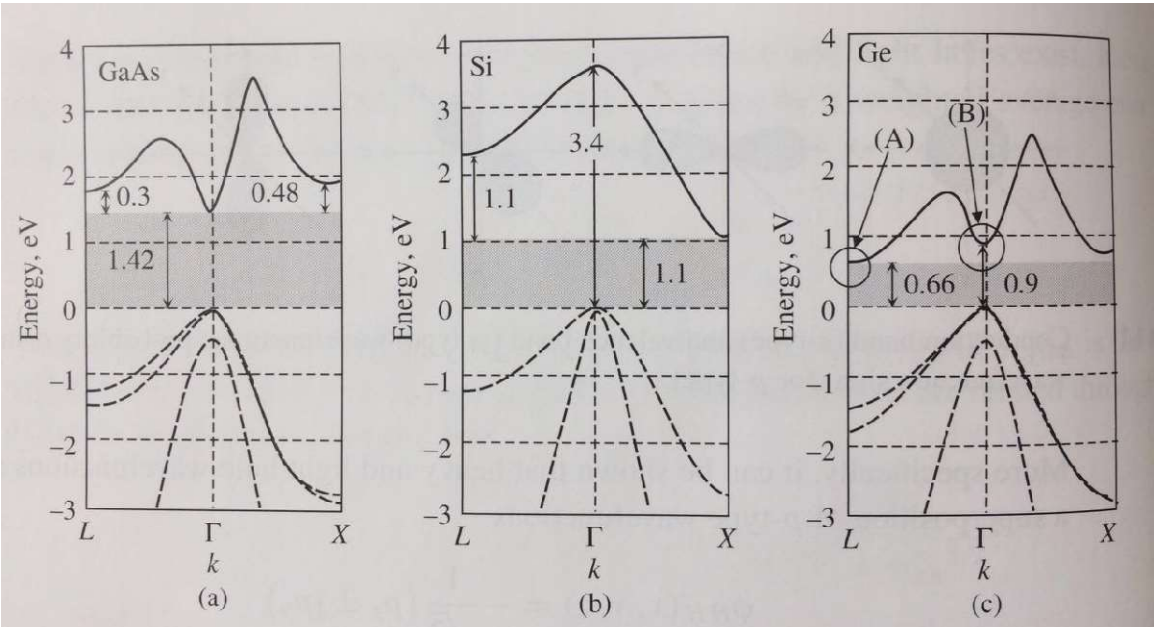


$$E_n = E_c + \frac{\hbar^2 k^2}{2m_n^*}$$

$$E_h = E_v - \frac{\hbar^2 k^2}{2m_h^*}$$

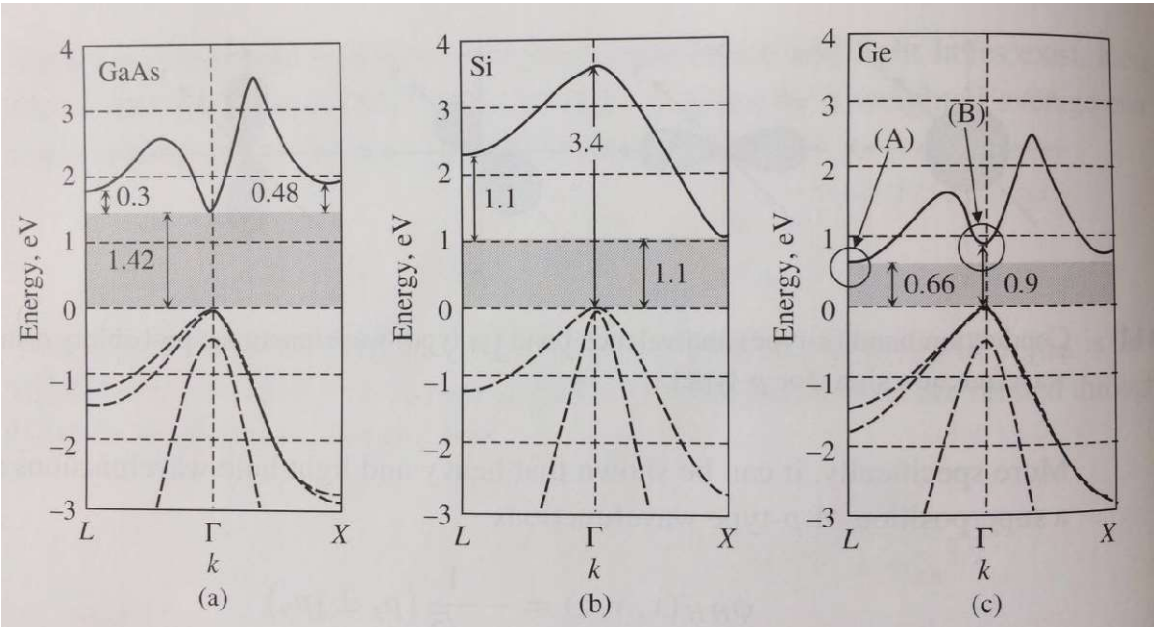
- The reduced mass is a mass considering the impact of the material potential field.

Direct- & indirect- bandgap semiconductors



- Direct bandgap (GaAs): the conduction band minimum and the valence band maximum has the same momentum at the Gamma point.
- Carriers interact directly with photons without momentum change.
- It is able to absorb and emit light efficiently.

Direct- & indirect- bandgap semiconductors

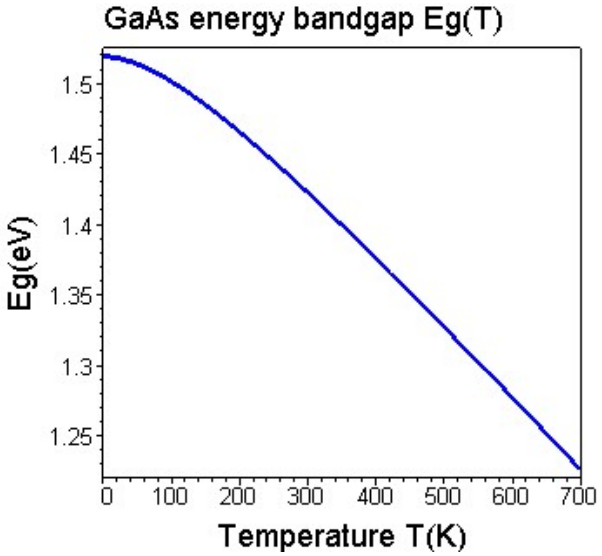


- Indirect bandgap (Si, Ge): the conduction band minimum and the valence band maximum has the different momentum.
- Carriers interact indirectly with photons with the help of phonons.
- It is able to absorb less efficiently but unable to emit light.

