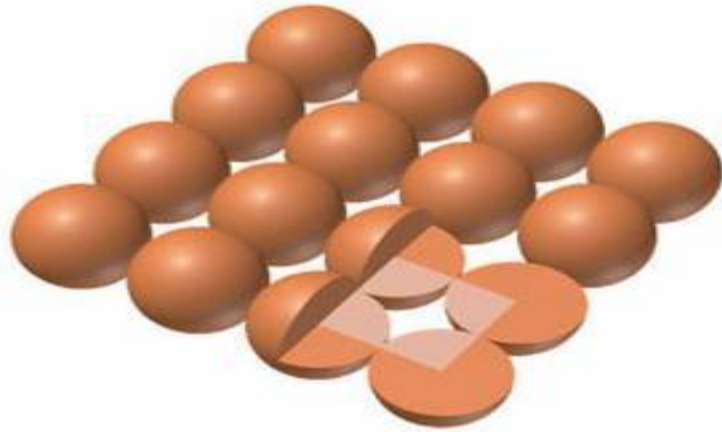


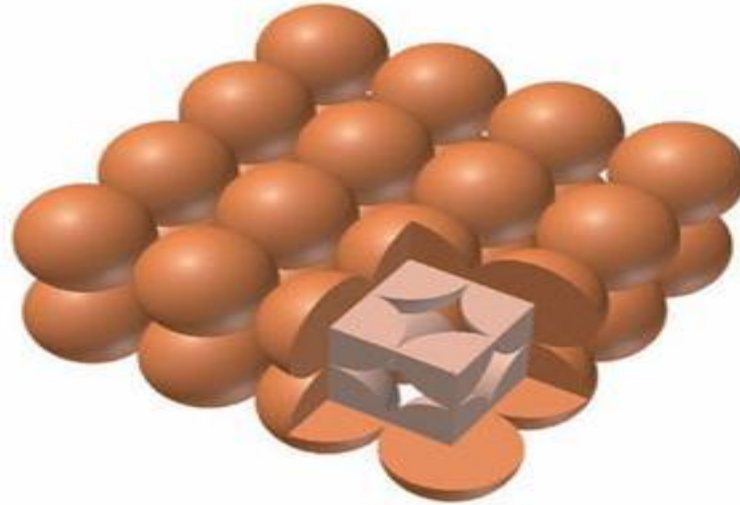
Engineered Materials (SC221)

Packing Fraction of single component crystal structures

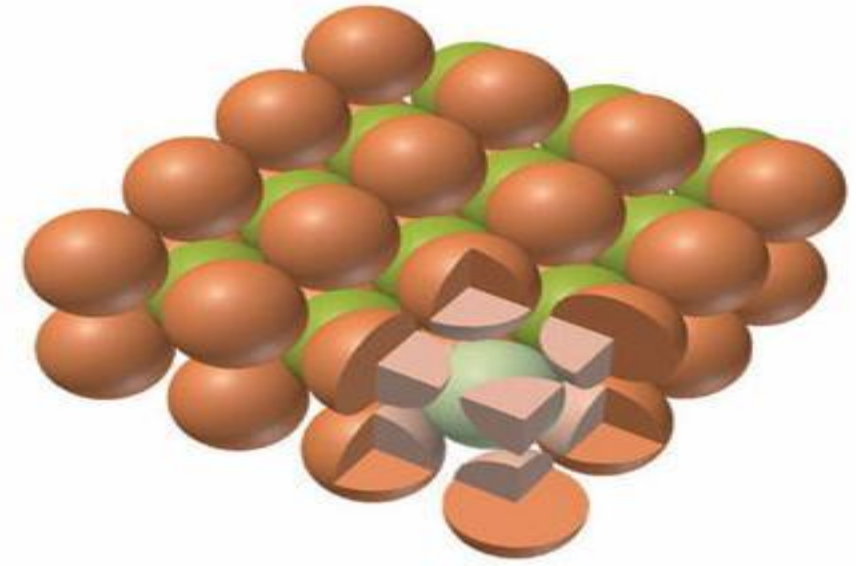
- Hexagonal close-packed (hcp): 0.74
- Face-centered cubic (fcc): 0.74
- Body-centered cubic (bcc): 0.68
- Simple cubic: 0.52
- Diamond cubic: 0.34



