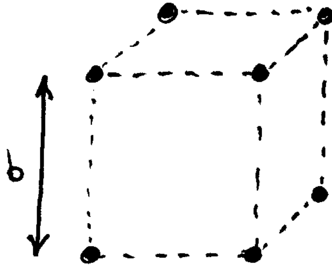
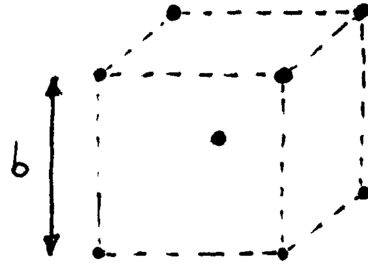
Quiz #1 Solutions Oct 5, 2001

1. a, b



SIMPLE CUBIC

Reciprocal Lattice Vectors: $(b\ 0\ 0)$ $(0\ b\ 0)$ $(0\ 0\ b)$



FCC → BCC

Reciprocal Lattice Vectors: $(\frac{b}{2}\ \frac{b}{2}\ -\frac{b}{2})$ $(\frac{b}{2}\ -\frac{b}{2}\ \frac{b}{2})$ $(-\frac{b}{2}\ \frac{b}{2}\ \frac{b}{2})$

Γ-point

$E_1 = 0$

non-degenerate

$E_2 = \frac{\hbar^2}{2m} b^2$

6-fold degenerate

$E_1 = 0$

non-degenerate

$E_2 = \frac{\hbar^2}{2m} \cdot 3\left(\frac{b}{2}\right)^2$

8-fold degenerate

X - point

$E_1 = \frac{\hbar^2}{2m} \cdot \left(\frac{b}{2}\right)^2$

6-fold degenerate

$E_2 = \frac{\hbar^2}{2m}\left[\left(\frac{b}{2}\right)^2 + b^2\right]$

24-fold degenerate

$E_1 = \frac{\hbar^2}{2m}\left(\frac{b}{2}\right)^2$

6-fold degenerate

$E_2 = \frac{\hbar^2}{2m} \cdot 2\left(\frac{b}{2}\right)^2$

12-fold degenerate

c. SIMPLE CUBIC

$E_1(\Gamma)$ - 1 level

$E_2(\Gamma)$ split into 4 in-plane and 2-axial levels

$E_1(X)$ - ″ - - ″ - - ″ - - ″ -

$E_2(X)$ split into 3 groups of 8 levels each.

FCC → BCC

$E_1(\Gamma)$ - 1 level

$E_2(\Gamma)$ - no splitting

$E_1(X)$ split into 4 in-plane and 2-axial levels.

$E_2(X)$ split into 4 in-plane and 8 off-plane levels.

2 a. There are 8 Co and 24 Sb atoms per unit cell.

b. The ratio of the elements is 1 Co to 3 Sb.
1 Co has 7 (d) or 9 (d+s) valence electrons and is missing 3 electrons to fill the d-orbitals
3 Sb's have 9 (p) valence electrons and are missing 9 electrons to fill the p-band.

From the above considerations, and knowing that Co is a metallic element we can expect Co to donate its 9 electrons to Sb×3

Bonding : Sb 5s, Sb 5p, Co 3p
Anti Bonding : Co 3d, Co 4s

Of course the actual bands might have contributions from several atomic orbitals. This is a first order approximation which neglects hybridization and covalent bonding.

c. $CoSb_3$ is a semiconductor.

d. There are 3 electron pockets and 1 hole pocket; all in the Γ-point

e. The mobility is inversely proportional to m^*. m^* is inversely proportional to the curvature of the band

[$CoSb_3$ has light electrons (similar to the holes) and heavy electrons.]

In general, the curvature of the valence and conduction bands at the Γ-point is high, which is expected from the small bandgap. One should expect a high mobility value, most probably larger than μ_{Cu} and similar to μ_{Si}

f. Dopants will fill the voids in the crystal structure. They don't influence significantly the band structure, as they do not bond to the adjacent atoms. They also do not scatter electrons significantly.