Bandgap energy

- The bandgap energy decreases with the increasing temperature

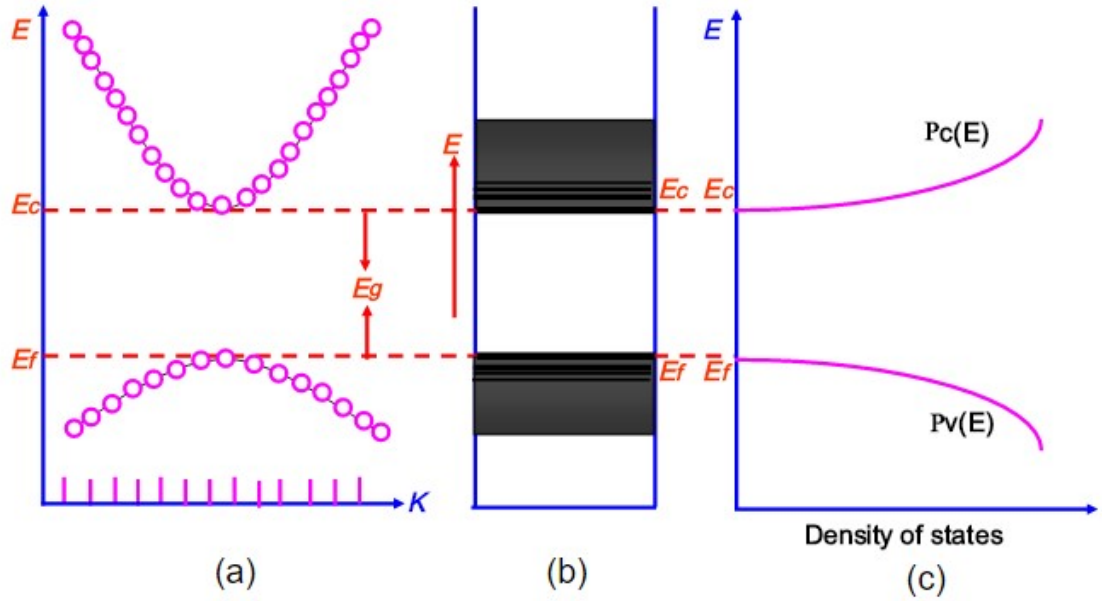
$$E_g = E_{g0} - \frac{aT^2}{T+b}$$



Material	Eg_0 (eV)	a	b
Si	1.17	4.37×10^{-4}	636
GaAs	1.52	5.41×10^{-4}	204
InP	1.42	4.91×10^{-4}	327

Density of states (DoS)

- The density of states (DOS) describes the number of states per unit volume per unit energy.



- For bulk semiconductor (3D):

$$D_c(E) = \frac{4\pi}{h^3}\left(2m_n^*\right)^{3/2}\sqrt{E - E_c}$$

$$D_v(E) = \frac{4\pi}{h^3}\left(2m_h^*\right)^{3/2}\sqrt{E_v - E}$$

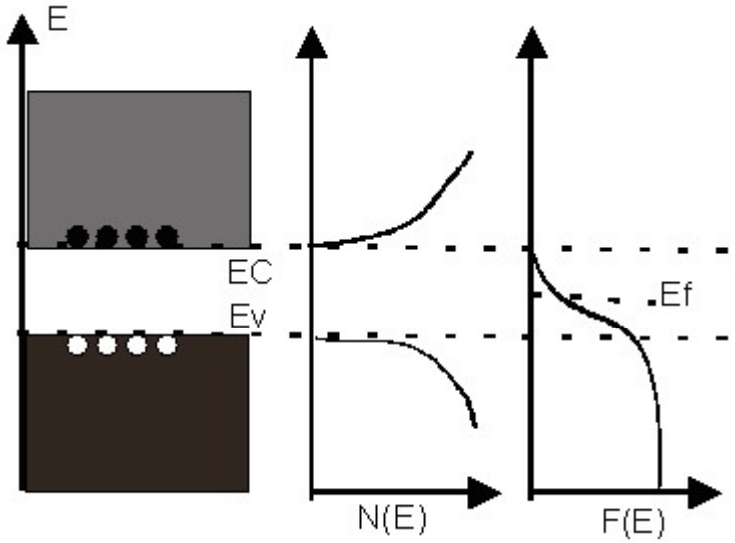
Occupation probability

- Under the thermal equilibrium condition, electrons and holes follow the Fermi-Dirac distribution.

$$f_n(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}$$

$$f_h(E) = \frac{1}{1+\exp\left(\frac{E_F-E}{k_BT}\right)}$$

$$= 1 - f_n(E)$$



- When the Fermi level is within the band gap, it approximately follows the Boltzman distribution:

$$f_n(E) \underset{E \gg E_F}{=} \exp\left(-\frac{E-E_F}{k_BT}\right)$$

Carrier densities

- The carrier density is determined by the density of states and the occupation probability.

$$n = \int_{E_c}^{\infty} N_c(E) f_n(E) dE = N_c \exp\left(\frac{E_F - E_C}{k_B T}\right)$$

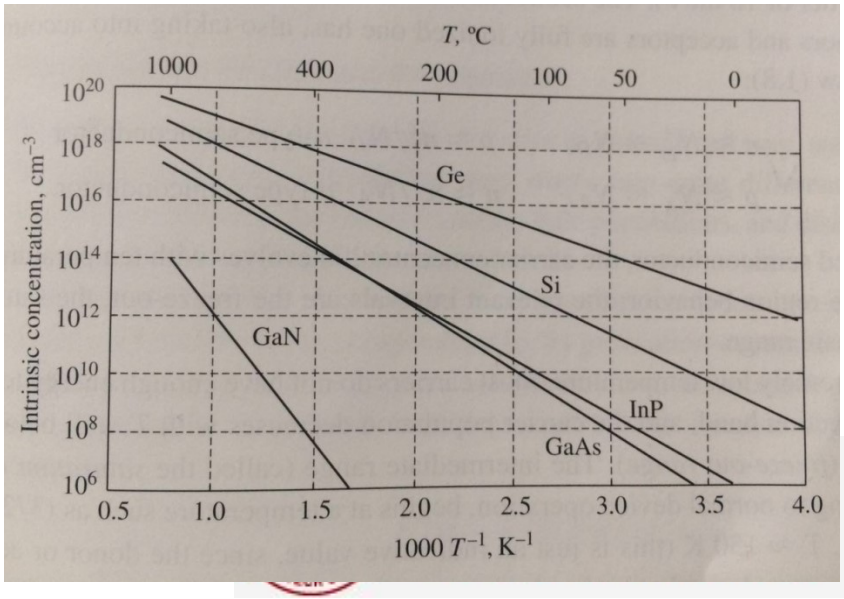
$$p = \int_{-\infty}^{E_v} N_v(E) f_h(E) dE = N_v \exp\left(\frac{E_V - E_F}{k_B T}\right)$$