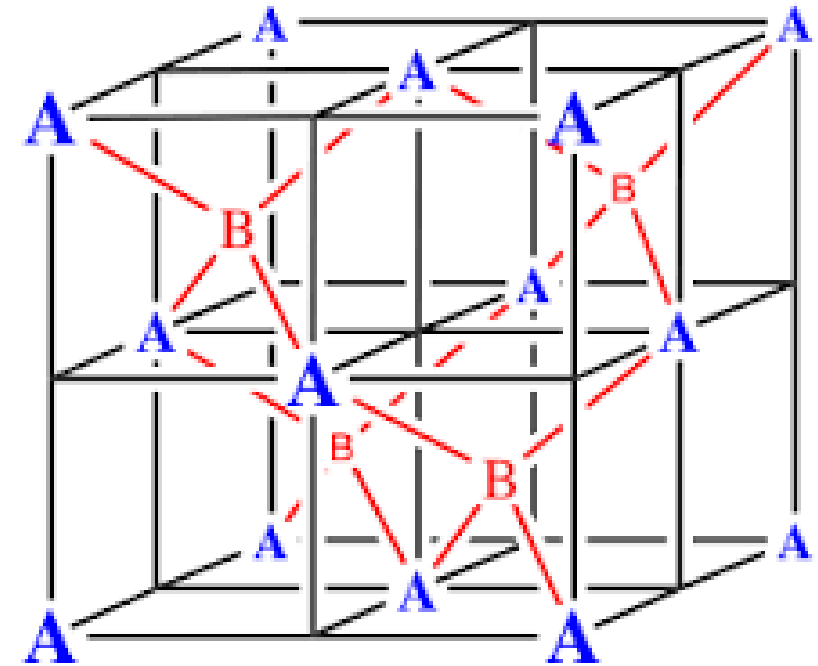
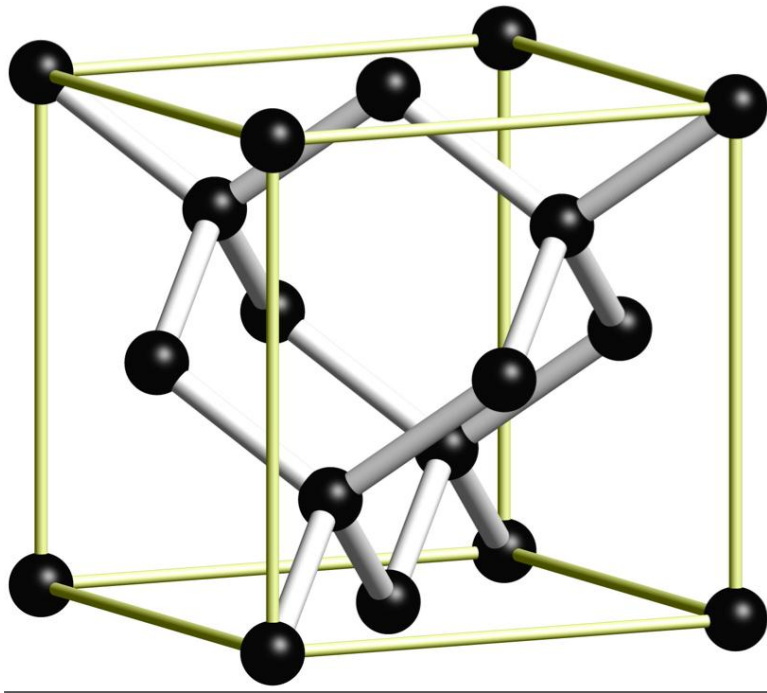
Simple cubic (52%)



Body-centered cubic (68%)



The number of atoms in the unit cell is not the same as the coordination number (number of nearest neighbours). In the **Body Centered Cubic (bcc)** structure above the number of atoms in the unit cell is 2 but the number of nearest neighbours is 8. The (bcc) structure is not as tightly packed as the (hcp) or (fcc) structures, with the atoms occupying only 68.02% of the available space.



The basis crystal structure of group IV crystals is a FCC.

<https://www.youtube.com/watch?v=n2yVr3UuuzY>

Si & Ge are Diamond Structure (Zincblende) crystals

Find out APF (atomic packing fraction) of Diamond structure.

Note in a FCC there are 4 atoms per unit cell, whereas in a diamond structure or a zincblende structure there are 8.

So APF will change.

Diamond is said to be the hardest material, yet its APF is even lower than that of a SC structure.

APF = vol. of atoms in unit cell/vol. of unit cell

$$= (z \times \text{vol. of one atom}) / \text{vol. of unit cell}$$

Density = mass of all atoms in the unit cell/vol. of the unit cell

$$= (z \times M) / (N_A \times a^3)$$

where M = molar mass of the atom/element

N_A = Avogadro number (no. of atoms per mole)

So, density is a function of i) a (lattice constant) and ii) ratio of M/N_A .

