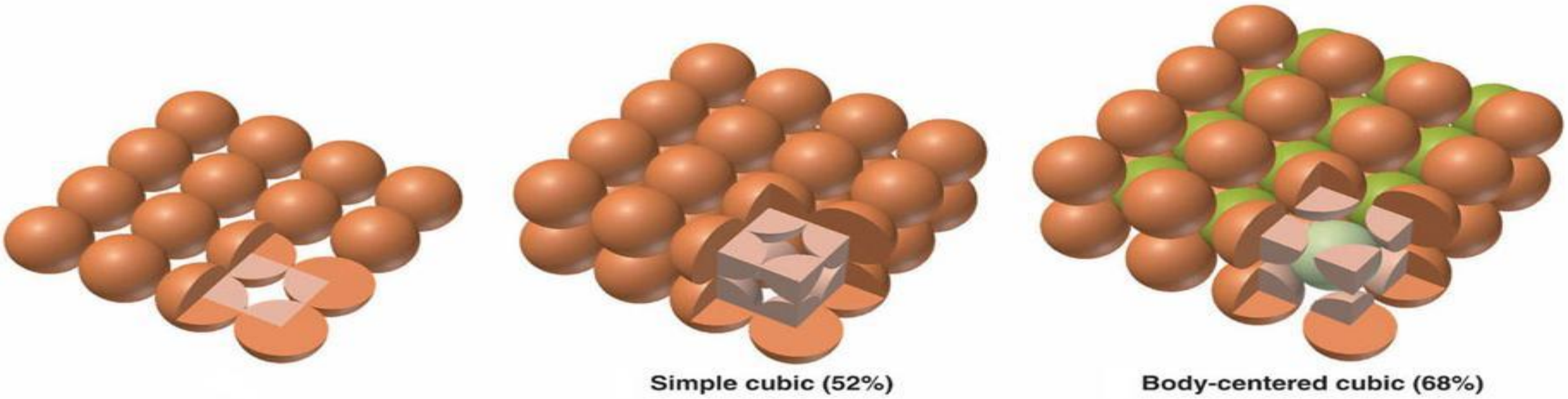
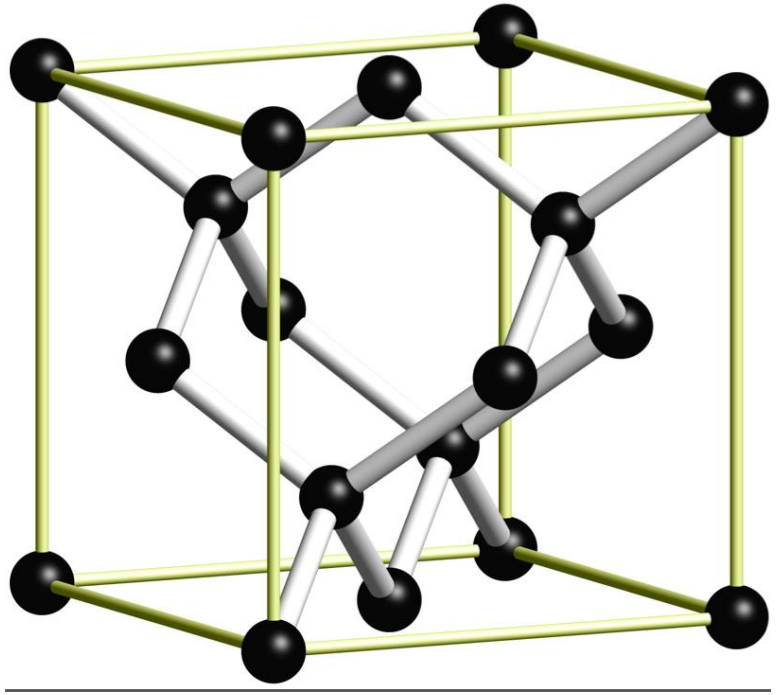
Engineered Materials (SC221)