with N_c, N_v the effective density of states

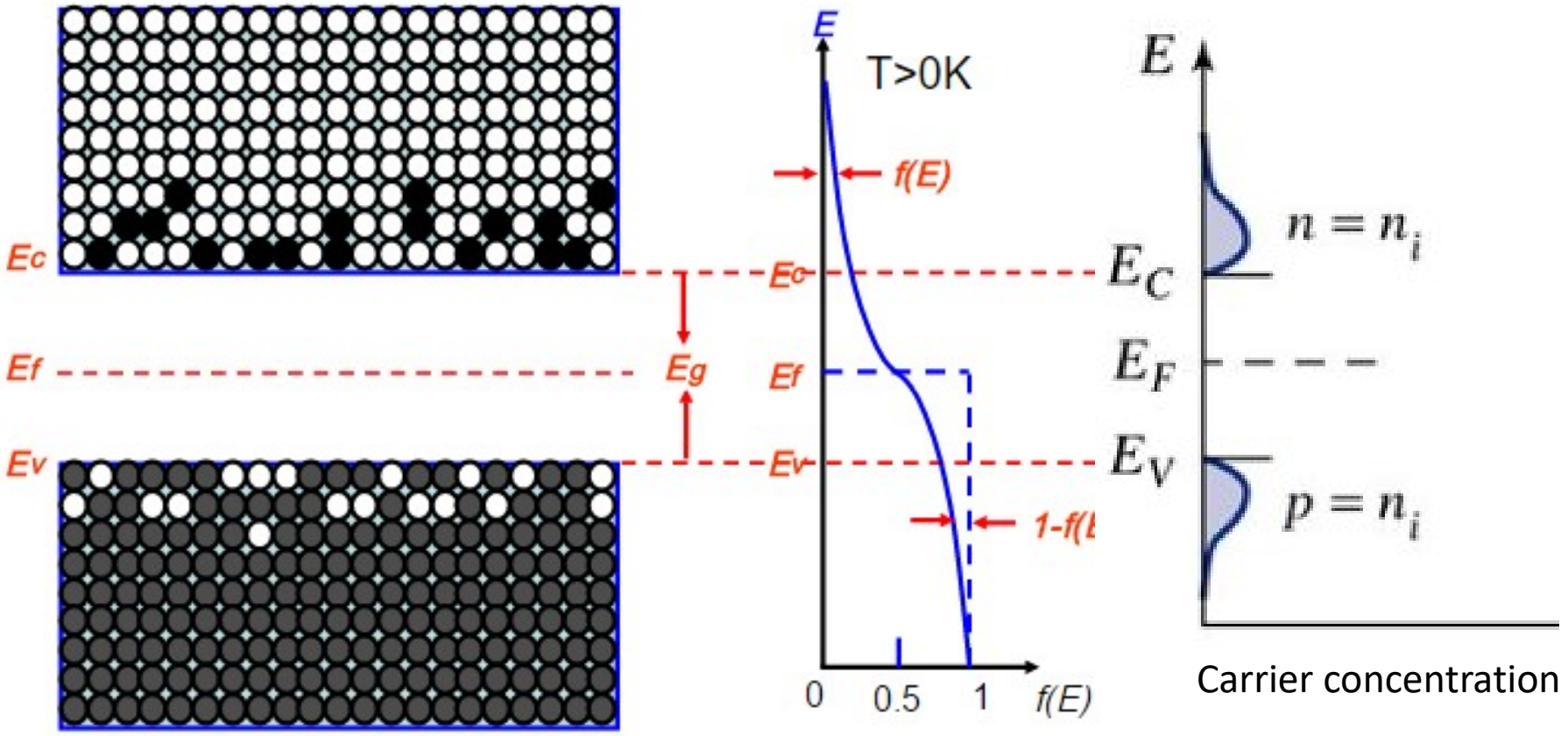
- In the intrinsic semiconductor, $n=n_i=p=p_i$; while the Fermi level is located at the midgap.

$$n_i = N_c \exp\left(\frac{E_{Fi} - E_c}{k_B T}\right) = p_i = N_v \exp\left(\frac{E_v - E_{Fi}}{k_B T}\right)$$

$$n_i p_i = n_i^2 = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right)$$



Carrier density



- Intrinsic (undoped) semiconductor

Mass action law

- In equilibrium conditions, the product of carrier densities n and p does not depend on the position of the Fermi level (while the Fermi level can be changed by the doping). This is coined the mass action law, which also holds for doped semiconductors.

$$np = n_i^2$$

Carrier densities in doped semiconductors

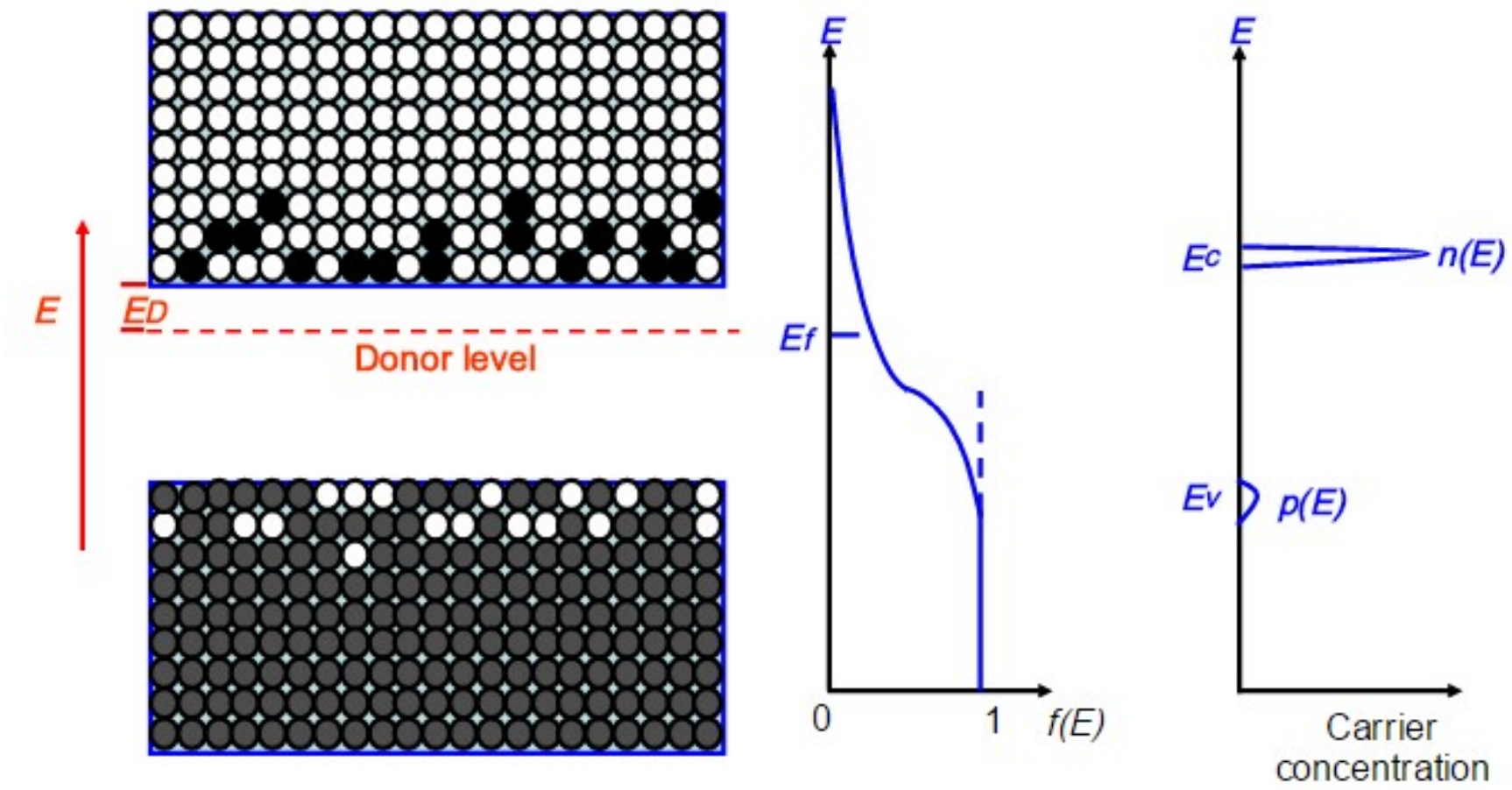
- N-type semiconductor is doped by a donor (density N_D) from, say group V, which provides extra electrons in the conduction band. The Fermi level becomes closer to the conduction band.