Material	'a' Lattice constant (Å)	Crystal structure	Atomic No.	M (in amu/mole)
C (diamond)	3.567	Diamond (FCC)	6	12
Si	5.431	Diamond (FCC)	14	28
Ge	5.658	Diamond (FCC)	32	72
GaAs	5.653	Zinc blende (FCC)		144
CdS	5.832	Zinc blende (FCC)		144
ZnS	5.42	Zinc blende (FCC)		97

Ref.: https://en.wikipedia.org/wiki/Lattice_constant

Considering the valence band and conduction band formation in Si and/or Ge crystals, how do you think they would conduct?

Or they are perfect insulators?

At absolute zero temperature semiconductors are perfect insulators.

At room temp.

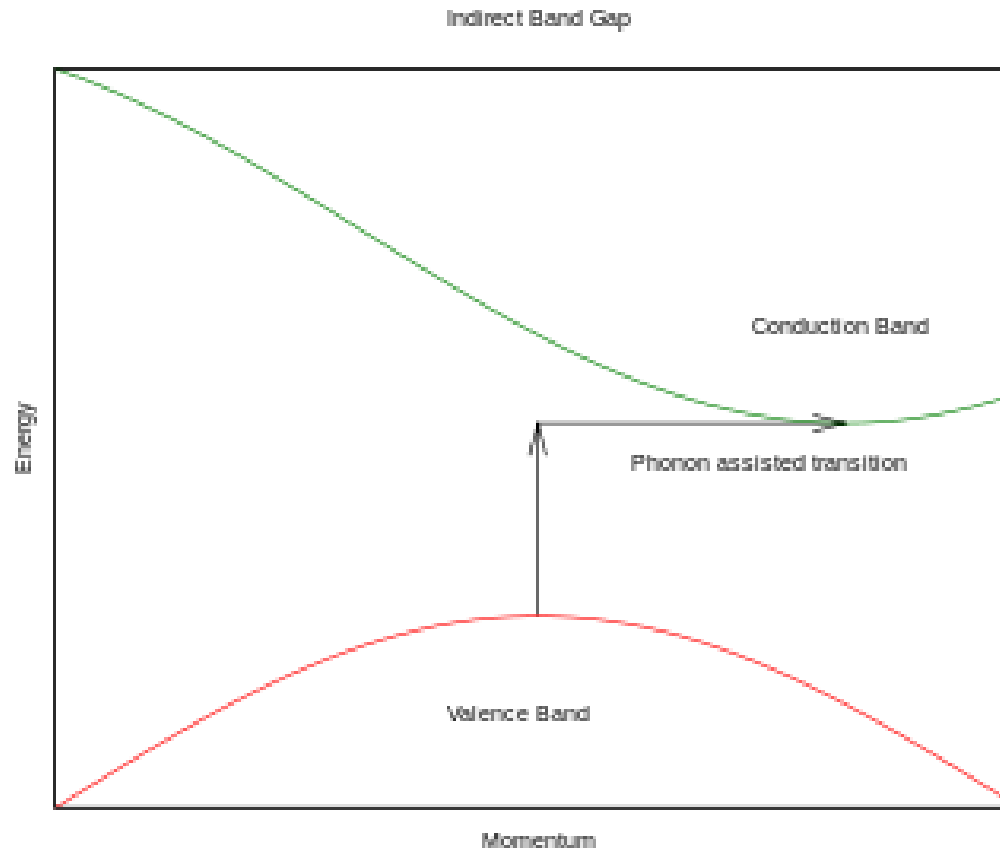
$$n_i = 1.5 * 10^{10} \text{ cm}^{-3} \text{ (Si)}$$

$$n_i = 12.5 * 10^{13} \text{ cm}^{-3} \text{ (Ge)}$$

$$n_i = 1.8 * 10^6 \text{ cm}^{-3} \text{ (GaAs)}$$

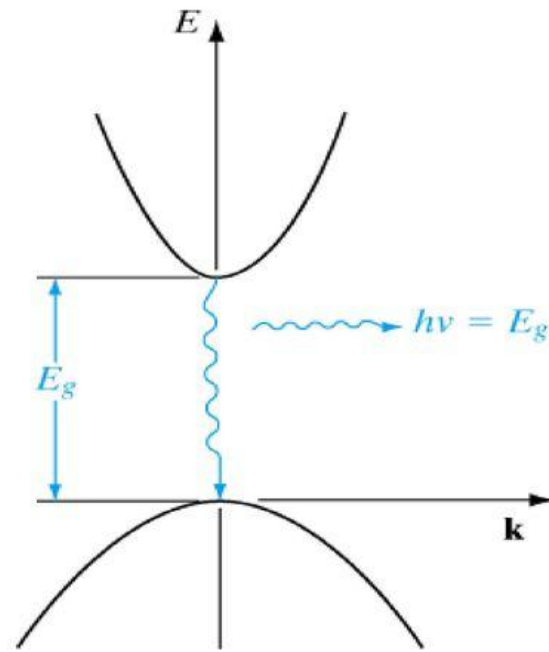
It rises with rise in temp.