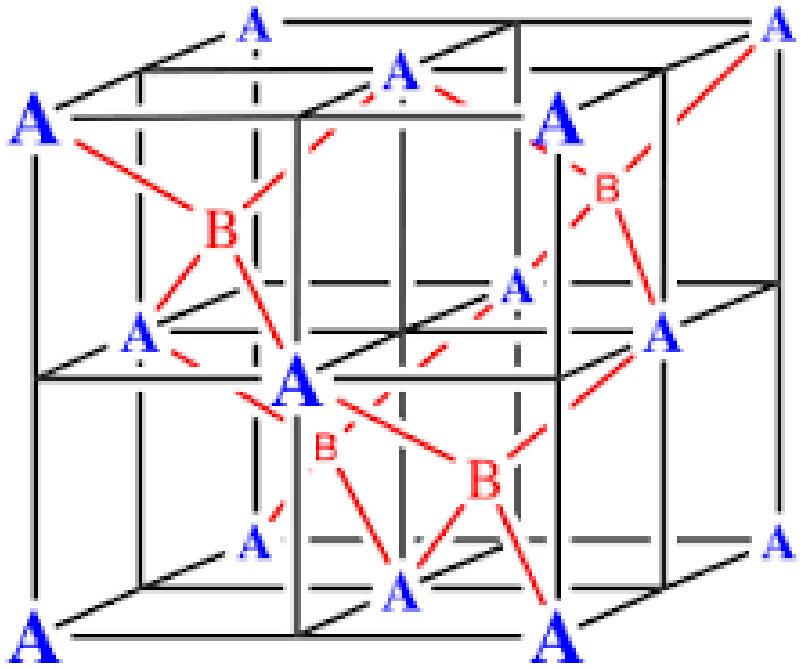
Packing Fraction of single component crystal structures

- 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



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 x vol. of one atom)/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.

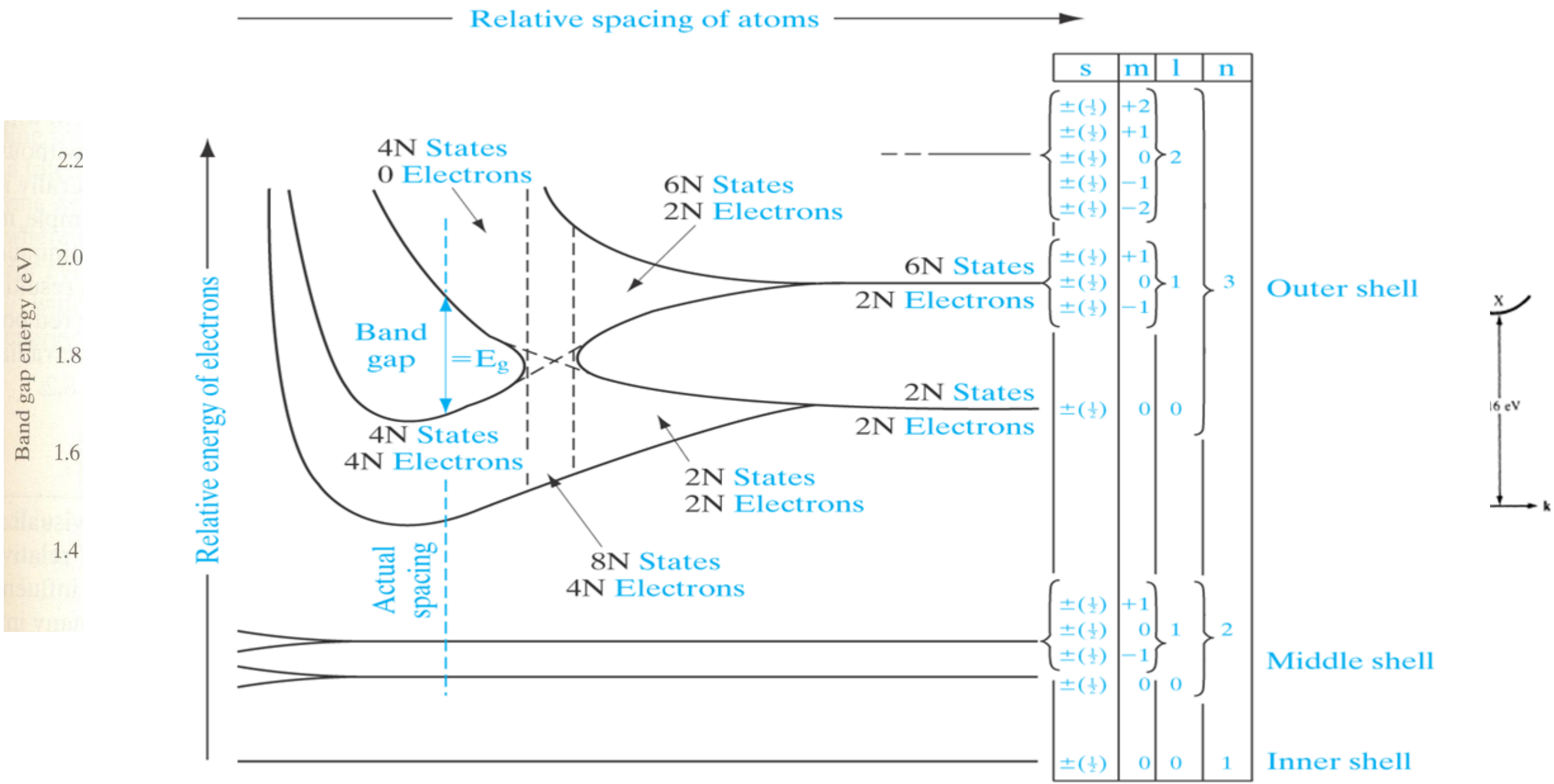
$n_i = 1.5*10^{10}$ cm^{-3} (Si)