$$n \approx N_D;\ p \approx n_i^2 / N_D$$

- P-type semiconductor is doped by an acceptor (density N_A) from, say group III, which provides extra holes in the valence band. The Fermi level becomes closer to the valence band.

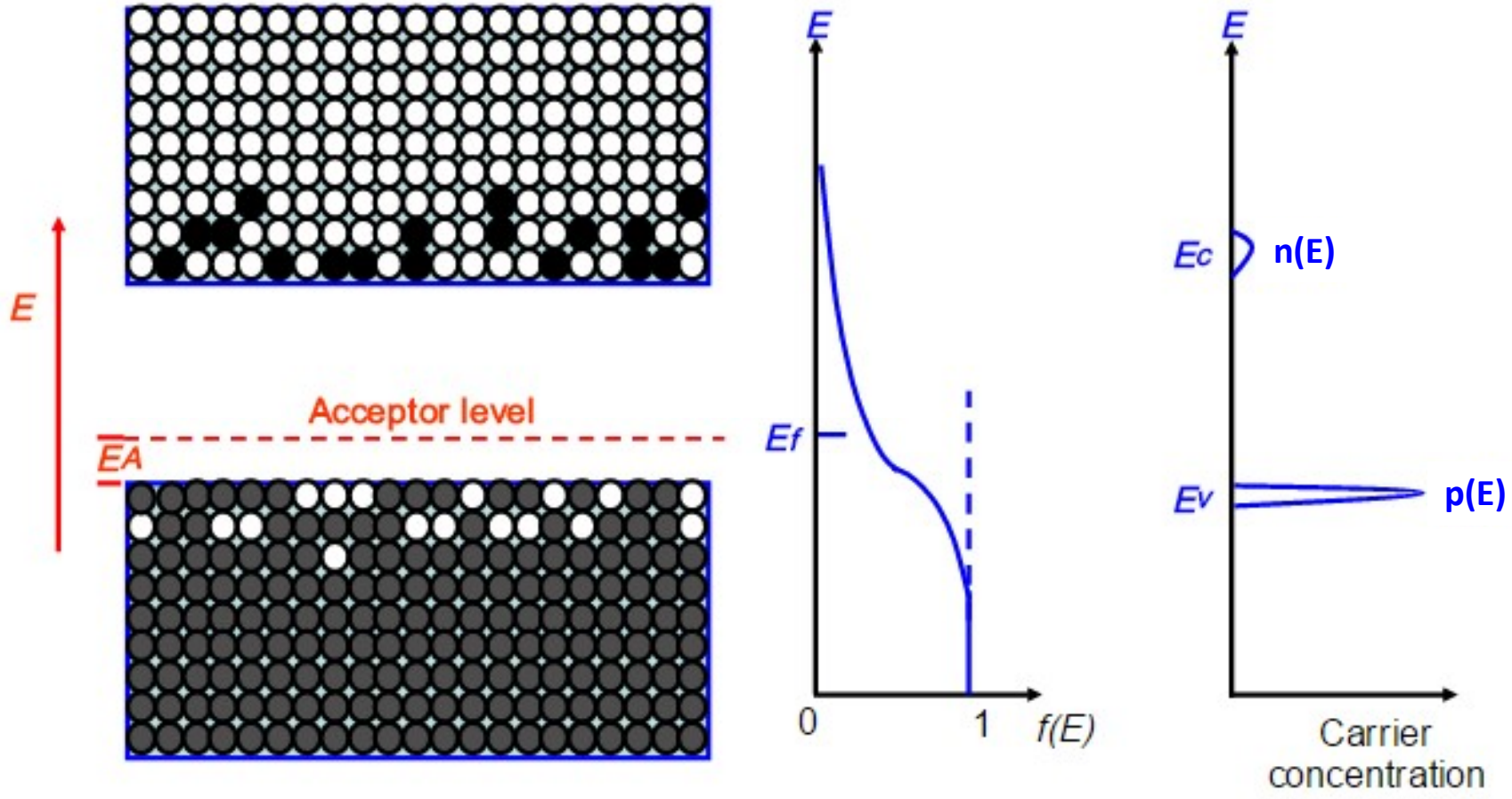
$$p \approx N_A;\ \mathrm{n} \approx n_i^2 / N_A$$

Carrier density



- N-type semiconductor

Carrier density



- P-type semiconductor

Quasi-equilibrium condition

- If the thermal equilibrium is perturbed by an external source (carrier injection), it will leads to carrier generation/recombination (GR) processes. It involves an exchange of energy and momentum with photons (radiative GR), phonons (thermal GR), or other electrons and holes (Auger recombination). This perturbed condition is described by a quasi-equilibrium distribution using two quasi-Fermi levels E_{Fn} and E_{Fh}:

$$f_n(E,E_{Fn})=\frac{1}{1+\exp\left(\frac{E-E_{Fn}}{k_BT}\right)};\quad f_p(E,E_{Fh})=\frac{1}{1+\exp\left(-\frac{E-E_{Fh}}{k_BT}\right)}$$