Why?

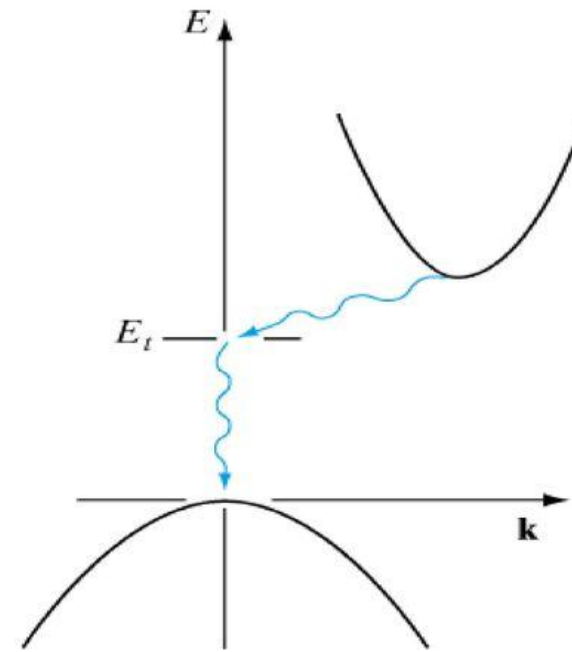


Energy vs. crystal momentum for a semiconductor with an indirect band gap, showing that an electron cannot shift from the highest-energy state in the valence band (red) to the lowest-energy state in the conduction band (green) without a change in momentum. Here, almost all of the energy comes from a photon (vertical arrow), while almost all of the momentum comes from a phonon (horizontal arrow).