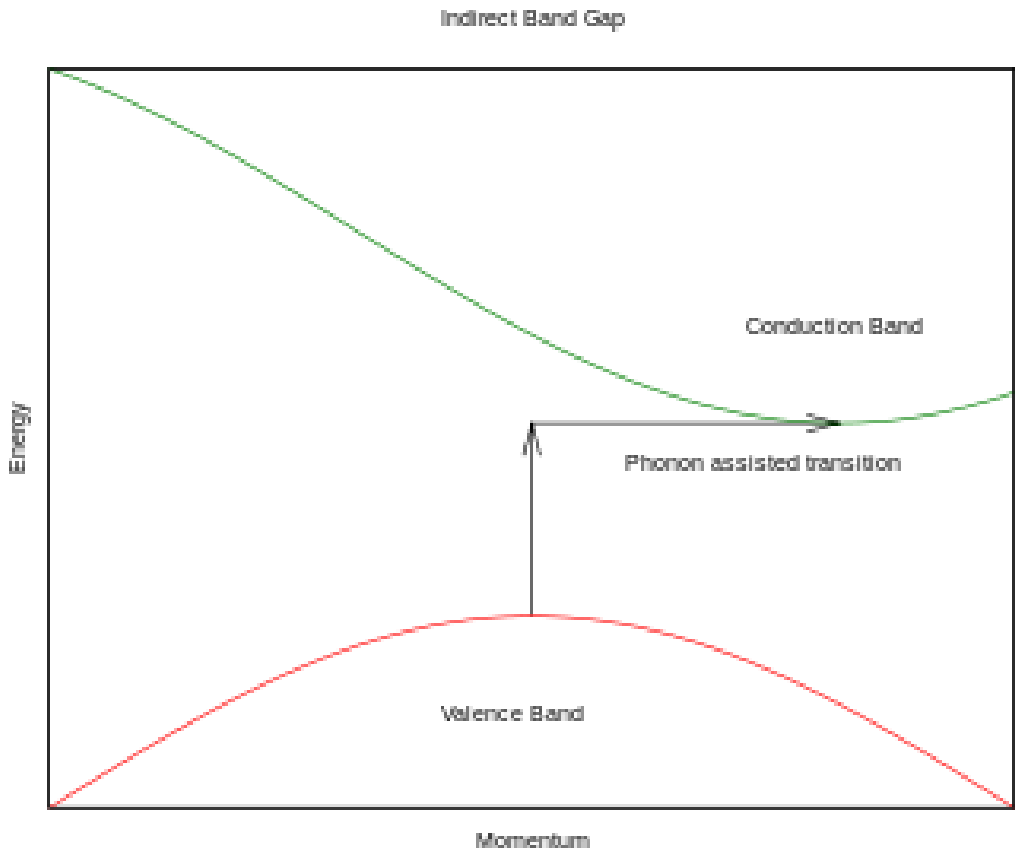
$n_i = 12.5*10^{13}$ cm^{-3} (Ge)