Quasi-equilibrium condition

- The carrier densities become

$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right); \quad p = N_v \exp\left(\frac{E_v - E_{Fh}}{k_B T}\right)$$

$$np = n_i^2 e \exp\left(\frac{E_{Fn} - E_{Fh}}{k_B T}\right)$$

- In case of carrier injection

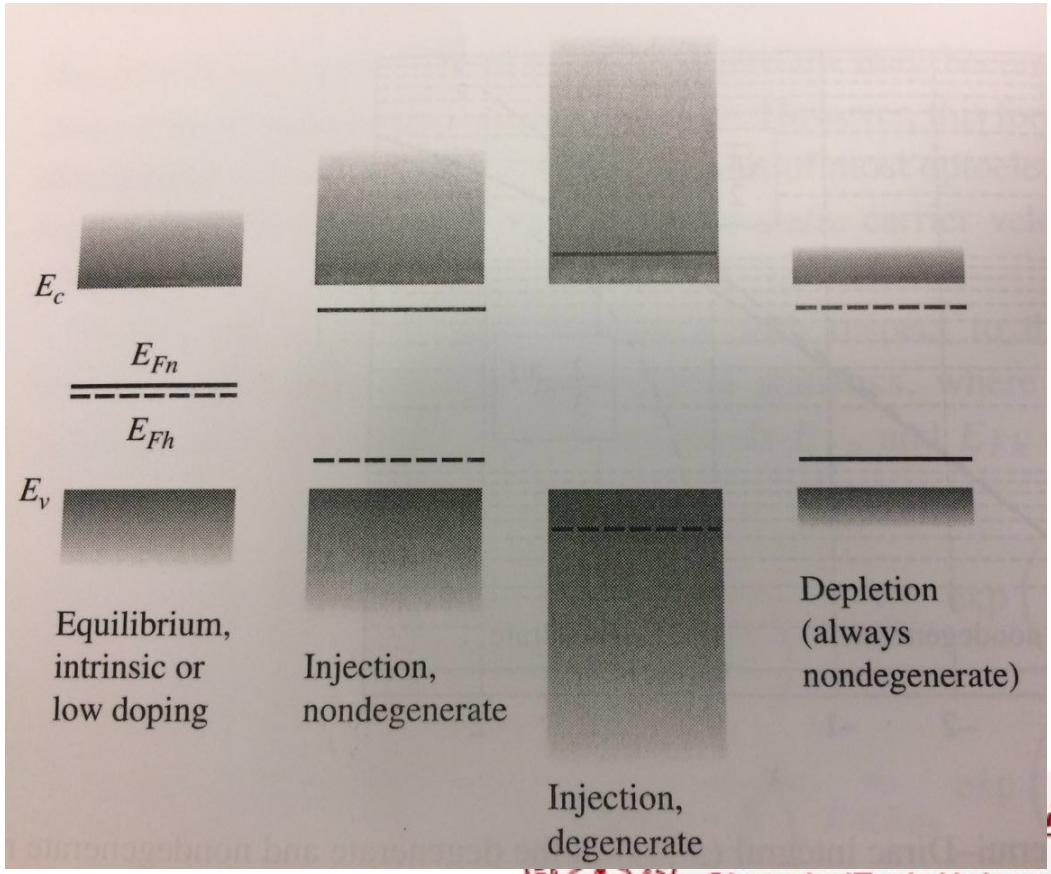
$$E_{Fn} > E_{Fh}$$

$$np > n_i^2$$

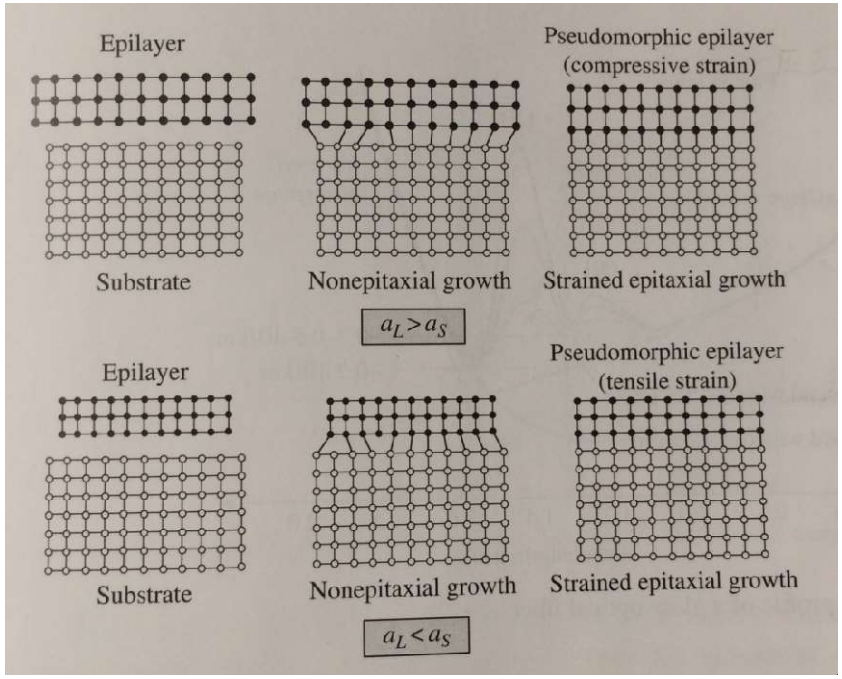
- In case of carrier depletion

$$E_{Fn} < E_{Fh}$$

$$np < n_i^2$$



Heterostructures



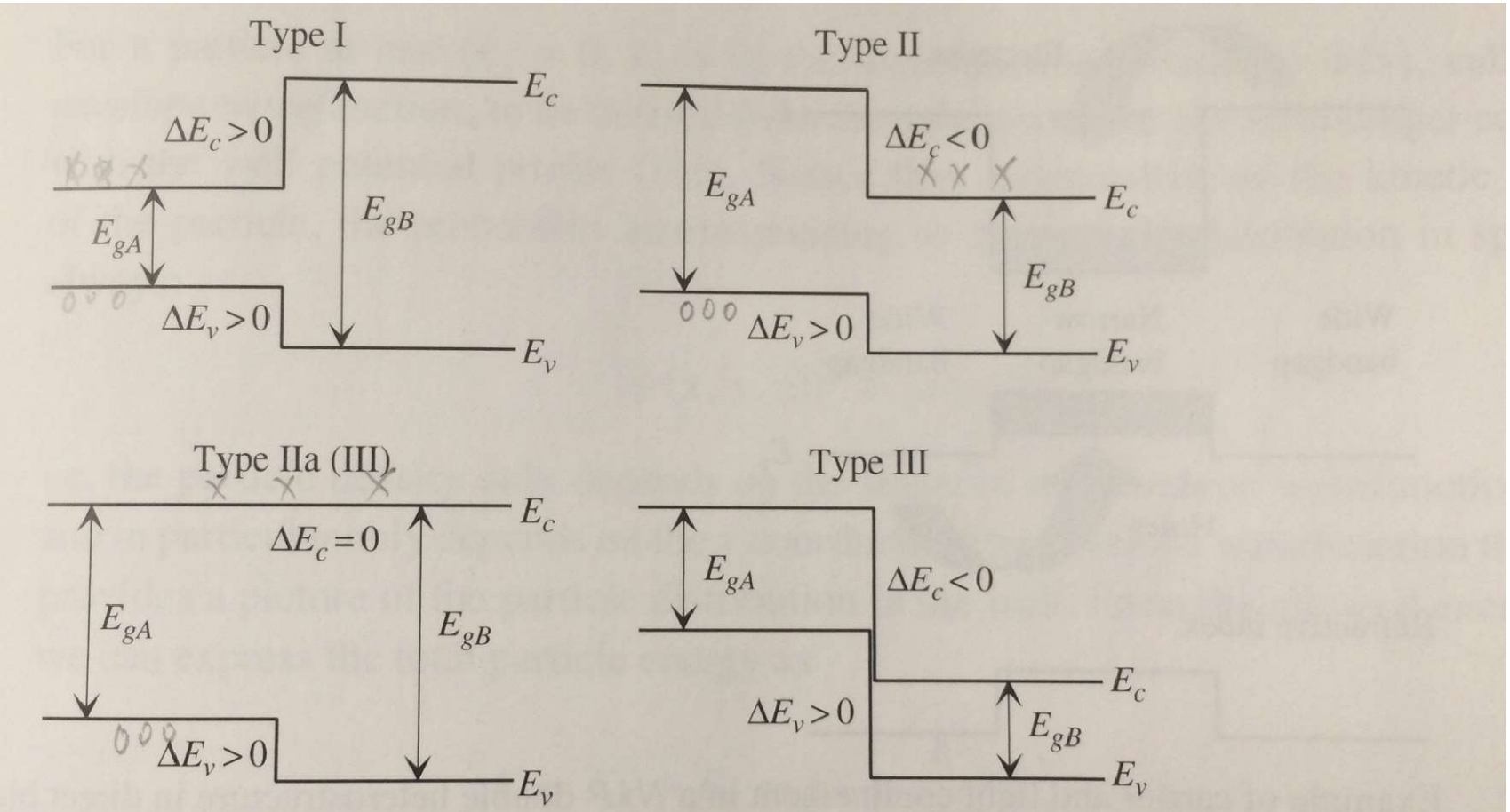
- Common substrates:

Si, GaAs, InP, SiC,