Source: https://en.wikipedia.org/wiki/Direct_and_indirect_band_gaps

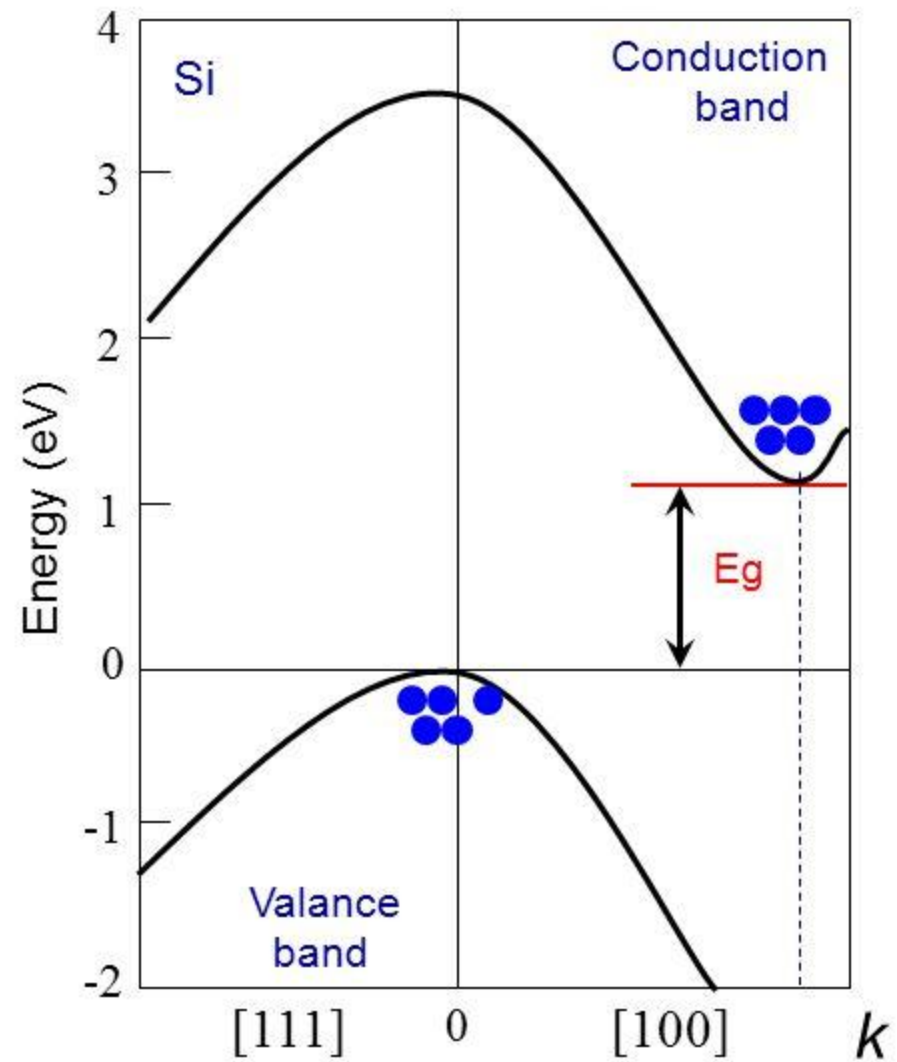
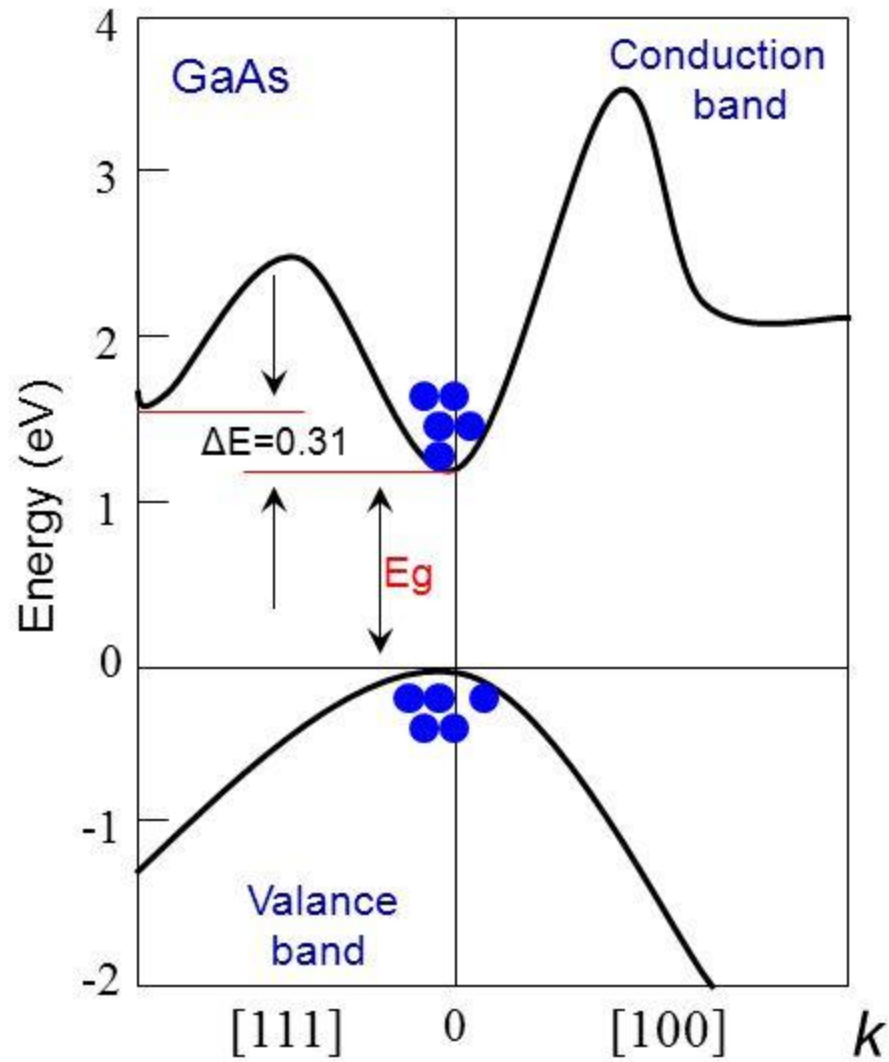