The dopants however serve as scattering centers for phonons since 1) their position is not periodic (not all the cages are filled), 2) their mass can differ significantly from the mass of Co and Sb, 3) they can absorb energy and rattle inside the void.

Thus, doping lower K without lowering σ, so $Z = \sigma S^2 / K$ increases.

3 a. There are 2 atoms per a^3 volume, $1e^-$ per atom.

$$\int_0^{E_F} g(E)\,dE = \frac{2}{a^3} \qquad g(E) = \frac{\sqrt{2m^3E}}{\pi^2\hbar^3}$$

$$\frac{\sqrt{2m^3}}{\pi^2\hbar^3}\cdot\frac{2}{3}E_F^{3/2} = \frac{2}{a^3}$$

$$E_F = \left[\frac{3\pi^2\hbar^3}{\sqrt{2m^3}\,a^3}\right]^{2/3}$$

b. assume lattice constant is $\left(\frac{a+b}{2}\right)$

$$E_F = \left[\frac{3\pi^2\hbar^3}{\sqrt{2m^3}\left(\frac{a+b}{2}\right)^3}\right]^{2/3}$$

c. There is 1 atom per a^2 area.

$$\int_0^{E_F} g(E)\,dE = \frac{1}{a^2} \qquad g(E) = \frac{m}{\pi\hbar^2}$$

$$E_F = \frac{\pi\hbar^2}{ma^2}$$

d. Carrier mobility will be the highest for (a), since in (b) there is an increase in scattering due to composition variations (neutral impurity scattering), and in (c) there is an increase in surface scattering.

4. a. $n = p = 0$ at $T = 0K$

$$n = 4\frac{\sqrt{2m_0^3}}{\pi^2\hbar^3}\cdot 0.01\cdot e^{E_F^e/kT}\cdot(kT)^{3/2}\int_0^\infty \sqrt{\epsilon}\, e^{-\epsilon}\, d\epsilon$$

$$p = 2\frac{\sqrt{2m_0^3}}{\pi^2\hbar^3}\, 0.1\, e^{E_F^h/kT}\,(kT)^{3/2}\int_0^\infty \sqrt{\epsilon}\, e^{-\epsilon}\, d\epsilon$$

① $$0.04\, e^{E_F^e/kT} = 0.2\, e^{E_F^h/kT}$$

$$E_F^e = E_F - E_C \qquad E_F^h = E_V - E_F$$

② $$E_F^e + E_F^h = E_V - E_C = -E_g$$

From ① + ② $$E_F^e - E_F^h = kT\ln\left(\frac{0.2}{0.04}\right) = kT\ln(5)$$

$$2E_F^e = kT\ln 5 - E_g$$

$$E_F^e = \frac{kT}{2}\ln 5 - \frac{1}{2}E_g$$

$$n = 0.04\,\frac{\sqrt{2m_0^3}}{\pi^2\hbar^3}\, e^{\frac{1}{2}\ln 5}\, e^{-\frac{1}{2}E_g/kT}\cdot(kT)^{3/2}\cdot\frac{\sqrt{\pi}}{2}$$

Low T means $kT \ll E_g$ so the Boltzman distribution can be used.

b. $\sigma = \sum_{pockets} \sigma_i = 4\sigma_e + 2\sigma_h$

$m_e^* = m_{et}$
$m_h^* = m_{hl}$ for the 100 direction

$$\sigma = 4\left(\frac{n}{4}\cdot\frac{e^2\tau_e}{0.01 m_0}\right) + 2\left(\frac{n}{2}\cdot\frac{e^2\tau_h}{m_0}\right)$$

$$= ne^2\left(\frac{100\tau_e}{m_0} + \frac{\tau_h}{m_0}\right)$$

from part (a)

c. The carrier concentration in semiconductors is lower than semimetals, and more strongly influenced by temperature.

S.C. $n\uparrow$ $T\uparrow$ S.M. $n \sim$ constant

Therefore, σ increases with temperature in semiconductors, while often decreases in semimetals due to increased scattering.