GaP, GaSb, CdTe

- Crystals with different lattice constants epitaxially grown together is called heterostructure/heterojunction. It improves electronic and optical properties, such as confinement of carriers and photons.
- Heterostructures can be lattice-matched or affected by a slight mismatch (maximum on the order of 1%), which induces tensile or compressive strain.

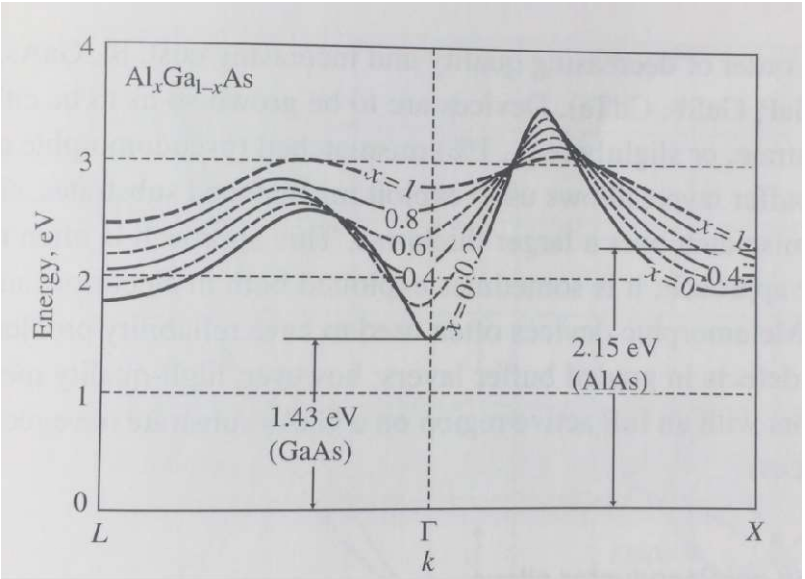
Heterostructures



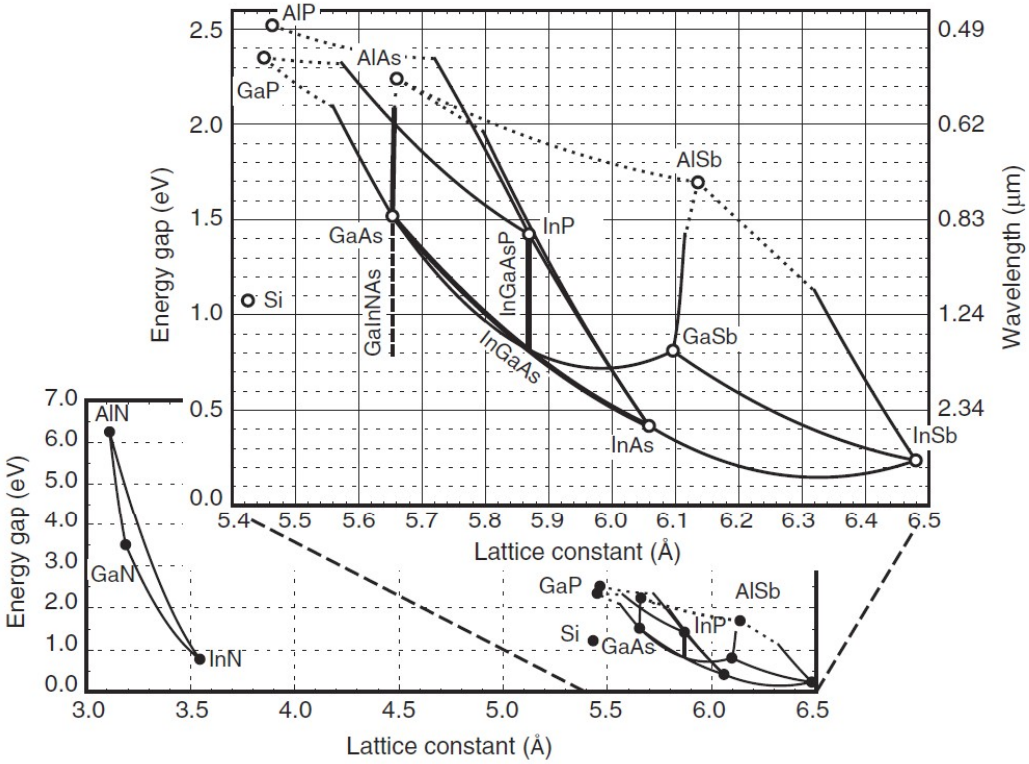
Classification of heterostructures according to band alignment; $\Delta E_j = E_{jB} - E_{jA}$.