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

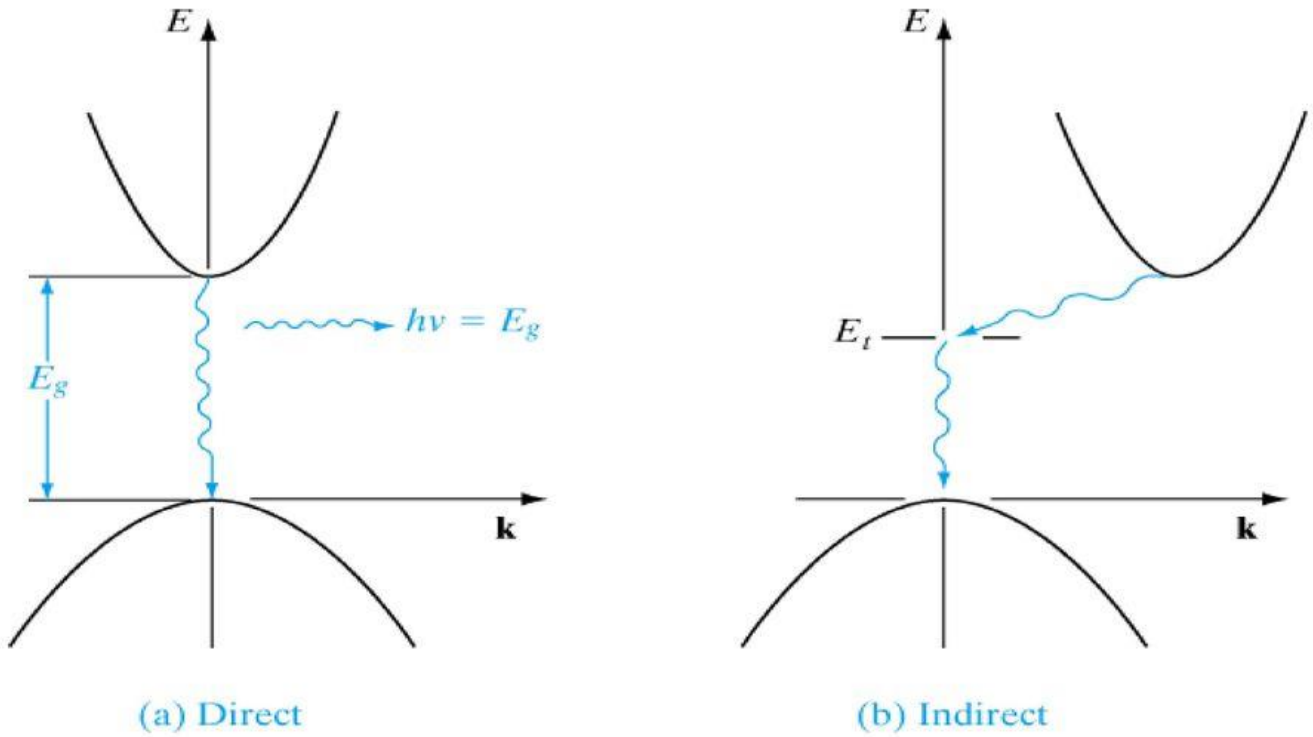
It rises with rise in temp.

Why?