(a) Direct

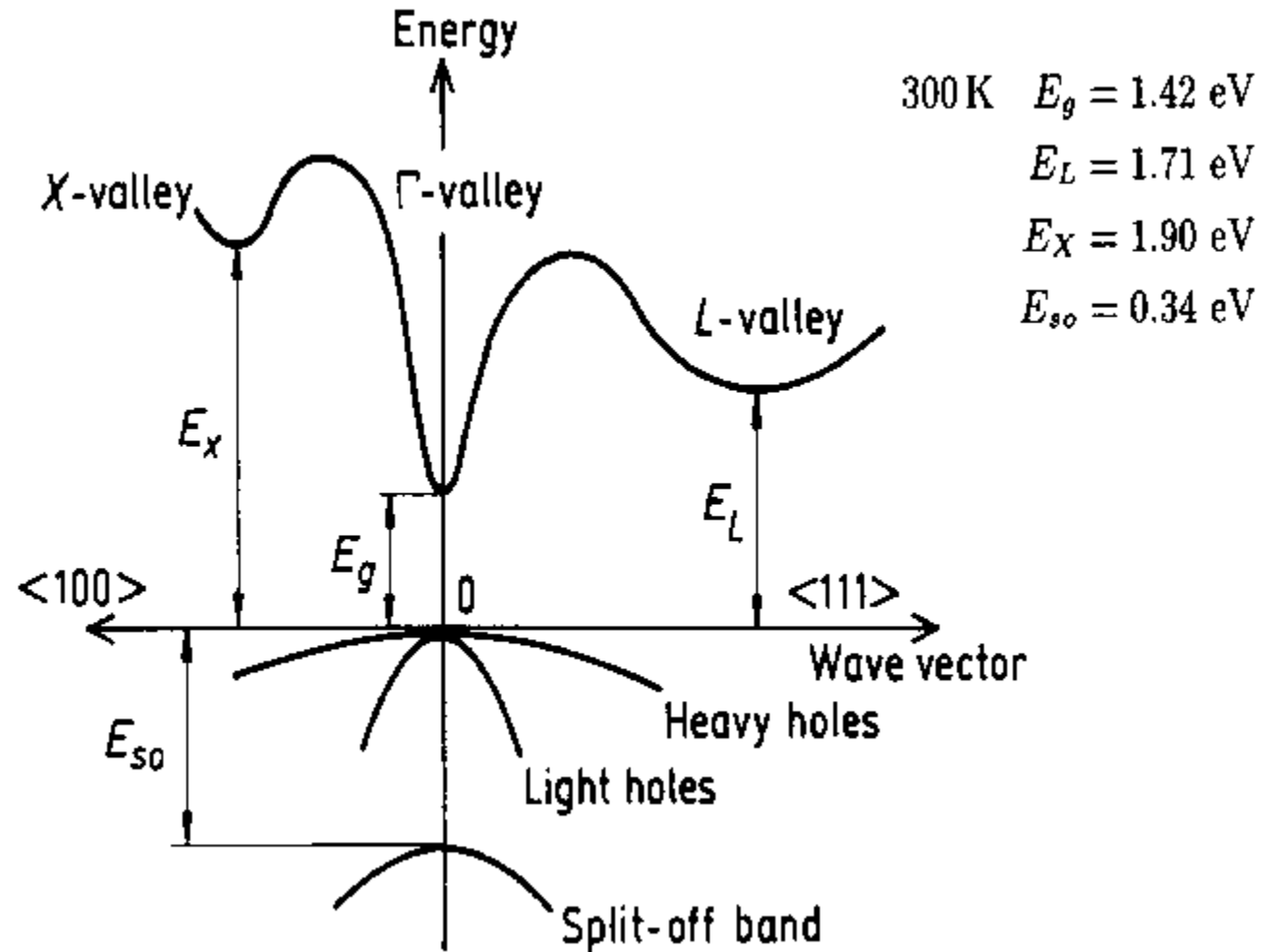


(b) Indirect

Direct and indirect electron transitions in semiconductors:
 (a) **direct transition with accompanying photon emission;**
 (b) **indirect transition via a defect level.**



Comparison between Direct and Indirect bandgap materials



This may be a situation which gives you an opportunity to engineer the material. In this example we may see how a $\text{Al}_x\text{Ga}_{1-x}\text{As}$ may be converted between GaAs ($x=0$) to AlAs ($x=1$) material.

In the ternary alloy $\text{Al}_x\text{Ga}_{1-x}\text{As}$ all of these conduction band minima move up relative to the valence band as the composition x varies from 0 (GaAs) to 1 (AlAs). However, the indirect minimum X moves up less than the others, and for compositions above about 38 percent Al this indirect minimum becomes the lowest-lying conduction band. Therefore, the ternary alloy AlGaAs is a direct semiconductor for Al compositions on the column III sublattice up to about 38 percent, and is an indirect semiconductor for higher Al mole fractions. The band gap energy E_g is shown in color on Fig. 3-6(c).

The variation of energy bands for the ternary alloy $\text{GaAs}_{1-x}\text{P}_x$ is generally similar to that of AlGaAs shown in Fig. 3-6. GaAsP is a direct semiconductor from GaAs to about $\text{GaAs}_{.55}\text{P}_{.45}$ and is indirect from this composition to GaP (see Fig. 6-19). This material is often used in visible LEDs.