Semiconductor compounds

- Compound Semiconductors: Offer high performance (optical characteristics, higher frequency, higher power) than elemental semiconductors and greater device design flexibility due to mixing of materials.
  - ✓ Binary: GaAs, SiC, etc...
  - ✓ Ternary: AlxGa1-xAs, InxGa1-xN where 0≤x ≤ 1
  - ✓ Quaternary: InxGa1-xAsyP1-y where 0 ≤ x ≤ 1 and 0 ≤ y ≤ 1
- The lattice constant and the bandgap energy are tuned by the element fractions.
- Tailoring the lattice constant is to achieve lattice matching to the substrate. Tailoring the bandgap energy is to get a certain photon wavelength.



Energy gap vs. lattice constant



- ✓ The lines represent tenary compounds
- ✓ The dashed lines are indirect gap
- ✓ The areas enclosed by lines are quaternaries.
- ✓ The enclosed area provides enough degrees of freedom to adjust the bandgap without changing the lattice constant.

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Compound semiconductor families

- III-V compounds: GaAs, InP, GaSb, InAs (direct bandgap);

  AlAs, GaP (Indirect bandgap);

- III-N compounds: GaN, InN, AlN (direct bandgap);

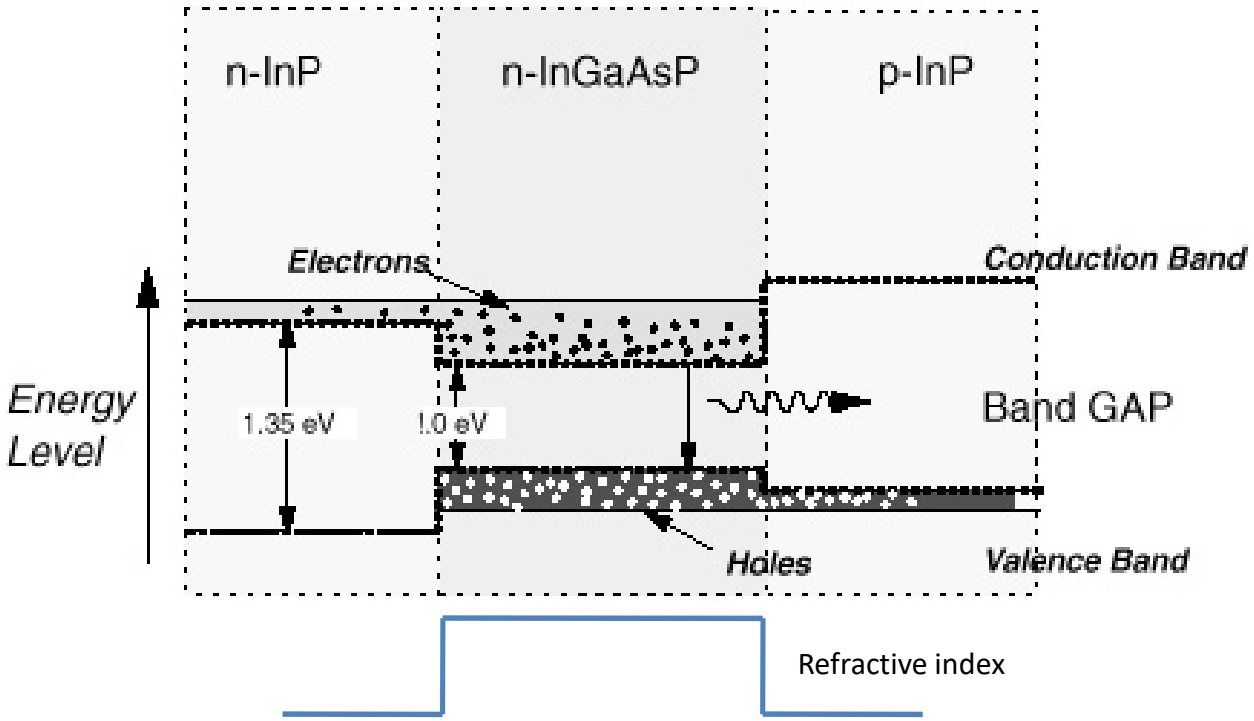
- II-VI compounds CdTe, HgTe, ZnS, CdSe, ZnO (direct bandgap);

- IV-IV compounds: SiC, SiGe (indirect bandgap);

- I-VII compounds: AgI, CuBr;

Double heterostructure

- The double heterostructure provides good electronic and optical properties

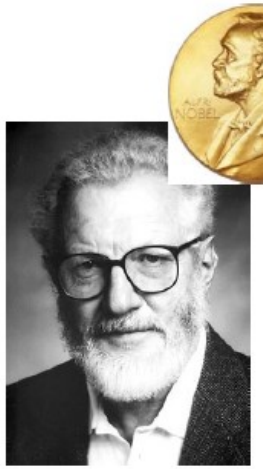


- The carrier confinement is achieved through different band gaps.
- The photon confinement is achieved through refractive index difference.
- The narrow gap material acts as active region in lasers.

The 2000 Nobel Prize in Physics

"For basic work on information and communication technology"

*"For developing **semiconductor heterostructures** used in high-speed opto-electronics"*