Relative spacing of atoms
Relative energy of electrons
Band gap energy (eV)
2.2
2.0
1.8
1.6
1.4
4N States
0 Electrons
6N States
2N Electrons
6N States
2N Electrons
Band
gap
$= E_g$
2N States
2N Electrons
4N States
4N Electrons
2N States
2N Electrons
8N States
4N Electrons
Actual
spacing
s
m
l
n
$\pm(\frac{1}{2})$ +2
$\pm(\frac{1}{2})$ +1
$\pm(\frac{1}{2})$ 0 2
$\pm(\frac{1}{2})$ −1
$\pm(\frac{1}{2})$ −2
$\pm(\frac{1}{2})$ +1
$\pm(\frac{1}{2})$ 0 1 3
$\pm(\frac{1}{2})$ −1
$\pm(\frac{1}{2})$ 0 0
Outer shell
$\pm(\frac{1}{2})$ +1
$\pm(\frac{1}{2})$ 0 1 2
$\pm(\frac{1}{2})$ −1
$\pm(\frac{1}{2})$ 0 0
Middle shell
$\pm(\frac{1}{2})$ 0 0 1
Inner shell
X
6 eV
k

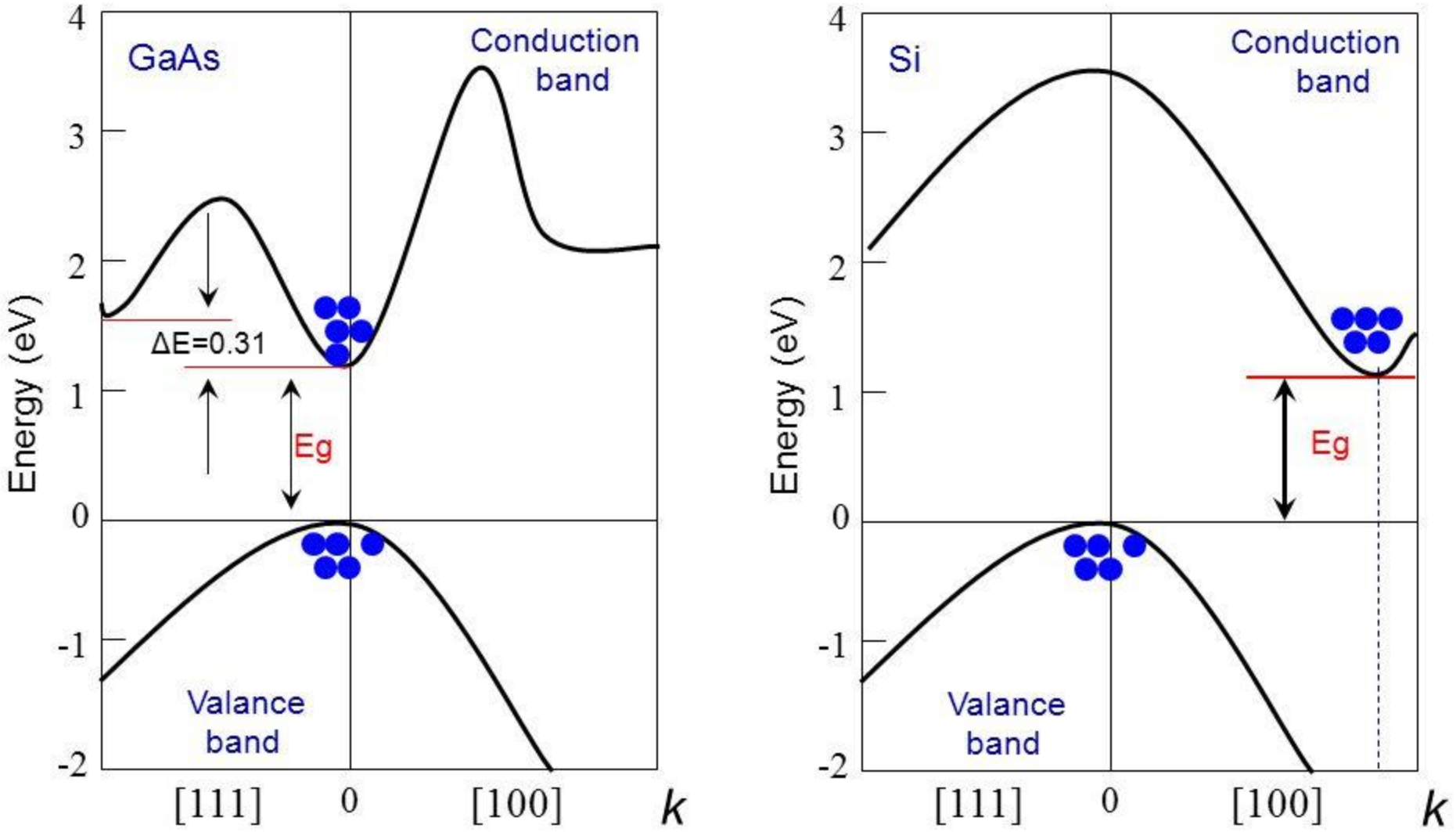


Energy vs. crystal momentum for a semiconductor with an indirect band gap, showing that an electron cannot shift from the highest-energy state in the valence band (red) to the lowest-energy state in the conduction band (green) without a change in momentum. Here, almost all of the energy comes from a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