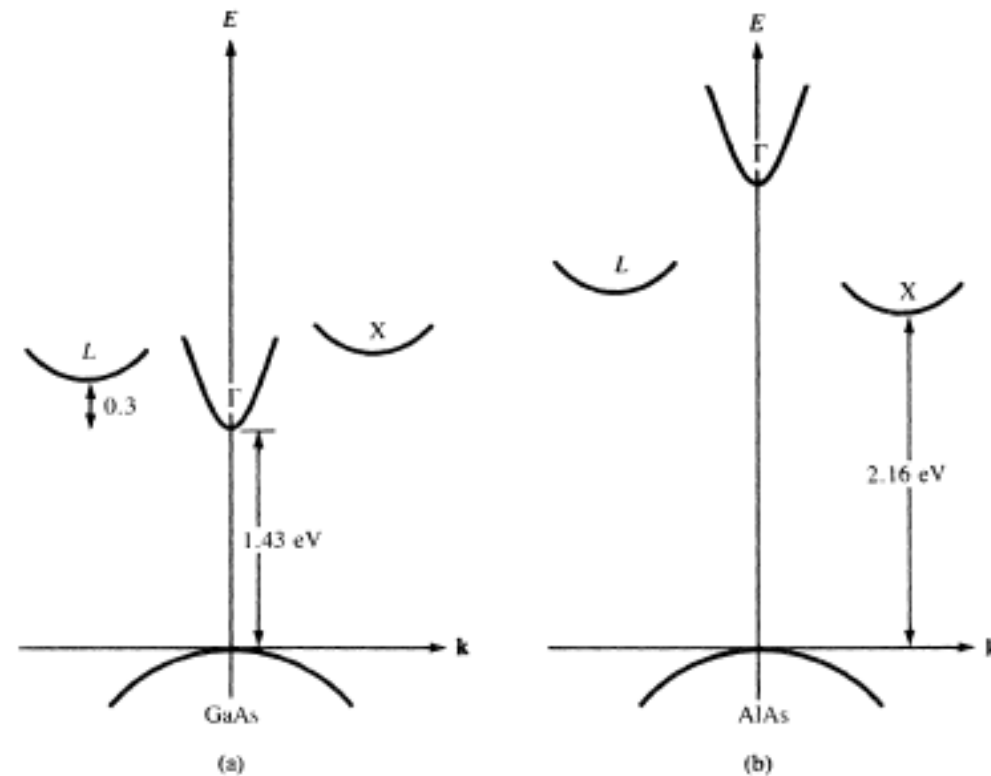
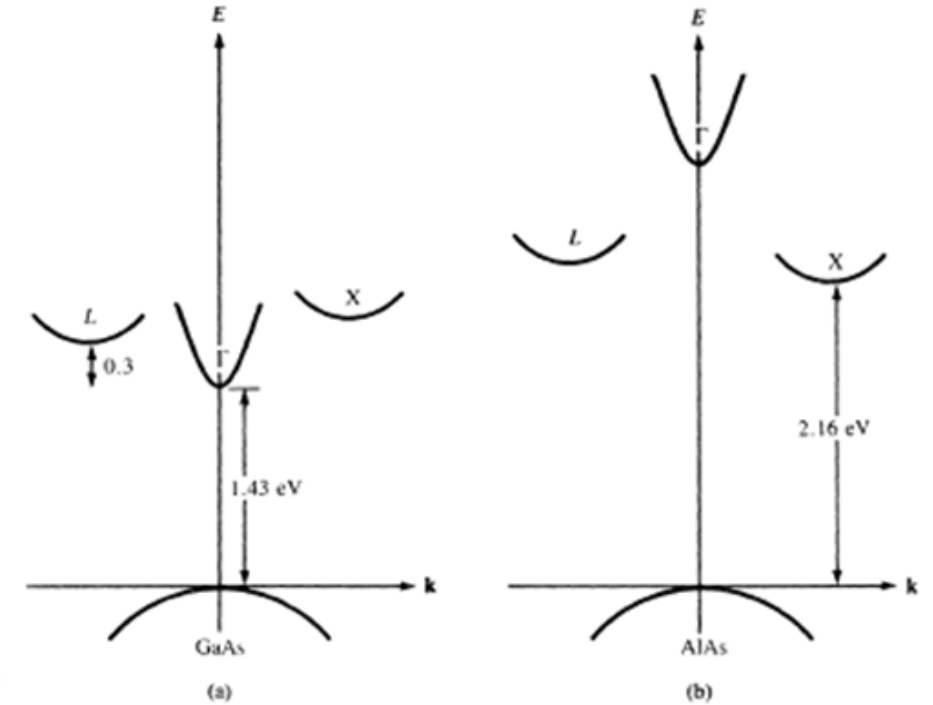
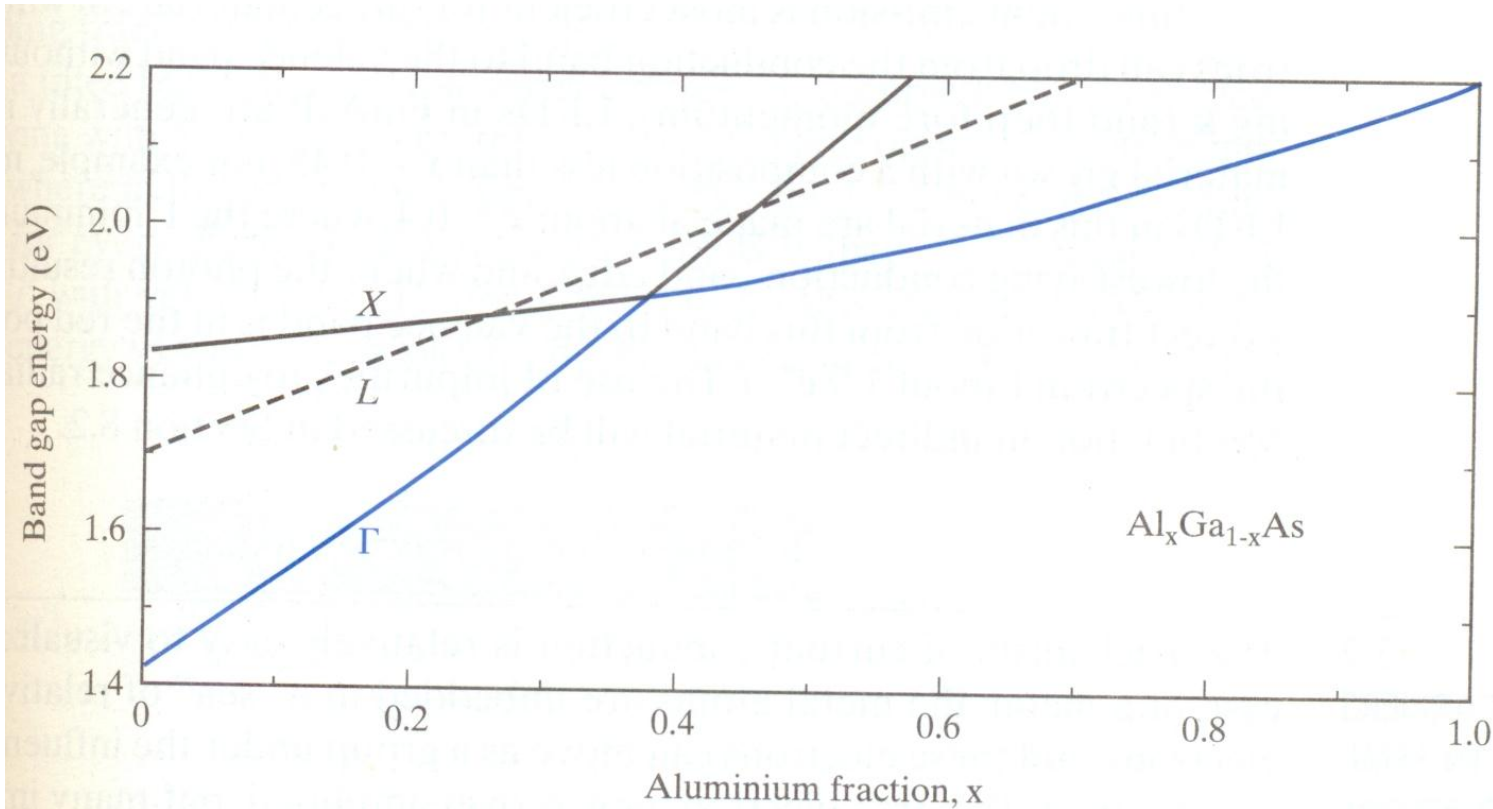


Figure 3-6
Variation of direct and indirect conduction bands in AlGaAs as a function of composition:
(a) the (E, k) diagram for GaAs, showing three minima in the conduction band;
(b) AlAs band diagram;



Source: Solid State Electronic Devices by Streetman and Banerjee. The smallest band gap, E_g (shown in colour), follows the direct Γ band up to $x=0.38$, and then follows the indirect X band.