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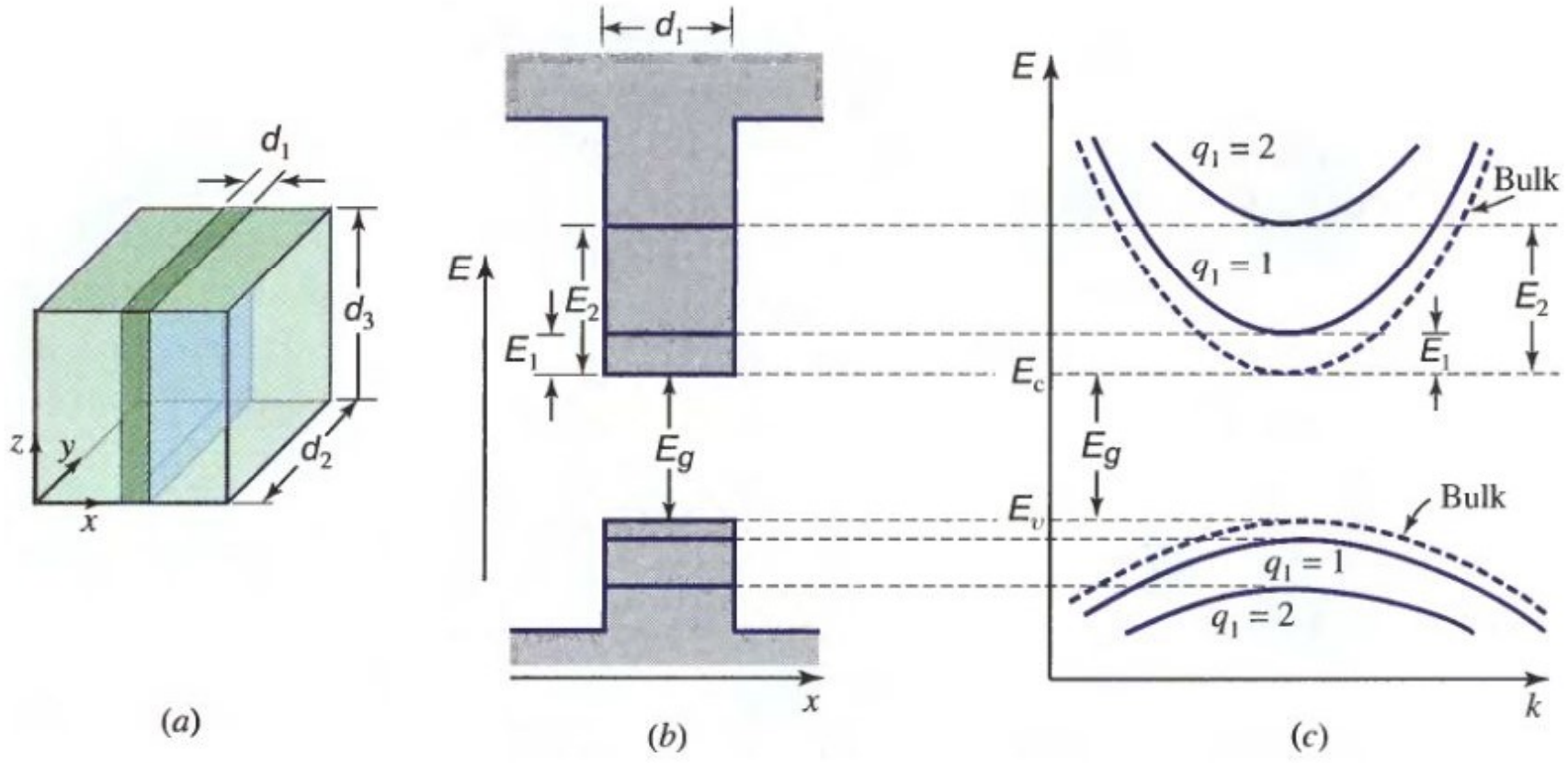
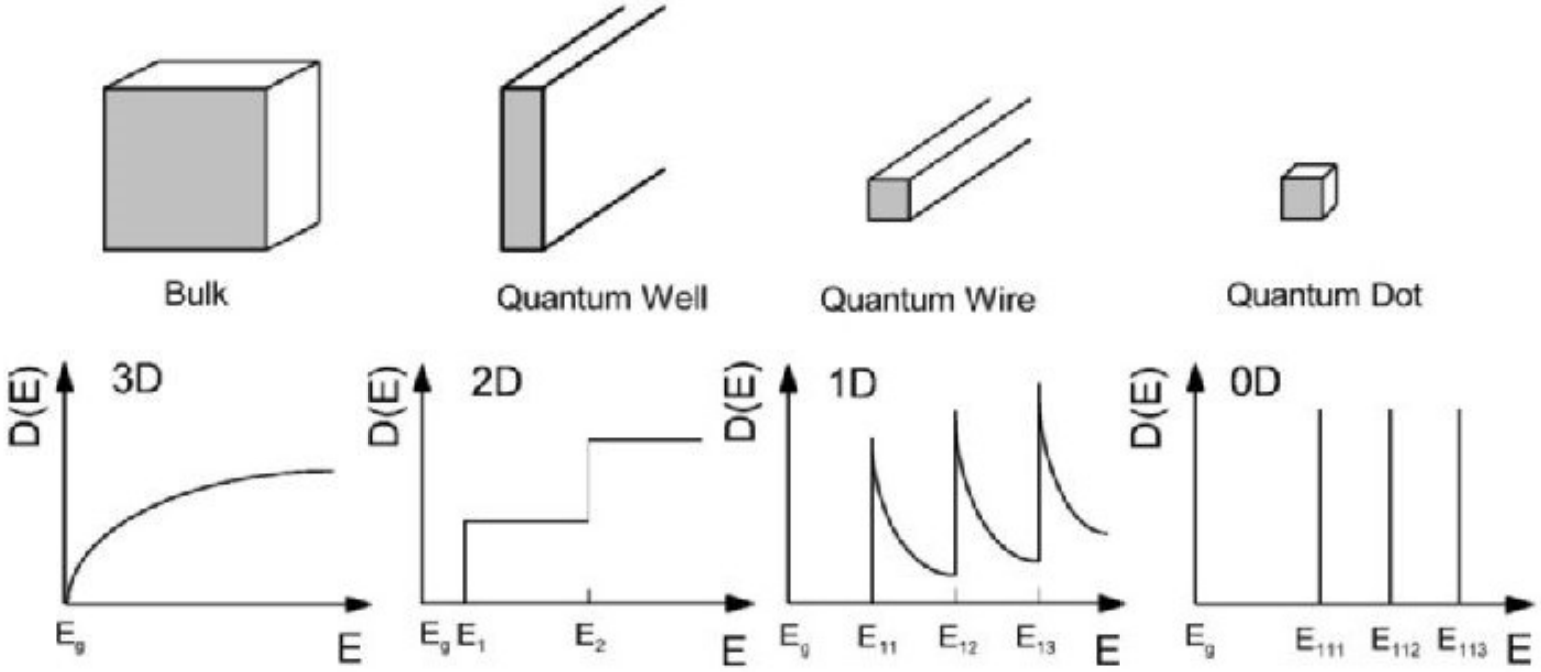
Quantum confinement

- When the size of the double heterostructure decreases to be less than 100 nm, the allowed energy levels of the confined carriers will be quantized, and the structure is called a quantum well, where sets of energy subbands appear.



Quantum confinement



$$E = E_c + \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$D_c(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c}$$

$$E = E_i + \frac{\hbar^2}{2m^*}\left(k_y^2 + k_z^2\right)$$

$$D_c(E) = \sum_{l=1}^{\infty}\frac{m^*}{\pi\hbar^2}\sigma\left(E - E_l\right)$$

σ is the Heaviside step function

$$E = E_{ij} + \frac{\hbar^2}{2m^*}\left(k_z^2\right)$$

$$D_c(E) = \sum_{l=1}^{\infty}\frac{m^*}{\pi\hbar}\sqrt{\frac{m^*}{2\left(E - E_l\right)}}\sigma\left(E - E_l\right)$$

$$E = E_{ijk}$$

$$D_c(E) = \delta\left(E - E_l\right)$$

δ is the delta function