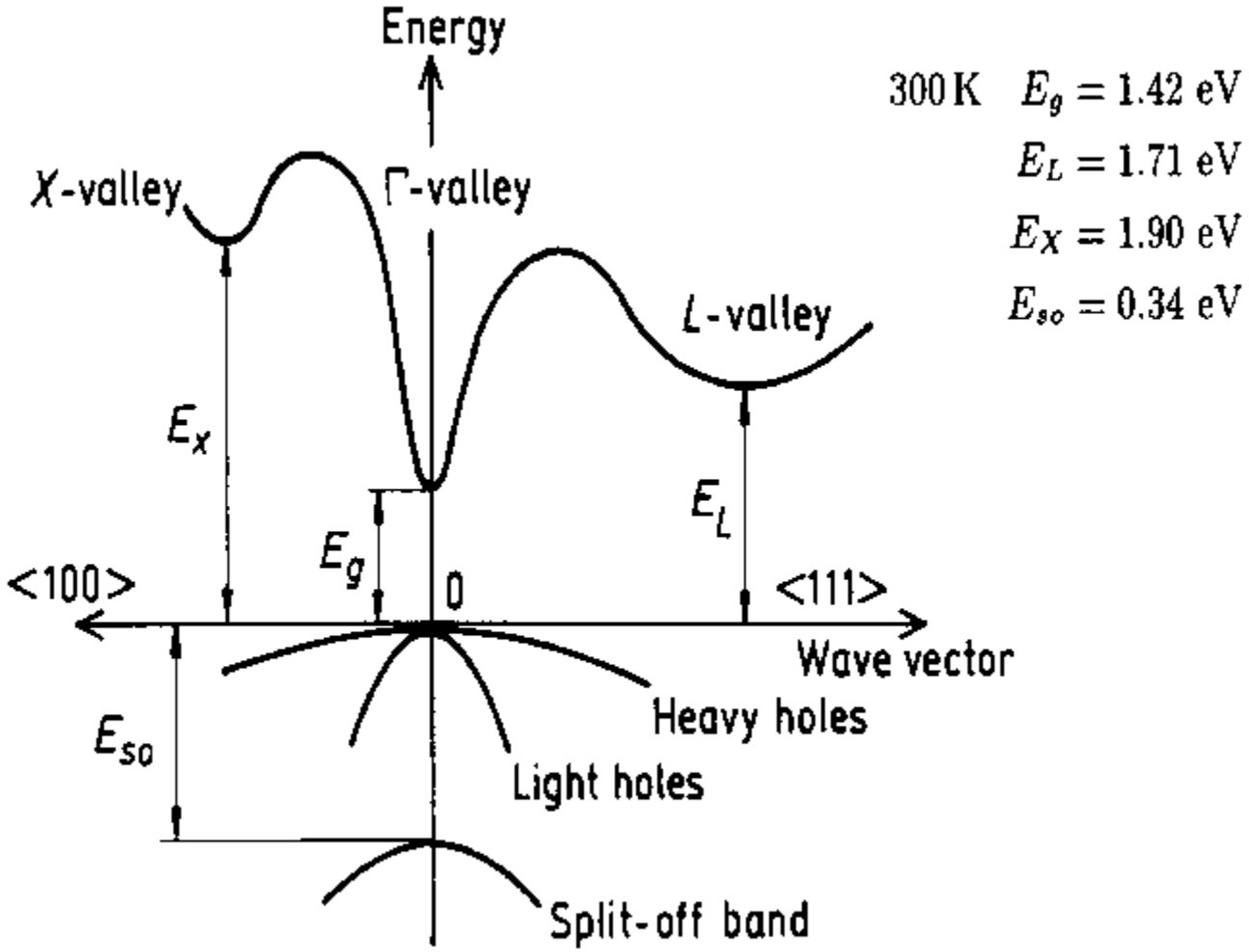


Direct and indirect electron transitions in semiconductors:
(a) direct transition with accompanying photon emission;
(b) indirect transition via a defect level.

Source: Solid State Electronic Devices by Streetman and Banerjee



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 $Al_xGa_{1-x}As$ may be converted between GaAs (x=0) to AlAs (x=1) material.

In the ternary alloy $Al_xGa_{1-x}As$ 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 $GaAs_{1-x}P_x$ is generally similar to that of AlGaAs shown in Fig. 3-6. GaAsP is a direct semiconductor from GaAs to about $GaAs_{.55}P_{.45}$ and is indirect from this composition to GaP (see Fig. 6-19). This material is often used in visible LEDs.

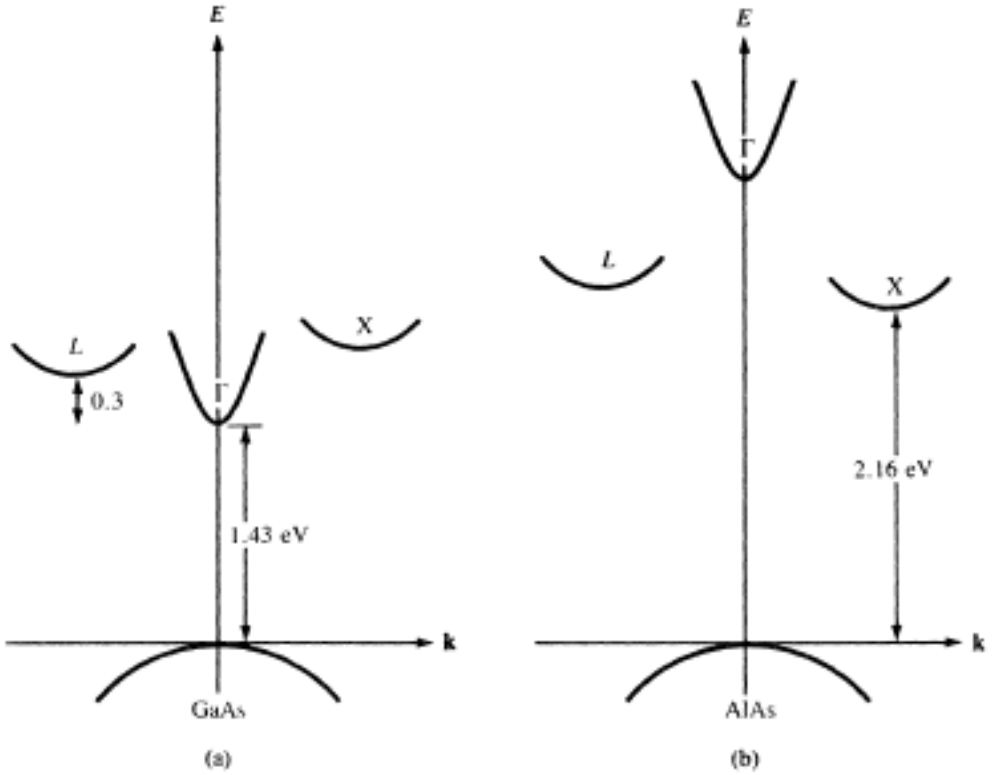


Figure 3-6
Variation of direct and indirect conduction bands in AlGaAs as a function of composition: (a) the $(E, \mathbf{k})$ diagram for GaAs, showing three minima in the conduction band; (b) AlAs band diagram;

Source: Solid State Electronic Devices by Streetman and Banerjee